

# Scale Dependence in Mechanical Behavior of Silicon Nanowires

by

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Koç University

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This is to certify that I have examined this copy of a doctoral dissertation by

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*To my Beloved Parents*

# ABSTRACT

## Scale Dependence in Mechanical Behavior of Silicon Nanowires

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Based on fabrication, characterization, and modeling, this thesis explores the multifaceted fundamentals of silicon nanowire mechanical behavior. Despite their significant potential as building blocks in nano electromechanical systems, studies on silicon nanowires have so far failed to converge to draw a comprehensive picture of the scale dependence of their fundamental mechanical properties. Aiming to clarify the existing lack of consensus in this field, nanowires obtained through top-down fabrication are tested *in-situ* in three-point bending configuration, where the monolithic technology provides i) well-defined boundary conditions without generating any interface, and hence any additional compliance, between nanowire samples and their supports and ii) ample space for accommodating bending deflections during testing. Metrology work is carried out for the quantification of both nanowire dimensions and intrinsic stresses. Bending behavior is then interpreted through a newly developed multiscale model that primarily incorporates the surface effect through surface-induced intrinsic stresses by considering the native oxide surface state and crystalline anisotropy of surfaces. This is achieved by a combined approach based on molecular dynamics simulations and modified core-shell model. Furthermore, the utilization of machine learning facilitated by comprehensive molecular dynamics simulations enhances the scope of the methodology established in this study, employing artificial intelligence as a practical instrument for understanding the nanomechanics of silicon nanowires. Finally, a thorough analysis of uncertainties attributed to the interplay between *processing-structure-property* in silicon nanowires is conducted.

The findings 1) bridge the 10-nm barrier that exists between computational and experimental studies due to various challenges in both realms; 2) link the evolution of the modulus of elasticity to nanowire critical dimension through the parameterization of surface inhomogeneity. A stiffening trend is quantified with increasing



critical dimension. Experimental trendlines are validated through independent analytical and machine learning methods enabled through atomistic simulations; 3) reveal theoretical strength limit achieved by nanowires below 20 nm. This robust finding is in stark contrast to a substantial body of literature on nanowires of similar dimensions reporting strength values ranging from a few MPa to 20 GPa; 4) yield a confidence level surpassing 95% for fracture strength and 85% for modulus of elasticity estimations of silicon nanowires via error analysis of systematic and random error sources; 5) shed light on the crucial influence of the native oxide on the mechanical properties of silicon nanowires.

Following the miniaturization trend in electronics as predicted by Moore's law, silicon nanowires due to their minuscule size resulting in exceptionally high resonance frequencies and significant surface-to-volume ratios emerge as primary candidates for transducers in the next generation of miniaturized sensors based on nano electromechanical systems. Employing a methodology that integrates comprehensive theoretical and multi-scale modeling along with state-of-the-art fabrication and characterization techniques, a series of enduring issues related to the interpretation of the scale effect in silicon nanowires have been conclusively resolved. The same approach can be applied to other low-dimensional materials including SiC, ZnO, core-shell and alloy nanowires as well as 2D materials including MoS<sub>2</sub> and WS<sub>2</sub>.

# ÖZETÇE

## Silikon Nanotellerde Mekanik Davranışın Ölçek Bağımlılığı

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Üretim, karakterizasyon ve modellemeye dayalı bu tez, silikon nanotel mekanik davranışının çok yönlü temellerini araştırmaktadır. Nano elektromekanik sistemlerde yapı taşları olarak önemli potansiyele sahip olmalarına rağmen, silikon nanoteller üzerine yapılan çalışmalar şu ana kadar temel mekanik özelliklerinin ölçeğe bağımlılığının kapsamlı bir resmini çizme konusunda yetersiz kalmıştır. Bu alandaki mevcut fikir birliği eksikliğini açıklığa kavuşturmak için yukarıdan aşağıya imalat yoluyla üretilen nanoteller, üç noktalı bükme konfigürasyonunda yerinde test edilir. Monolitik teknoloji, i) nanotel numuneleri ve bunların destekleri arasında herhangi bir arayüz veya ek uyum oluşturmada iyi tanımlanmış sınır koşulları ve ii) test sırasında bükülme sapmalarını karşılamak için yeterli alan sağlamaktadır. Hem nanotel boyutlarını hem de içsel gerilimleri ölçmek için metroloji çalışması yürütülmüştür. Eğilme davranışı daha sonra, doğal oksit yüzeyinin durumunu ve yüzey kristalinde var olan anizotropiyi dikkate alırken, öncelikle yüzey kaynaklı içsel gerilimler aracılığıyla yüzey etkisini birleştiren yeni geliştirilmiş çok ölçekli bir model kullanılarak yorumlanır. Bu model, moleküler dinamik simülasyonlara ve değiştirilmiş çekirdek-kabuk modeline dayalı birleşik bir yaklaşıma dayanmaktadır. Ek olarak, kapsamlı moleküler dinamik simülasyonlarının mümkün kıldığı makine öğreniminin kullanımı, bu çalışmada geliştirilen ve silikon nanotellerin nanomekaniğini anlamak için yapay zekayı pratik bir araç olarak kullanan metodolojinin kapsamını genişletmektedir. Son olarak silikon nanotellerdeki işlem-yapı-özellik etkileşimiyle ilgili belirsizliklerin kapsamlı bir analizi gerçekleştirilir. Bulgular şu şekildedir: 1) Hesaplamalı ve deneysel çalışmalarda çeşitli zorluklar nedeniyle var olan 10 nm'lik bariyeri aşmak; 2) Yüzey homojensizliğinin parametreleştirilmesi, elastisite modülünün değişimini nanotellerin kritik boyutuna bağlamamıza olanak tanır. Sertleşme eğilimi, kritik boyutun arttırılmasıyla ölçülmüştür. Atomistik simülasyonların mümkün

kıldığı bağımsız analitik ve makine öğrenme yöntemleri kullanılarak deneysel eğilim çizgileri doğrulanmıştır; 3) 20 nm'den küçük nanoteller için teorik güç sınırı ortaya çıkarılmıştır. Bu sağlam bulgu, birkaç MPa'dan 20 GPa'ya kadar değişen güç değerleri bildiren, benzer boyutlardaki nanoteller hakkında önemli miktarda literatürle tam bir tezat oluşturmaktadır; 4) Sistematik ve rastgele hata kaynaklarının hata analizi yoluyla silikon nanotellerin kırılma mukavemeti için %95'in üzerinde ve elastisite modülünün tahminleri için %85'in üzerinde bir güven düzeyi elde edilmiştir; 5) Doğal oksit tabakasının silikon nanotellerin mekanik özelliklerini nasıl etkilediğine ışık tutmaktadır. Moore yasasının elektronikte öngördüğü minyatürleştirme eğilimini takiben, silikon nanoteller, olağanüstü yüksek rezonans frekansları ve önemli yüzey-hacim oranları ile sonuçlanan çok küçük boyutları nedeniyle nano elektromekanik sistemlere dayalı yeni nesil minyatür sensörlerde dönüştürücüler için birincil adaylar olarak ortaya çıkmaktadır. Silikon nanotellerdeki ölçek etkisinin yorumlanmasına ilişkin uzun zamandır devam eden bir dizi sorun, kapsamlı teorik ve çok ölçekli modellemenin yanı sıra en ileri üretim ve karakterizasyon tekniklerini içeren bir metodoloji kullanılarak kesin olarak açıklığa kavuşturulmuştur. Aynı yöntem, SiC, ZnO, çekirdek kabuğu ve alaşım nanotelleri gibi diğer düşük boyutlu malzemelerin yanı sıra MoS<sub>2</sub> ve WS<sub>2</sub> gibi 2 boyutlu malzemelerle de kullanılabilime potansiyeline sahiptir.

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## ABBREVIATIONS

|        |                                                  |
|--------|--------------------------------------------------|
| NW     | Nanowire                                         |
| NEMS   | Nanoelectromechanical System                     |
| IC     | Integrated Circuit                               |
| MEMS   | Microelectromechanical System                    |
| Si     | Silicon                                          |
| CD     | Critical Dimension                               |
| sSOI   | Strained Silicon-On-Insulator                    |
| RIE    | Reactive Ion Etching                             |
| MD     | Molecular Dynamics                               |
| TEM    | Transmission Electron Microscopy                 |
| LPCVD  | Low-Pressure Chemical Vapor Deposition           |
| LTO    | Low-Temperature Oxide                            |
| e-beam | Electron-Beam                                    |
| DRIE   | Deep Reactive Ion Etching                        |
| ICP    | Inductively Coupled Plasma                       |
| EB     | Euler-Bernoulli                                  |
| LO     | Longitudinal Optical                             |
| FET    | Field Effect Transistor                          |
| VLS    | Vapor-Liquid-Solid                               |
| PDP    | Phonon Deformation Profile                       |
| SST    | Stress Shift Coefficient                         |
| ReaxFF | Reactive Force Field                             |
| PDF    | Pair Distribution Function                       |
| IoT    | Internet of Things                               |
| HR-TEM | High-Resolution Transmission Electron Microscope |



|       |                                   |
|-------|-----------------------------------|
| FIB   | Focused Ion Beam                  |
| SEM   | Scanning Electron Microscopy      |
| M-CS  | Modified Core-Shell               |
| CS    | Core-Shell                        |
| PCC   | Pearson's Correlation Coefficient |
| SCS   | Single-Crystal-Si                 |
| DFT   | Density Functional Theory         |
| ML    | Machine learning                  |
| RF    | Random Forest                     |
| KNN   | K-Nearest Neighbors               |
| LR    | Linear Regression                 |
| DT    | Decision Trees                    |
| MLP   | Multi-Layer Perceptron            |
| SVM   | Support Vector Machines           |
| AR    | Aspect Ratio                      |
| ROI   | Region Of Interest                |
| GIS   | Gas Injection System              |
| SW    | Stillinger-Weber                  |
| m-SW  | Modified Stillinger-Weber         |
| TM    | Tersoff-Munetoh                   |
| TT3   | Tersoff-T3                        |
| TD    | Top-Down                          |
| BU    | Bottom-Up                         |
| HSQ   | Hydrogen SilsesQuioxane           |
| BC    | Boundary Conditions               |
| MEAM  | Modified Embedded Atom Method     |
| RMSE  | Root Mean Squared Error           |
| MAE   | Mean Absolute Error               |
| $R^2$ | Coefficient of Efficiency         |

|        |                                                   |
|--------|---------------------------------------------------|
| BDT    | Brittle-to-Ductile Transition                     |
| CG     | Conjugate Gradient                                |
| YL     | Young-Laplace                                     |
| SCREAM | Single-Crystal Reactive Etching And Metallization |
| PR     | PhotoResist                                       |
| BOX    | Buried Oxide                                      |
| VASP   | Vienna Ab-initio Simulation Package               |
| PBE    | Perdew, Burke, and Ernzerhof                      |
| GGA    | Generalized Gradient Approximation                |
| PAW    | Project Augmented Wave                            |
| 1-D    | One-Dimensional                                   |

## Chapter 1

# INTRODUCTION

Nanowires (NWs) are pivotal elements in various technological advancements spanning nanoelectronics, nanoelectromechanical systems (NEMS), mass spectrometry, and biomedical sensors [Arjmand et al., 2022, Iakab et al., 2019, Sage et al., 2018, Alaca and Karimzadehkhoei, 2023, Zhang et al., 2010b, Zafar et al., 2018, Jia et al., 2019, Lu and Lieber, 2010, Yang et al., 2006, Wang et al., 2016b, Sang et al., 2016, Ambhorkar et al., 2018, Karimzadehkhoei et al., 2023, Nehra et al., 2020, Chen et al., 2024, Espinosa et al., 2012, Ghosh, 2023]. Their high sensitivity, ease of integration, and compatibility with integrated circuits (ICs) render them indispensable in NEMS, where mechanical stresses significantly influence their performance [Nasr Esfahani and Alaca, 2019, Cakirlar et al., 2022, Yang et al., 2022, Seike et al., 2007, Fan et al., 2017, Minamisawa et al., 2012, Geiger et al., 2015, Cullinan et al., 2012, Fleetwood, 2023, Gu et al., 2023, Meng and Li, 2020, Qu, 2016, Templeman et al., 2020, Zhu et al., 2020]. Tensile strain, for instance, enhances transconductance and alters dopant diffusion mechanisms, while intrinsic stresses can induce buckling, impacting mechanical behavior [Nasr Esfahani et al., 2022, Calahorra et al., 2015, Allain et al., 2012, Zare Pakzad et al., 2023c, Zare Pakzad et al., 2021]. Embedded stresses, crucial for piezoresistive transduction in NEMS, pose a significant challenge, necessitating thorough characterization for sensor applications [Zhu et al., 2019, Nasr Esfahani and Alaca, 2019, Nasr Esfahani et al., 2022, Fiorillo et al., 2018, Fukata and Jevasuwan, 2024, Rojo et al., 2013, Samykano, 2021, Tran et al., 2023, Wang et al., 2019]. The potential for utilization of NWs extends to fields like field effect transistors, energy conversion, and storage, with surface-related properties playing a crucial role in their mechanical behavior [Nehra et al., 2020, Alaca and

Karimzadehkhoei, 2023, Karimzadehkhoei et al., 2023, Zafar et al., 2018, Goktas et al., 2018, Stokes et al., 2023]. Surface-to-volume ratios dictate size-dependent mechanical properties, influencing fracture strength and quality factor, prompting extensive experimental and computational exploration [Stassi et al., 2021, Yang et al., 2002, Cui et al., 2003, Zare Pakzad et al., 2023c, Pakzad et al., 2021, Pakzad et al., 2023a, Chen et al., 2017, Gerberich et al., 2017, Han et al., 2023]. In the realm of high-performance devices, NWs and nanotubes offer versatility across electronics, energy, sensing, and communication domains [Wang et al., 2017, Ahoulou et al., 2021, Akbari-Saatlu et al., 2020, Ambhorkar et al., 2018, Arjmand et al., 2022, Barlian et al., 2009, Chen et al., 2024, Espinosa et al., 2013, Goktas et al., 2018, McIntyre and i Morral, 2020]. Applications ranging from gate-all-around transistors to next-gen mass spectrometers underscore the potential for extreme miniaturization, enhancing sensitivity and power efficiency [Chen et al., 2024, Dasgupta et al., 2014, Goktas et al., 2018, Verma et al., 2021]. Feasible integration with electronics, mature fabrication techniques, and transduction via piezoresistivity position silicon (Si) NWs at the forefront of this miniaturization drive, emphasizing the importance of understanding scale effects in NEMS design and implementation [Petersen, 1982, Cui et al., 2023, Nasr Esfahani and Alaca, 2019, Alaca and Karimzadehkhoei, 2023, Zare Pakzad et al., 2023c, Dasgupta et al., 2014, Wang et al., 2017, Fukata et al., 2017, Furmanchuk et al., 2012, Gadea et al., 2018, Hsu et al., 2023, Hwang et al., 2023, Namazu, 2023, Namdari et al., 2016, Raman et al., 2023, Solanki and Um, 2018, Sreejith et al., 2023, Tintelott et al., 2021, Yang and Chandran, 2023, Yang et al., 2022].

Experimental techniques for characterizing the elastic and strength properties of Si NWs are widely utilized in scientific missions [Mead et al., 2023, Espinosa et al., 2013, Zare Pakzad et al., 2023b, Elhebeary and Saif, 2018, Wollschläger et al., 2016]. Various testing techniques, including bending, uniaxial loading, indentation, and resonance, address specific aspects of these requirements with varying degrees of success [Nasr Esfahani and Alaca, 2019, Wang et al., 2017, Yang et al., 2022, Pantano and Kuljanishvili, 2020]. The tests involve loading Si NWs with exter-

nal force-sensing probes or integrating them into micro electromechanical systems (MEMS) for exposure to bending loads [Sohail and Afzaal, 2019, Elhebeary and Saif, 2017b, Jayaram, 2022, Kawamoto et al., 2013, Namazu, 2023, Pantano et al., 2012, Pantano and Kuljanishvili, 2020, Zhu and Chang, 2015]. However, interpreting the resulting load-displacement data requires appropriate models due to the complex experimental aspects, particularly nanometrology-related challenges [Liu and Li, 2022, Kawamoto et al., 2013, Namazu, 2023, Pantano and Kuljanishvili, 2020, Xie et al., 2023]. Without reliable nanomechanical models, quantifying basic properties like stiffness and strength becomes challenging, leading to conflicting observations and a broad range of estimations between experimental and computational findings [Zare Pakzad et al., 2023c, Zare Pakzad et al., 2021, Momeni et al., 2020, Jin et al., 2023, Wang et al., 2023]. The lack of a sound modeling approach underscores the need for more robust methodologies to enhance the accuracy of characterization [Nasr Esfahani and Alaca, 2019, Wang et al., 2017, Zare Pakzad et al., 2023c]. In this respect, experimental challenges include rigorous requirements for reliable testing, such as sample alignment and boundary conditions imposition [Solanki and Um, 2018, Nasr Esfahani and Alaca, 2019, Zare Pakzad et al., 2023c, Espinosa et al., 2013, Wang et al., 2017, Elhebeary and Saif, 2017b]. Additionally, challenges related to processing and metrology, such as sample preparation, device calibration, setup resolution, and *in-situ* characterization, contribute to significant spread in measurements [Li et al., 2020, Elhebeary and Saif, 2017b, Espinosa et al., 2013, Nasr Esfahani et al., 2022]. As a result, Si NW strength reports cover several orders of magnitude, ranging from 100 MPa to 21 GPa below the critical dimension of 400 nm [Nasr Esfahani and Alaca, 2019, Zhu and Chang, 2015, DelRio et al., 2015]. Theoretical and modeling approaches, such as molecular dynamics (MD) simulations and *ab initio* methods, offer powerful tools for studying mechanical properties but also yield a wide range of estimations due to inconsistent use of constitutive models, particularly regarding surface bond reconstruction and nonlinearity in elasticity, highlighting the need for detailed examination and revisitation in modeling approaches [Park et al., 2009, Pakzad et al., 2023b, Pakzad et al., 2024, Pakzad et al., 2023a, Schaible, 1999].

Modeling size-dependent mechanical properties of Si NWs has been primarily conducted through MD simulations, considering parameters such as NW diameter and geometrical shape [Xu and Kim, 2019, Xu, 2020, Pakzad et al., 2021, Pakzad et al., 2023b, Pakzad et al., 2024, Pakzad et al., 2023a, Schaible, 1999]. In this context, MD simulations uncover the correlation between surface stress and bulk elastic modulus in NWs [Lao et al., 2013, Li and Sun, 2012, Park et al., 2009, Schaible, 1999]. Surface-related properties, including surface stress and side surface crystalline orientations, have also been addressed, with both atomic simulations and continuum formulation employed to account for size dependence [Zare Pakzad et al., 2023c, Pakzad et al., 2021, Pakzad et al., 2023a, Agrawal et al., 2008, Miller and Shenoy, 2000, Izumi et al., 2004]. However, most studies, both MD and continuum, have focused on unreconstructed and passivated Si NW surfaces while neglecting the presence of the native oxide layer, known as amorphous silicon dioxide ( $\text{aSiO}_2$ ), which significantly affects local structure and introduces defects [Pakzad et al., 2024, Pakzad et al., 2023b, Nasr Esfahani et al., 2022, Zare Pakzad et al., 2023c]. Despite the expected influence of the native oxide on Si NW mechanical behavior, limited research has been reported, although studies have shown compressive stress near the  $\text{aSiO}_2/\text{Si}$  interface and a reduction in NW stiffness due to the oxide layer [Nasr Esfahani et al., 2022, Zare Pakzad et al., 2023c]. Models often struggle with adequately describing surface-related phenomena and inconsistently using surface models and nonlinear elasticity [He and Lilley, 2008, Song et al., 2011, Zare Pakzad et al., 2021, Zare Pakzad et al., 2023c, Zhan and Gu, 2012]. Effective models should incorporate parameters related to the native oxide's presence, appropriate interatomic potentials for surface stress and elasticity, and considerations for structural aspects like finite deformation and intrinsic stresses [Nasr Esfahani et al., 2022, Zare Pakzad et al., 2023c, Pakzad et al., 2023a]. The native oxide,  $\text{aSiO}_2$ , affects Si NW structure by introducing defects and interfaces, with recent studies revealing tensile intrinsic stresses and reductions in modulus of elasticity and ultimate strength due to native oxide formation [Pakzad et al., 2024, Nasr Esfahani et al., 2022, Zare Pakzad et al., 2023c]. Introducing appropriate interatomic

potentials is crucial for accurately simulating surface stress and elasticity, yet various degrees of success have been observed in estimating size-dependent NW properties [Nasr Esfahani and Alaca, 2019, Zare Pakzad et al., 2023c, Pakzad et al., 2023b, Pakzad et al., 2024, Barrios et al., 2023]. Additionally, other structural aspects such as finite deformation, intrinsic stresses, and boundary conditions must be properly modeled for mechanical consistency and relevance to experimental conditions, considering uncertainties associated with boundary conditions impacting the load-displacement relationship [Wang et al., 2017, Zare Pakzad et al., 2023c].

Regarding this matter, the mechanical characteristics of Si NWs have gained significant attention, with various inconsistencies observed among reported trends concerning the relationship between mechanical behavior and scale [Nasr Esfahani and Alaca, 2019, Yang et al., 2022, Zare Pakzad et al., 2023c]. Additionally, the majority of nanomechanical tests conducted on Si NWs have focused on critical dimensions (CDs) exceeding 10 nm, while computational investigations have primarily been constrained to CDs below 10 nm [Nasr Esfahani and Alaca, 2019, Yang et al., 2022, Zare Pakzad et al., 2023c, Pakzad et al., 2024]. This dimensional discrepancy between experimental and computational approaches has delayed the establishment of a shared foundation, thus impeding progress toward comprehending the size dependence in Si NW mechanical properties [Nasr Esfahani and Alaca, 2019]. Comprehending the impact of the native oxide in generating intrinsic stress [Nasr Esfahani et al., 2022] along with size-dependent mechanical properties of Si NWs [Zare Pakzad et al., 2023c] is pivotal for the prospective integration of NWs as fundamental mechanical components. This understanding will aid in advancing the shift from MEMS to NEMS, facilitating the development of highly precise sensor platforms through ultimate miniaturization [Arjmand et al., 2022, Iakab et al., 2019, Sage et al., 2018, Alaca and Karimzadehkhoei, 2023, Zafar et al., 2018, Jia et al., 2019, Wang et al., 2016b, Sang et al., 2016, Ambhorkar et al., 2018, Karimzadehkhoei et al., 2023, Nehra et al., 2020, Chen et al., 2024, Espinosa et al., 2012, Ghosh, 2023]. In line with Moore's law driving electronics miniaturization, Si NWs, with their small dimensions resulting in high resonance

frequencies and significant surface-to-volume ratios, emerge as top candidates for transducers in the next generation miniaturized sensors based on NEMS [Petersen, 1982, Cui et al., 2023, Nasr Esfahani and Alaca, 2019, Alaca and Karimzadehkhoei, 2023, Zare Pakzad et al., 2023c, Dasgupta et al., 2014, Wang et al., 2017, Fukata et al., 2017, Furmanchuk et al., 2012, Gadea et al., 2018, Hsu et al., 2023, Hwang et al., 2023, Namazu, 2023, Namdari et al., 2016, Raman et al., 2023, Solanki and Um, 2018, Sreejith et al., 2023, Tintelott et al., 2021, Yang and Chandran, 2023, Yang et al., 2022]. In the context of this thesis, the interpretation of the scale effect is accomplished through an integrated approach utilizing MD simulations and the modified core-shell model. Additionally, the incorporation of machine learning (ML), enabled by extensive MD simulations, broadens the applicability of the methodology established in this research, employing artificial intelligence as a practical tool for comprehending the nanomechanics of Si NWs. Lastly, a comprehensive analysis of uncertainties arising from the interplay between *processing, structure, and property* in Si NWs is performed. Employing an integrated methodology within the context of this thesis combining theoretical modeling, multi-scale simulations, advanced fabrication, and multi-modal characterization techniques, a series of enduring issues related to the interpretation of the scale effect in Si NWs have been conclusively addressed.



## Chapter 2

# EFFECT OF NATIVE OXIDE ON STRESS IN SILICON NANOWIRES: IMPLICATIONS FOR NANOELECTROMECHANICAL SYSTEMS

### 2.1 Overview

Understanding the origins of intrinsic stress in Si nanowires is crucial for their successful utilization as transducer building blocks in next-generation, miniaturized sensors based on nanoelectromechanical systems. With their small size leading to ultra-high resonance frequencies and extreme surface-to-volume ratios, silicon nanowires raise new opportunities regarding sensitivity, precision and speed in both physical and biochemical sensing. With silicon optoelectromechanical properties strongly dependent on the level of nanowire intrinsic stress, various studies have been devoted to the measurement of such stresses generated, for example, as a result of harsh fabrication processes. However, due to enormous nanowire surface area, even the native oxide that is conventionally considered as a benign surface condition can cause significant stresses. To address this issue, a combination of nanomechanical characterization and atomistic simulation approaches is developed. Relying only on low-temperature processes, the fabrication approach yields monolithic nanowires with optimum boundary conditions, where nanowires and support architecture are etched within the same silicon crystal. Resulting nanowires are characterized by transmission electron microscopy and micro-Raman spectroscopy. The interpretation of results is carried out through molecular dynamics simulations with ReaxFF potential facilitating the incorporation of humidity and temperature, thereby providing a close replica of the actual oxidation environment – in contrast to previous dry oxidation or self-limiting thermal oxidation studies. As a result, consensus on

significant intrinsic tensile stresses on the order of 100 MPa – 1 GPa was achieved as a function of nanowire critical dimension and aspect ratio. The understanding developed herein regarding the role of native oxide played in the generation of nanowire intrinsic stresses is important for the design and development of silicon-based nanoelectromechanical systems.

## **2.2 Introduction**

Nanowires (NWs) are considered as the central building block of a series of disruptive technologies and device concepts addressing a wide range of applications in nanoelectronics [Jia et al., 2019, Lu and Lieber, 2010] and nanoelectromechanical systems (NEMS) such as mass spectrometers [Sage et al., 2018, Yang et al., 2006], biomedical and physical sensors [Wang et al., 2016b, Sang et al., 2016, Ambhorkar et al., 2018]. Silicon NWs (Si NWs) have received a particular attention in NEMS due to their high sensitivity, ease of integration and compatibility with integrated circuits (ICs) [Nasr Esfahani and Alaca, 2019, Weber et al., 2014]. Mechanical stresses are especially critical in this respect, as they are known to contribute to the optoelectromechanical performance of Si NWs. For example, inducing tensile strain in Si NWs is reported to enhance transconductance [Seike et al., 2007, Minamisawa et al., 2012], and to improve thermal [Fan et al., 2017] and optical properties [Geiger et al., 2015]. Such intrinsic stresses can lead to buckling of suspended Si NWs [Alain et al., 2012] with a direct impact on their mechanical behavior [Calahorra et al., 2015]. The intrinsic stress can also change the dopant diffusion mechanisms in Si NWs [Prüßing et al., 2022]. Furthermore, with piezoresistivity as the leading transduction technique in NEMS [Zhu et al., 2019], the characterization of embedded stresses in these miniscule structures becomes a technologically relevant task and an immediate challenge for the use of Si NWs in sensors.

For this purpose, Raman spectroscopy is widely employed to measure uniaxial stresses in NWs [Nugent and Praver, 1998, De Wolf, 1996, Harris et al., 2004] with a series of studies specifically addressing Si NWs [Spejo et al., 2020, Suess et al., 2014, Minamisawa et al., 2012, Park et al., 2015]. Although Raman techniques have

demonstrated a strain up to 4.5% in Si NWs patterned on highly strained silicon-on-insulator (sSOI) substrates [Hashemi et al., 2009, Spejo et al., 2020, Suess et al., 2014, Minamisawa et al., 2012], the level of strain reported for Si NWs fabricated on stress-free substrates is limited to 0.048% [Park et al., 2015]. In addition to Raman spectroscopy, X-ray diffraction approaches have been utilized to measure strain in Si NWs. For example, a strain of 0.04% was measured, whose origin was traced back to the catalyst residues used during the growth processes [Dupre et al., 2012, Buttard et al., 2011]. Recently, a scanning X-ray diffraction microscopy technique was employed for mapping in-plane crystalline strain in suspended Si NWs, reporting a strain level of 0.025% [Dolabella et al., 2020].

Regarding the origin of the intrinsic stress, the formation of the native oxide layer on Si NW surface has to be studied as one of the major causes in addition to stress generation due to fabrication processes such as reactive ion etching (RIE), die bonding and wafer bonding [Fan et al., 2017, Beccari et al., 2022, Toda et al., 2010, Poborchii et al., 2013]. The presence of native oxide is of paramount importance in Si NWs compared to larger Si structures utilized in microelectromechanical systems (MEMS), as the oxide thickness becomes comparable to the critical dimensions (CDs) of the nanostructure [Allain et al., 2012, Toda et al., 2010, Poborchii et al., 2013]. For example, the effect of native oxide on the mechanical behavior of Si nanoresonators was linked to dissipation mechanisms [Tao et al., 2015] and initial stresses [Beccari et al., 2022]. As native oxide is a very thin layer of amorphous SiO<sub>2</sub> forming on Si surfaces at ambient temperatures upon contact with air, it has an entirely different growth mechanism compared to that of thermal oxides [Morita et al., 1990, Steinruck et al., 2014]. In this respect, previous works reported a strain up to 0.05% in Si NWs, which increases to 0.5% [Takeuchi et al., 2009] or 160 MPa [Calahorra et al., 2015] of stress in thermally oxidized Si NWs depending on their surface condition. The initial formation of the native oxide layer on Si surfaces and the kinetics of its growth have been the subject of various studies, where parameters such as Si doping level, NW shape, and crystal orientation were found to alter the thickness of the oxide layer in a range between 0.3 nm to 5 nm [Philipp and Taft,

1982, Han et al., 2013, McDowell et al., 2011]. The intrinsic stress in Si NWs has been predominantly the main focus of various studies, where pre-strained substrates and thermally oxidized processes are used for fabrication [Minamisawa et al., 2012, Spejo et al., 2020]. Although a limited number of studies have presumed native oxide as a possible cause of intrinsic stress [Fan et al., 2017, Beccari et al., 2022, Toda et al., 2010, Poborchii et al., 2013], an in-depth study dedicated specifically to NWs is required to closely examine this link.

Understanding the role played by native oxide on the generation of intrinsic stress is a critical aspect of the future use of NWs as mechanical building blocks and will thus contribute to the transition from MEMS to NEMS as a high-precision sensor platform of ultimate miniaturization. For this purpose, a recently developed monolithic technology based on low-temperature processes is employed to fabricate Si NWs suspended between two microscale supports [Tasdemir et al., 2018]. Micro-Raman spectroscopy is used to measure the uniaxial stresses in the Si NWs. Finally, an interpretation through modelling is achieved using reactive molecular dynamics (MD) for native oxide formation and intrinsic stress quantification. In the remainder of this work, the fabrication method will be discussed first followed by the micro-Raman measurement technique. After MD simulations are described, the work is concluded with a discussion on the native-oxide-induced stress in Si NWs.

## **2.3 Methods and Materials**

### *2.3.1 Fabrication*

This study uses a recently developed monolithic method to fabricate Si NWs suspended between two microscale pillars [Tasdemir et al., 2018, Zare Pakzad et al., 2021]. The fabrication process starts with a p-type,  $\langle 100 \rangle$  Si wafer of 100-mm diameter, 525- $\mu\text{m}$  thickness and a resistivity range of 0.1–100  $\Omega\text{cm}$ . In this process, 33 nanoscale features are patterned using electron-beam (e-beam) lithography in a 200-nm-thick hydrogen silsesquioxane (HSQ) resist (Figure 2.1 (a)). Then, the substrate is etched via RIE in  $\text{Cl}_2$  plasma to form a Si protrusion on the surface (Fig-

ure 2.1 (b)). The e-beam lithography defines the NW width, while the RIE process determines the same thickness for all patterned nanoscale features regardless of their in-plane dimension. The process is followed by the coating of a low-temperature oxide (LTO) film as the passivation layer via low-pressure chemical vapor deposition (LPCVD) (Figure 2.1 (c)). The LTO layer is then removed from lateral surfaces in a fluoroform plasma using inductively coupled plasma (ICP)-based etching (Figure 2.1 (d)). The Si protrusion, which will turn into a Si NW at the end of the process, is protected over all of its three surfaces. This is followed by deep reactive ion etching (DRIE) that releases the protrusion in the form of a Si NW (Figure 2.1 (e)). This is achieved as undercuts associated with DRIE scallops from both sides are extensive enough to completely remove the Si column that extends beneath the Si surface protrusion. It is this same DRIE process, during which pillars that serve as microscale support columns of the Si NW are also generated. Finally, the e-beam resist and LTO film encapsulating NWs are removed by HF vapor etching (Figure 2.1 (f)). Figure 2.1 (g) demonstrates the multiscale nature of the fabrication technology as structures with a three-order-of-magnitude scale difference are obtained in a single batch. The technique was previously shown to work successfully up to an etch depth of  $40\text{ }\mu\text{m}$  [Esfahani et al., 2017b] and its various applications in MEMS [Esfahani et al., 2017a, Yilmaz et al., 2017] and nanomechanical resonators [Esfahani et al., 2018] were demonstrated. One sample Si NW suspended  $10\text{ }\mu\text{m}$  above the substrate surface is shown in the micrograph in Figure 2.1 (g). Si NW surfaces then gradually oxidize, as a result of which Si NW assumes the cross-section presented in Figure 2.1 (h). The presence of the uniform native oxide layer around the Si core was previously demonstrated in a cross-sectional transmission electron microscopy (TEM) study [Wollschläger et al., 2016] and will be further elaborated below.

### 2.3.2 Raman Measurement

In order to quantify the intrinsic stress in suspended Si NWs, a home-built micro-Raman setup is employed with a Princeton Instruments SP-2500 spectrometer as shown in Figure 2.1 (i). A laser with a wavelength of  $488\text{ nm}$  is used as the excita-

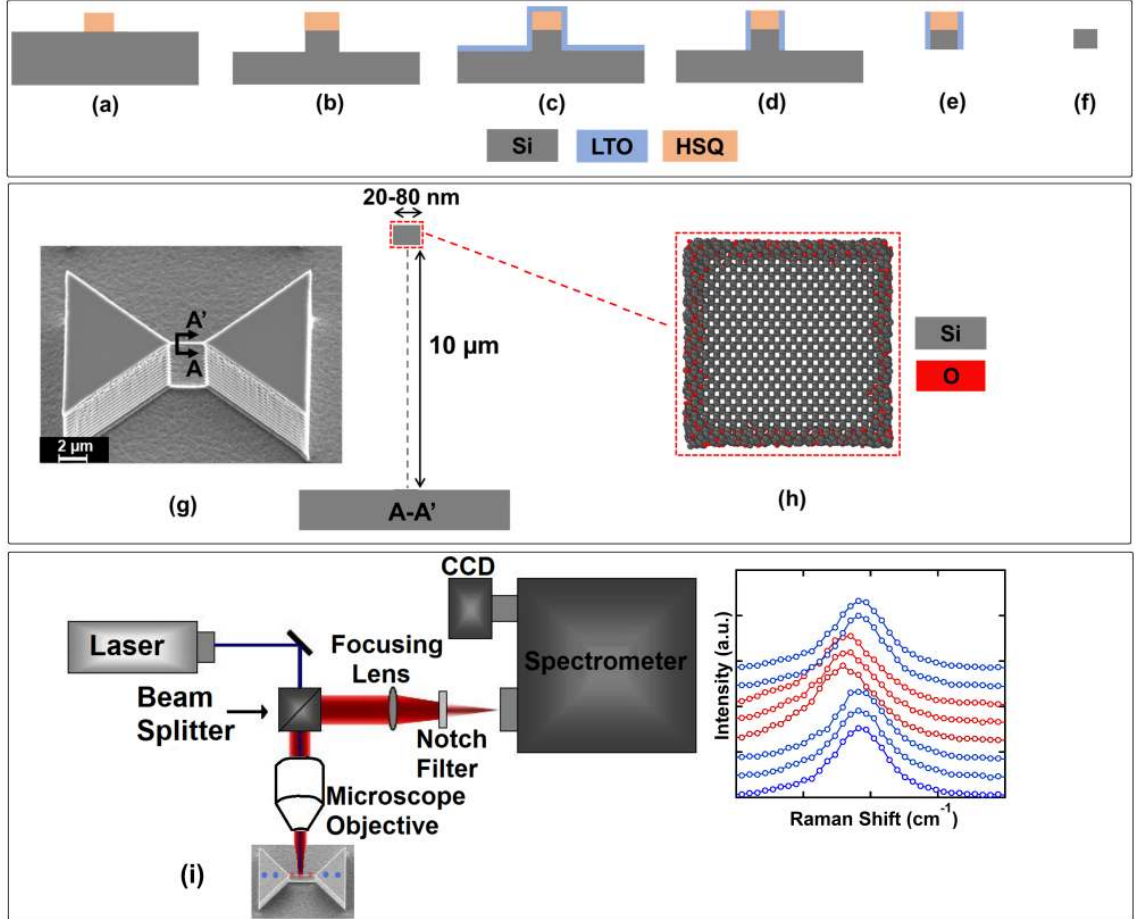


Figure 2.1: (a-f) Process flow for suspended Si NWs. (a) High-resolution patterning through electron-beam lithography. (b) Anisotropic etching step forming the surface protrusion, the precursor line for the future Si NW. (c) Conformal coating of low-temperature oxide (LTO). (d) LTO removal from horizontal surfaces. (e) DRIE with adequate undercut to release the Si NW. (f) Etching of protective layers. (g) Electron micrograph of a Si NW anchored between two 10-μm-thick triangular supports along with a schematic – not drawn to scale – showing the multiscale architecture in the A-A' cross-section. (h) A schematic representation of Si NW cross-section with native oxide (Si and oxygen atoms are shown as gray and red spheres, respectively.) (i) Raman measurement setup consists of a laser source integrated with a beam splitter and a microscope, providing a spot size of 1 μm. A set of data obtained at locations indicated by blue and red dots on the micrograph is also provided as a plot of intensity vs. Raman shift.

tion source. The laser beam is passed to a beam splitter followed by a microscope objective lens to create a spot size of 1  $\mu\text{m}$ . The scattered light is collected through a focusing lens and passed into a notch filter and then guided to the spectrometer. The microscope integrated with the measurement setup enables focusing of the micro-spot on NWs and facilitates a line scanning system to analyze the Raman shift along the entire length of suspended Si NWs with a high spatial resolution.

The Raman shift,  $\Delta\omega$ , is commonly used to measure stress by linking the longitudinal optical (LO) mode obtained in backscattering configuration with stress components in the Si NW [Spejo et al., 2020]. In our case,  $\Delta\omega$  is defined as the shift between the unstrained Si peak,  $\omega_0$ , and the LO shifted strained Si peak,  $\omega_i$ , as given in Equation 2.1.

$$\Delta\omega = \omega_i - \omega_0 = \frac{1}{2\omega_0} \left[ [pS_{12} + q(S_{11} + S_{12})](\sigma_{xx} + \sigma_{yy}) + (pS_{11} + 2qS_{12})\sigma_{zz} \right] \quad (2.1)$$

where  $S_{11}$  and  $S_{12}$  are elastic constants and  $p$  and  $q$  are phonon deformation profiles (PDPs). This model is valid for samples with negligible shear stress with  $\sigma_{xx}$ ,  $\sigma_{yy}$ , and  $\sigma_{zz}$  representing normal stress components along  $x$ ,  $y$ , and  $z$  directions, respectively. For a NW along the  $x$  axis,  $\sigma_{yy}$  and  $\sigma_{zz}$  are negligible and Equation 2.1 can be simplified as Equation 2.2.

$$\Delta\omega = \frac{1}{2\omega_0} \left[ [pS_{12} + q(S_{11} + S_{12})] \right] \sigma_{xx} = (SSC)\sigma_{xx} \quad (2.2)$$

Relating the Raman shift to the uniaxial stress along the NW, the stress shift coefficient (SSC) of Equation 2.2 is an important parameter. A wide range of SSC is reported for Si NWs, where SSC of  $-1.93 \times 10^{-9} \text{cm}^{-1} \text{Pa}^{-1}$  is recommended for NWs in sub-100 nm thickness [Spejo et al., 2020]. Therefore, the Raman shift given in Equation 2.2 can be written as Equation 2.3.

$$\Delta\omega[\text{cm}^{-1}] = -1.93 \times 10^{-9} \times (\sigma_{xx}[\text{Pa}]) \quad (2.3)$$

### 2.3.3 Atomic Simulations

In the final phase of fabrication, Si NWs encapsulated within various oxide layers (e-beam resist, HSQ and LTO) are treated in HF vapor as discussed in relation to Figure 2.1 (f). After this stage, Si NW surfaces exposed to ambient conditions gradually oxidize. This oxide coating as well as the crystalline nature of the Si core were verified previously in a high-resolution TEM study [Wollschläger et al., 2016]. To study the effect of the resulting structure on Si NW intrinsic stresses, MD simulations are carried out. To this end, the oxidation of  $\langle 110 \rangle$  Si NWs is modelled using the reactive force field (ReaxFF) interatomic potential [Van Duin et al., 2003]. A detailed description of the force field as developed for Si-SiO<sub>2</sub> can be found elsewhere [Khalilov et al., 2011, Neyts et al., 2011, Khalilov et al., 2012a]. The force field parameters employed by Newsome *et al.* [Newsome et al., 2012] are used in this work. The choice of ReaxFF is based on the fact that it has been parameterized and previously proven to accurately describe oxide formation process by oxygen and water molecules [Newsome et al., 2012]. A similar oxidation mechanism previously implemented by Khalilov et al. [Khalilov et al., 2012a, Khalilov et al., 2012b] on Si surfaces is utilized here to obtain native oxide formation at ambient temperature with humidity effect. In this model, Si NWs, oxygen, and water molecules (42% relative humidity) are defined in a periodic simulation box as depicted in Figure 2.2 (a) and Figure 2.2 (b). Both ends of the NW are fixed to mimic the type of support in the fabricated architecture of Figure 2.1 (g). The simulation box is relaxed at a temperature of 25 °C and under a pressure of 1 atm for 600 ps using isobaric ensemble (NPT) with a time step of 1 fs. The resulting stress state in the Si NW,  $\pi_{ij}$ , is then calculated using the virial theorem [Zimmerman et al., 2004] as

$$\sigma_{ij} = \frac{1}{2\Omega_o} \left[ \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \frac{1}{r^{\alpha\beta}} \frac{\partial V(r^{\alpha\beta})}{\partial r} (v_i^{\alpha\beta} v_j^{\alpha\beta}) \right] \quad (2.4)$$

where  $\Omega_o$  stands for the atomic volume in an undeformed system with  $N$  as the total number of atoms. Atomic distances between atoms  $\alpha$  and  $\beta$  are represented as  $r^{\alpha\beta}$ .  $v_j^\alpha$  stands for the position of atom  $\alpha$  along  $j$  direction, *i.e.*,  $v_j^{\alpha\beta} = v_j^\alpha - v_j^\beta$  and  $V$



represents the interatomic potential.

## 2.4 Results

Si NWs with a nominal width ( $W$ ) of 20 nm and 80 nm are fabricated with an aspect ratio (AR) of 75, 100 and 150, where AR is defined by the NW length-to-width ratio. Thanks to this chosen set of CDs, results of this study remain relevant both for the application of Si-based nanoelectromechanical systems [Sage et al., 2018, Yang et al., 2006] as well as for the verification through atomistic simulations. NWs are suspended 10  $\mu\text{m}$  above the substrate surface and supported by microscale pillars at both ends. Micrographs in Figure 2.2 (c) and Figure 2.2 (d) depict Si NWs with  $W$  of 20 nm and 80 nm, respectively. Both NWs have an AR of 75 translating into a Si NW length of 1.5  $\mu\text{m}$  in Figure 2.2 (c), and 6  $\mu\text{m}$  in Figure 2.2 (d). The cross-section of each NW is also studied as presented by the corresponding lower micrographs (TEM images). An initial protrusion with a thickness of about 70 nm obtained during the RIE process (Figure 2.1 (b)) leads to rectangle and square cross-sections of NWs with a nominal width of 20 nm and 80 nm, respectively. Both micrographs exhibit a uniform native oxide layer of 3–3.5 nm thickness.

Raman measurements carried out on both types of NWs under ambient conditions are initiated through mapping scattered beams for Si NWs and micro-pillars. The optical microscope in the Raman measurement setup is a navigation system for laser beam positioning. Figure 2.3 (a) depicts one such optical image of the Si NW of Figure 2.2 (d). The resulting normalized Raman intensity obtained for this Si NW is shown in Figure 2.3 (b). This indicates a successful confocal beam scattering from the suspended NW, and hence, the obtained spectra can be considered for calculating the NW Raman shift. In the next step, laser-related effects are eliminated from Raman measurements, where the laser power can cause a Raman shift due to local heating of the NW [Piscanec et al., 2003]. In this respect, Raman measurements are carried out on NWs with a series of different laser powers, the results of which are then compared with those of the bulk Si (Figure 2.3 (c)). A significant heat effect is observed for any laser power in excess of 5 mW. To eliminate heating effects, all

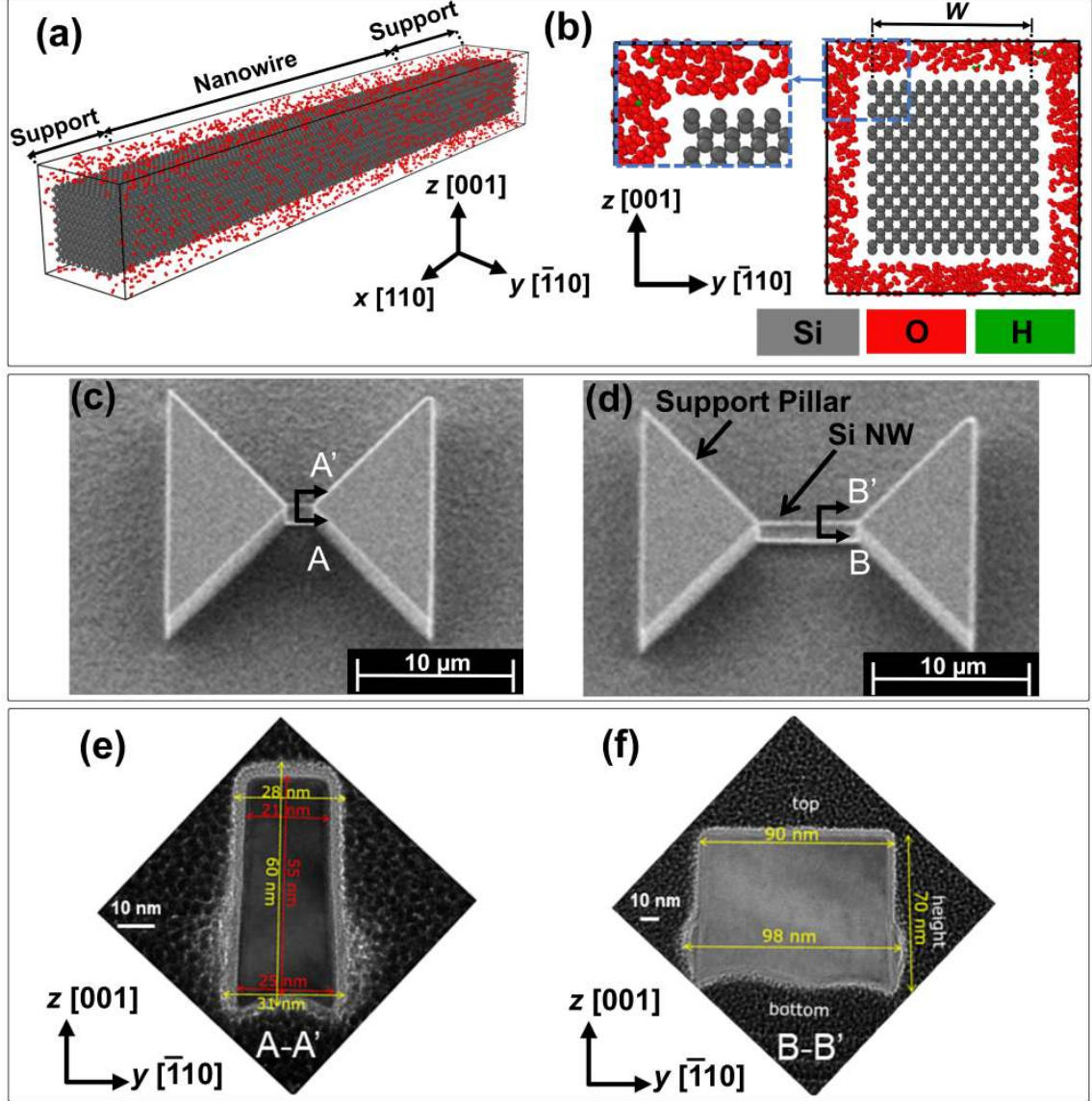


Figure 2.2: (a) A schematic showing the MD simulation of a Si NW with oxygen and water molecules resembling ambient oxidation under 42% humidity. Silicon, oxygen, and hydrogen atoms are represented with gray, red, and green spheres, respectively. (b) Cross-sectional image of a Si NW of width  $W$  with its long axis in  $\langle 110 \rangle$ . SEM images of Si NWs with (c) a nominal width,  $W$ , of 20 nm and a length of 1.5  $\mu\text{m}$  and (d) a nominal width,  $W$ , of 80 nm and a length of 6  $\mu\text{m}$ , suspended between triangular micro-pillars. Cross-sectional TEM images of Si NWs with (e) a nominal width,  $W$ , of 20 nm and (f) a nominal width,  $W$ , of 80 nm reveal the dimensions of the Si core as well as the native oxide envelope.

Raman measurements are carried out at a power of 2 mW.

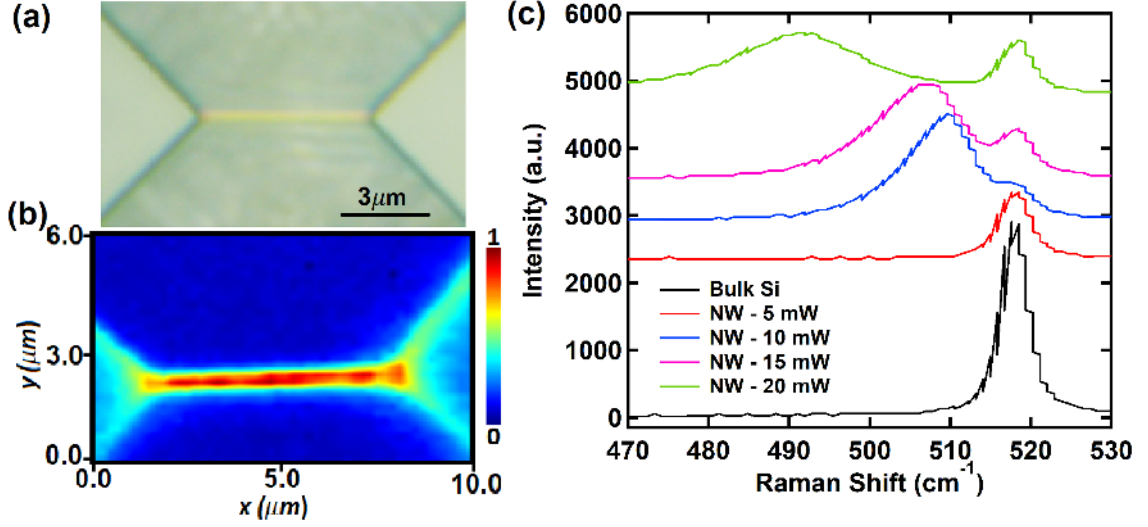


Figure 2.3: (a) Optical micrograph of a Si NW with a width of 80 nm and a length of 6 μm. (b) Mapped Raman intensity of the NW. (c) Raman spectra of bulk Si and the Si NW for a set of laser powers.

After the calibration of the laser power, line scans are carried out along NWs measuring the Raman shift of the bulk as well as the NW. Raman spectra for the NW in  $x$ -direction are recorded, which corresponds to a line-scan along the NW as shown in Figure 2.3 (b) with the associated Raman intensity. Figure 2.4 (a) and Figure 2.4 (b) exhibit Raman spectra obtained from such line scans of Si NWs with  $W$  of 20 nm and 80 nm, respectively. The shaded colors defined on the attached micrographs indicate the location of Raman spectra measured through a line scan, where blue and red curves represent micropillars and Si NWs, respectively. The Gaussian model is used for fitting the Raman peaks of NWs under tension [Chen et al., 2010], while the Lorentzian line shape is considered mainly for homogenous systems [Meier, 2005, Chen et al., 2010]. In this respect, the Gaussian fit is employed here to predict the Raman shift in a line scan. Figure 2.4 (c) and Figure 2.4 (d) exhibit the Raman shifts with the same color code along the NW longitudinal axis ( $x$ -direction) for the 20-nm and 80-nm NW, respectively. A fairly narrow distribution of the peaks is obtained in both cases. Results show Raman spectra with a peak

intensity at  $519.1 \text{ cm}^{-1}$  on Si micropillars, while spectra from suspended NWs shift towards lower wavenumbers. An average downshift of  $1.0 \text{ cm}^{-1}$  is observed for both NWs. This shift towards lower wavenumbers indicates a tensile intrinsic stress along the NW axis.

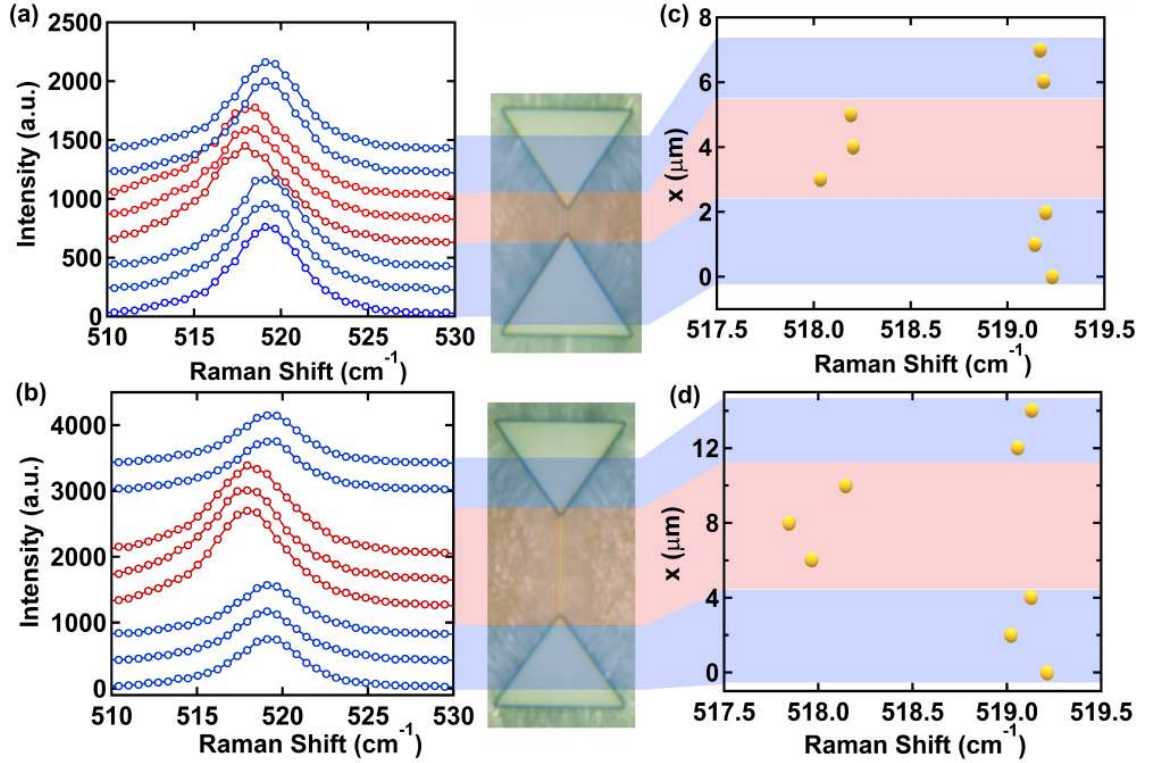


Figure 2.4: Raman spectra measured through a line scan on suspended Si NWs with a width of (a) 20 nm and (b) 80 nm of AR of 75. Insets show the corresponding micrographs, where blue and red indicate micro-pillars and Si NW, respectively. Raman shifts extracted from panels (a) and (b) are provided with the same color code in (c) and (d), respectively.

Finally, Raman spectra for each NW of different ARs are obtained by the same line scan measurement technique. Gaussian fits are performed on the data to estimate the Raman peak shift for each spectrum. Figure 2.5 shows the resulting Raman shifts for micro-pillars and suspended NWs as a function of AR. A total of 33 NWs are tested for proper statistical treatment of the findings as reflected by the error bars of Figure 2.5. Results in Figure 2.5 (a) indicate a Raman peak of  $519.0 \pm 0.3 \text{ cm}^{-1}$  for micropillars regardless of NW size. On the contrary, a lower Raman

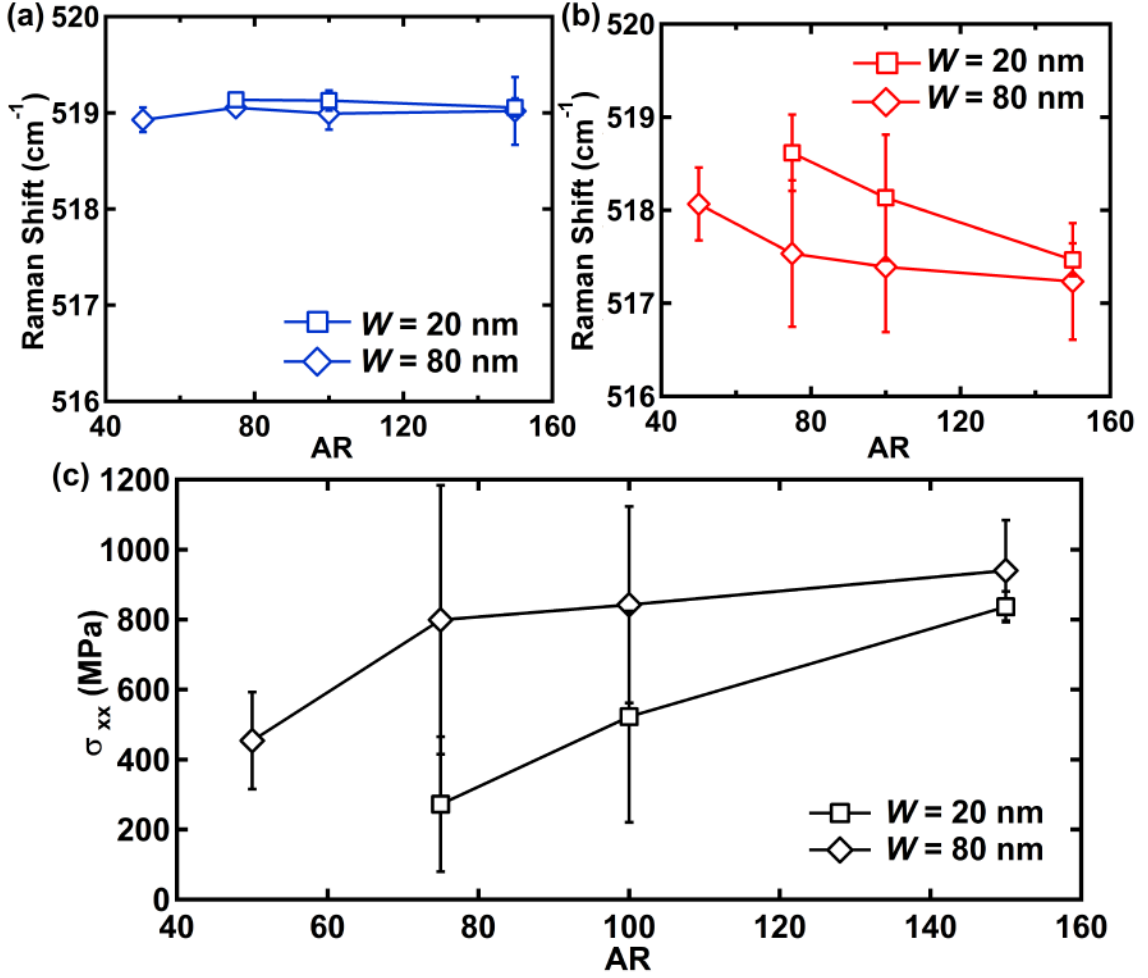


Figure 2.5: Raman peak shifts obtained in line scans as a function of AR for (a) micro-pillar supports and (b) suspended NWs. (c) Uniaxial stress in suspended Si NWs as a function of AR.

peak shift is observed for Si NWs with increasing NW AR (Figure 2.5 (b)). In this respect, the Raman shift in Si NWs with  $W = 80$  nm reduces from  $518.0 \text{ cm}^{-1}$  to  $517.2 \text{ cm}^{-1}$  with the AR changing from 50 to 150. Compared to NWs with  $W = 80$  nm, a larger change in the Raman shift is obtained in Si NWs with  $W = 20$  nm, where increasing AR from 75 to 150 reduces the Raman peak shift from  $518.6 \text{ cm}^{-1}$  to  $517.4 \text{ cm}^{-1}$ .

At this stage, the uniaxial stress in Si NWs can be calculated via Eq. (3). Figure 2.5 (c) depicts the resulting uniaxial stress values as a function of AR. A tensile stress of 431 MPa is obtained for Si NWs with  $W$  of 80 nm and AR of

50, while it reaches 892 MPa for an AR of 150. A similar size-dependent uniaxial stress is observed for Si NWs with  $W$  of 20 nm, where the tensile stress increases from 258 MPa to 794 MPa with AR increasing from 75 to 150. Compared to the measurement uncertainty, the trends exhibited for NWs with different widths are found to be significant with the highest standard deviation of 364 MPa and 287 MPa obtained for  $W$  of 80 nm and 20 nm, respectively. This stress range corresponds to an intrinsic strain of up to  $0.5\% \pm 0.2\%$ .

It is to be emphasized that the associated fabrication technology is based on low temperature, top-down processes on Si substrates to minimize any fabrication-induced stresses in Si NWs, while previous studies reporting residual stresses in Si NWs employed pre-strained substrates [Spejo et al., 2020, Suess et al., 2014, Minamisawa et al., 2012] or used high temperature processes [Fan et al., 2017]. Some studies presumed native oxide formation as the origin of intrinsic stress in Si NWs [Fan et al., 2017, Toda et al., 2010, Poborchii et al., 2013], where the transition in the crystal structure between amorphous  $\text{SiO}_2$  to crystalline Si is attributed to the residual stresses in NWs [Beccari et al., 2022, Toda et al., 2010]. To the best of our knowledge, findings in this work represent the first study reporting intrinsic stresses in top-down Si NWs fabricated neither via high-temperature processes nor using pre-strained substrates.

It is observed that the strain levels reported here are comparable to those reported by a number of previous studies on top-down fabricated Si NWs using high-temperature processes [Fan et al., 2017], while the measured strain in this study is significantly lower than those works using pre-strained substrates [Suess et al., 2014, Minamisawa et al., 2012, Spejo et al., 2020]. However, it remains significant compared to others, especially those achieved through X-ray diffraction techniques [Dolabella et al., 2020]. Despite lower strain levels on the order of 0.025% were reported by the latter, an important tilt magnitude in the crystal lattice was detected [Dolabella et al., 2020]. The difference between the nature of X-ray and Raman measurements previously attracted attention in the field of intrinsic stress measurement of nanostructures [Marola et al., 2021]. Such discrepancies can be linked to

differences between the measurement methods, effects of diffuse scattering as well as defect state of the material and surface defects.

Apart from the intrinsic stress magnitude, the effect of NW size surfaced as another observation that was not reported before. Data in Figure 2.5 (c) reveals clear trends regarding the size effect, where increasing both NW width,  $W$ , and AR leads to higher intrinsic stresses. The effect of AR is especially significant for smaller, *i.e.*  $W = 20$  nm, NWs. Regarding the NW width, previous studies using pre-strained substrates and high-temperature processes reported the opposite trend as a function of  $W$  [Minamisawa et al., 2012, Allain et al., 2012]. The expansion during the thermal oxidation process at high temperatures and associated stresses are considered as the main contributing factors for such intrinsic stresses in Si NWs [Fan et al., 2017]. The residual stresses as a direct impact of lithography resist curing [Liou and Pretzer, 1998] and LTO deposition [Kakiuchi et al., 2007] are found to be negligible compared to the stresses measured in this study. Furthermore, compressive stresses are reported as a result of etching processes in Si nanostructures [Poborchii et al., 2007]. Thus, high tensile stresses encountered in this work verify the surface state – rather than the fabrication itself – is responsible for the generation of intrinsic stresses. Representing the state of the art, the present technology comes as close to eliminating fabrication-related stresses as possible. To our knowledge, there is no top-down alternative that would match the success of this technology in thick SOI wafers.

Taking the aforementioned indicators into consideration, the formation of native oxide on Si NW surfaces following the final oxide removal step of Figure 2.1 (f) via HF vapor etch is considered as the main reason behind the observed tensile stresses in this work. Therefore, MD simulations are employed to study the effect of surface oxidation on the generation of intrinsic stresses in suspended Si NWs. Such simulations can serve as a powerful tool for the interpretation of the above measurement results, as - to the best of our knowledge - no previous MD treatment of the native oxide growth problem exists for Si NWs. Prior MD studies focused on native oxide growth mechanisms investigating chemical composition (stoichiometry)



[Khalilov et al., 2013a], incident particle impact (oxygen atom or oxygen molecule) [Khalilov et al., 2013b], and oxide thickness [Khalilov et al., 2017], while the majority mainly focused on the stresses in thermally oxidized Si NWs [Ohta et al., 2007, Uematsu et al., 2004, Han et al., 2013]. Moreover, a series of studies employed MD to model stress distribution in Si-SiO<sub>2</sub> interface reporting a compressive stress concentrated on the oxide region in the vicinity of the interface [Ohta et al., 2007]. In addition, the ReaxFF potential was employed to model thermal oxide formation on Si NWs using chemical reactions at high temperatures up to 1200 K. A compressive stress of 7-8 GPa was reported in thermal oxide, while Si NWs were found to be under a tensile stress of 2-3 GPa [Khalilov et al., 2013a]. Another study modeled the interfacial stresses during self-limiting oxidation of Si NWs reporting a change in the residual stress from 3.2 GPa to 2 GPa by increasing the temperature from 300 K up to 700 K [Khalilov et al., 2013b].

In contrast to MD studies on the thermal oxidation, the present study employs the ReaxFF potential to model the native oxide formation under ambient conditions replicating the oxidation after etching of protective layers during the fabrication process shown in Figure 2.1 (f), where Si NWs are doubly clamped between micropillars. For this purpose, reactive MD simulations are carried out on Si NWs with both ends fixed over a certain support region, the length of which is set to the 1/8th of NW length replicating the fixed-fixed boundary condition for the Si NW. Periodic boundary condition is defined along all directions. In the first step, the oxide formation on Si NW surfaces is studied through measuring pair distribution functions (PDF). Figure 2.6 (a) demonstrates the magnitude of the pair distribution for Si-O bonds over the simulation time. Oxidation starts off over the first 20 ps with a high rate and reaches the steady state after 60 ps for all  $W$  values involved. Figure 2.6 (b) depicts the PDF of Si-O bonds at 40 ps as a function of the bond length ( $r_{Si-O}$ ). A peak at 1.7 Å is observed for the PDF of oxide. An average Si-O bond length was reported previously as about 1.60 Å using MD simulations [Hung and Hong, 2009], while bond length measurements yield values between 1.55 Å and 1.75 Å for different polymorphs of SiO<sub>2</sub> [Meade et al., 1992]. The native oxide thickness is mea-



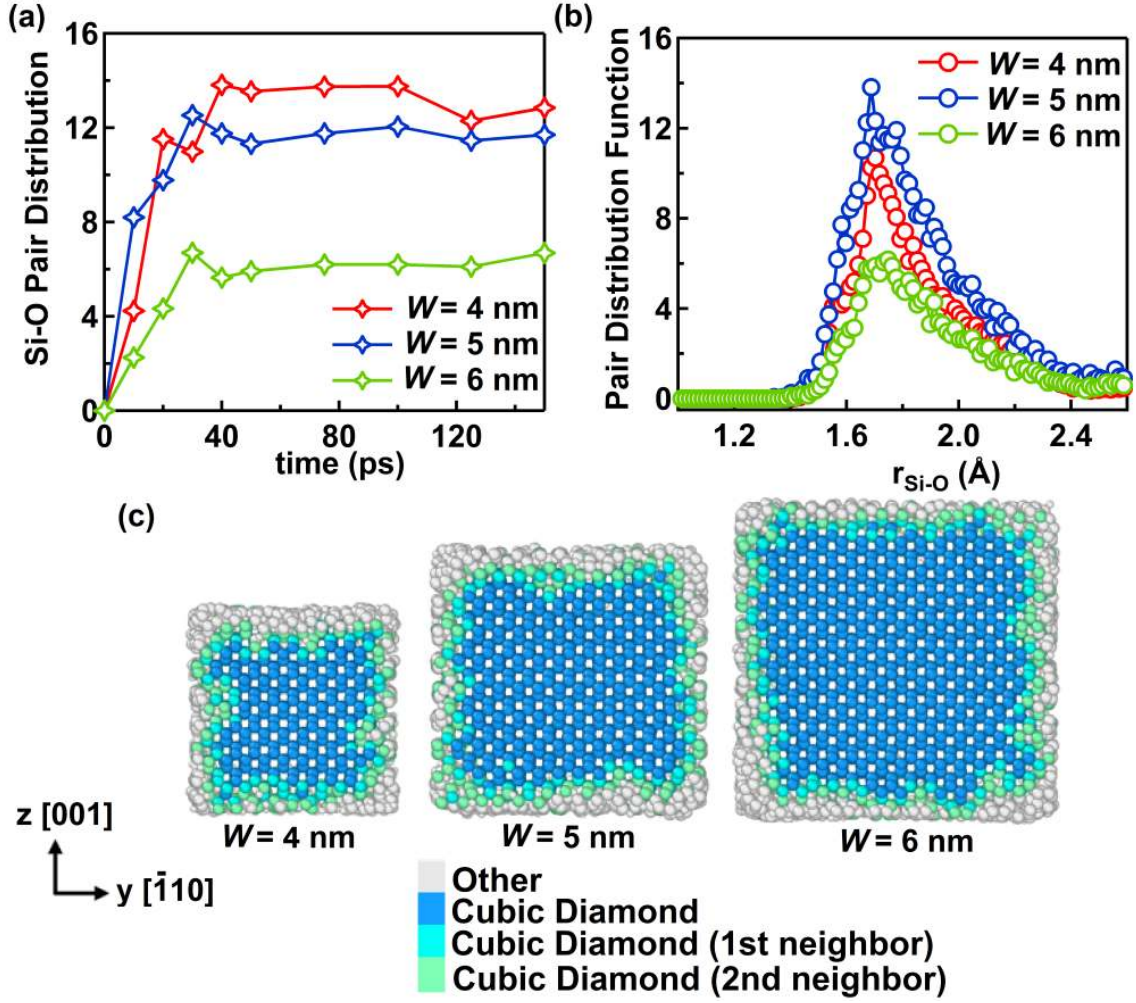


Figure 2.6: (a) The magnitude of the Si-O pair distribution as a function of time (AR=7.5), (b) PDF of Si-O for Si NWs at 40 ps. (c) Atomic structure of Si NWs upon oxidation. Diamond cubic crystal structure is retained within the crystalline core of Si NW.

sured using the diamond crystal structure analysis while identifying the core Si and native oxide regions [Maras et al., 2016]. Figure 2.6 (c) demonstrates the diamond cubic crystal in core Si, while an amorphous native oxide layer is formed around NWs. Results show a native oxide with a thickness ranging between 0.5 nm up to 1.1 nm encapsulating the Si crystal, which is comparable to previous experimental observations [Ma et al., 2003, McDowell et al., 2011, Matteini et al., 2015] as well as MD simulations [Khalilov et al., 2012b, Khalilov et al., 2013a, Khalilov et al., 2013b, Ohta et al., 2007, Pakzad et al., 2021].

Following the oxidation process reaching its steady state, atomic stresses are computed along the longitudinal direction ( $x$ -axis) as described by Equation 2.4. Figure 2.7 (a) and Figure 2.7 (b) depict the distribution of this uniaxial stress component for  $AR = 7.5$ . For  $W = 4$  nm (Figure 2.7 (a)), an average tensile stress of 2.9 GPa is observed along the support regions, while this tensile stress drops to an average value of 2.3 GPa within the NW zone. Although there is a certain variation in  $\sigma_{xx}$ , as it drops from 2.6 GPa at the fixed end of the NW zone to 2.0 GPa at the midspan, there is a clear reduction compared to the stress within the support region. The same trend is obtained for Si NWs of  $W = 6$  nm (Figure 2.7 (b)), where a tensile stress of 1.0 GPa obtained in the support region drops to 0.2 GPa within the NW. Raman measurements of Figure 2.4 can be successfully captured by oxidation simulations at room temperature. Hence, both sign and magnitude of the stress induced through the formation of native oxide around a Si NW can be captured by reactive MD simulations. In contrast to previous studies based on high-temperature (thermal) oxidation, the present approach uses reactive atomic simulations for capturing the native oxide growth on Si NWs at the end of the fabrication process (following Figure 2.1 (f)) at room temperature. Although there is an order of magnitude scale difference between fabricated Si NWs and atomic simulations, both experimental and modelling studies yielded stresses of the same sign, *i.e.* tensile, and order, *i.e.* 100 MPa - 1 GPa. Having employed state-of-the-art fabrication, measurement and computational tools, this scale difference is kept at a minimum. With such verification, the resulting effect of native oxide formation is established as a significant and relevant issue for the performance of Si-based nanoelectromechanical systems.

After calculating the stress profile along Si NWs through reactive MD simulations, the size effect is similarly studied by plotting average  $\sigma_{xx}$  as a function AR (Figure 2.7 (c)). A considerable size-dependent stress is evident for Si NWs with  $W$  less than 6 nm. The uniaxial stress changes from 2.1 GPa to 0.4 GPa with AR increasing from 7.5 to 12 for  $W = 4$  nm. The stress level reduces with increasing NW width, while its variations also become less sensitive to AR. The stress level

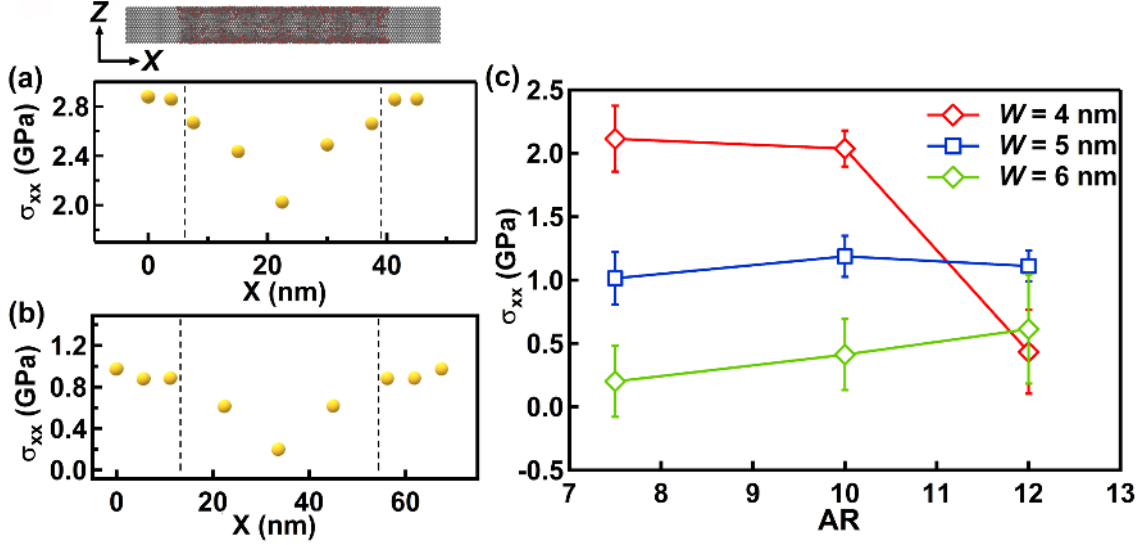


Figure 2.7: Sample stress distributions along Si NWs with AR of 7.5 and  $W$  of (a) 4 nm and (b) 6 nm. Significant tensile stresses are observed with their magnitude decreasing with increasing  $W$ . (c) MD prediction of average uniaxial stress in Si NWs as a function of AR. Stress level increases significantly with reducing  $W$ .

observed in this work is comparable to previous MD studies on thermally oxidized Si NWs [Ohta et al., 2007, Uematsu et al., 2004, Han et al., 2013]. For instance, a tensile stress of 3-6 GPa is obtained in MD simulations of Si NWs with thermal oxide [Ohta et al., 2007], while a lower tensile stress in a range of 100 MPa to 2.0 GPa is predicted through finite element modeling of oxidized Si nanobeams [Han et al., 2013]. Although trends in AR and  $W$  dependence established here cannot directly translate into the observed behavior at the nanoscale, both experimental observations and MD simulations exhibit a considerable tensile stress as a result of native oxide formation in Si NWs. Hence, a strong link between the measured stress profiles obtained through micro-Raman technique (Figure 2.5 (c)) and Si NW surface state is established validating the hypothesis on native oxide effect considerations in a series of previous studies [Fan et al., 2017, Beccari et al., 2022, Toda et al., 2010, Poborchii et al., 2013]. The use of a low-temperature monolithic technology has provided a direct link between the surface state and intrinsic stress measurements. The comparison of MD results with experimental data has revealed a series of

similar trends. Measured stress levels are found to be comparable to those predicted by MD simulations. Here, atomic simulations are utilized to interpret and verify experimental observations on the effect of native oxide on stress in Si NWs. With work in both compartments carried out using state-of-the-art tools and techniques, an exemplary correspondence is obtained, although a series of further benchmark studies is required to understand the size effect on the mechanical properties of Si NWs and its implications for intrinsic stresses.

## **2.5 Conclusion**

Following the miniaturization trend in electronics as predicted by the Moore's Law, electromechanical systems are also under a similar transition fueled by the request for ultrafast and low-power sensors. With their small size leading to ultrahigh resonance frequencies and extreme surface-to-volume ratios, Si NWs are leading candidates for transducer building blocks in next-generation, miniaturized sensors based on NEMS. Although top-down fabrication of Si NWs in NEMS follow the footsteps of transistor manufacturing, the associated challenges are unique, as extreme topographies have to be utilized, and hence, their full utilization necessitates rigorous technology development. In this respect, the role played by the native oxide on the generation of intrinsic stresses is a critical issue. Although its presence in MEMS can be neglected, Si NWs with their immense surface-to-volume ratio are affected by all surface conditions including the native oxide.

This study aims to investigate the impact of native oxide on the embedded stress in Si nanostructures. In this respect, a recently developed technology is utilized to fabricate suspended Si NWs, which involved a combination of high-resolution lithography and a two-stage etching. No high-temperature processes were utilized during fabrication, and pristine Si NWs were left to oxidize under ambient conditions after a final thorough cleaning stage involving HF vapor etching. This led to the formation of native oxide on all Si NW surfaces as verified by high-resolution TEM. Si NWs of two different nominal widths of 20 nm and 80 nm were fabricated with ARs of 75, 100 and 150. TEM measurements revealed a uniform native oxide layer

of 3–3.5 nm thickness. For the characterization of intrinsic stresses in Si NWs, a Micro-Raman-spectroscopy-based approach was developed and applied to a set of 33 samples. A downshift was consistently observed in Si NWs representing a tensile intrinsic stress. For 80-nm Si NWs, this tensile stress was observed to change from 431 MPa to 892 MPa with increasing AR from 50 to 150. In parallel, a tensile stress of 258 MPa was observed for 20-nm Si NWs of AR of 75, which increased to 794 MPa for AR of 150. For the interpretation of measurements, a reactive MD simulation had to be developed for the modeling of the formation of native oxide around Si NWs. Si NWs with nominal widths of 4, 5, and 6 nm and AR of 7.5, 10, 12 and 15 were modeled using the ReaxFF potential.

Results exhibited tensile stresses in the range of 100 MPa to 2.0 GPa. Both the sign and the magnitude of stresses induced by the formation of native oxide around a Si NW could thus be captured. Hence, experimental measurements and computational simulations indicate a significant tensile stress in Si NWs as a direct outcome of native oxide formation. It was shown for the first time that room-temperature formation of native oxide can generate significant stresses in Si NWs. This result was achieved through careful development of both the fabrication and modelling approaches, where the first suppresses any unintended sources of stress generation and ensures correct boundary conditions, while the latter – having taken temperature and humidity effects into account – provides a close replica of the oxidation environment under ambient conditions. Therefore, the simulation approach utilized here can replace those reported in previous dry oxidation or self-limiting thermal oxidation studies. The understanding developed herein regarding the role of native oxide played in the generation of Si NW intrinsic stresses is important for the design and development of future NEMS sensors.

## Chapter 3

# A NEW CHARACTERIZATION APPROACH TO STUDY THE MECHANICAL BEHAVIOR OF SI NWS

### 3.1 Overview

This work proposes a new approach to characterize the mechanical properties of nanowires based on a combination of nanomechanical measurements and models. Silicon nanowires with a critical dimension of 90 nm and a length of 8  $\mu\text{m}$  obtained through a monolithic process are characterized through *in-situ* three-point bending tests. A nonlinear nanomechanical model is developed to evaluate the mechanical behavior of nanowires. In this model, the intrinsic stress and surface parameters are examined based on Raman spectroscopy measurements and molecular dynamics simulations, respectively. This work demonstrates a new approach to measure the mechanical properties of Si nanowires by considering the surface effect and intrinsic stresses. The presented technique can be used to address the existing discrepancies between numerical estimations and experimental measurements on the modulus of elasticity of silicon nanowires.

### 3.2 Introduction

Nanowires (NWs) are frequently employed as fundamental components in innovative devices including gate-all-around transistors, next-generation mass spectrometers and solar cells [Wang et al., 2017, Song et al., 2012]. This trend is further consolidated by the emergence of Internet of Things, (IoT), with the integration of various sensors quickly becoming a challenge for semiconductor manufacturing [Nasr Esfahani and Alaca, 2019]. Despite all their promising aspects, the level of commercialization of such new technologies remains surprisingly low.

There has been a vast effort towards the characterization of materials behavior at the nanoscale, while a series of contradictory findings were reported in experimental and computational studies. Measurements of mechanical properties such as the modulus of elasticity appear to be affected by the shape, size, crystal orientation and surface state of NWs as possible causes of discrepancy [Wang et al., 2017, Nasr Esfahani and Alaca, 2019]. For example, the size effect on the modulus of elasticity of  $\langle 111 \rangle$  Si NWs is reported to be more drastic compared to those reported for  $\langle 100 \rangle$  and  $\langle 110 \rangle$  crystal orientations highlighting the effect of orientation on the size-dependent elastic behavior [Nasr Esfahani and Alaca, 2019]. Significant improvement remains to be accomplished regarding the optimization of NW fabrication technologies, physical characterization tests and integration techniques.

Mechanical characterization is an important aspect of the feasibility study for the use of NWs as the central building block of nanoelectromechanical systems (NEMS). Nanomechanical testing is carried out mainly through tensile/buckling, bending and nanoindentation tests, where the NW size is found to be a critical factor affecting mechanical properties [Nasr Esfahani and Alaca, 2019]. Understanding the size effect on the NW mechanical response requires a comprehensive characterization approach to address existing contradictions in the literature. For instance, theoretical calculations predict the size-dependent elastic properties for NWs with cross-sectional dimensions less than about 10 nm [Kang and Cai, 2010]. However, experimental measurements report contradictory findings as a result of particular NW diameter, defect density, loading type and loading conditions [Tang et al., 2012]. This study investigates one such case, where the modulus of elasticity of Si NWs with a critical dimension of 90 nm is estimated via three-point bending testing. Testing effort is accompanied by a comprehensive nonlinear model of NW bending, considering all relevant effects including large deformation, intrinsic stresses, and surface parameters. In this respect, the presence of intrinsic stresses is studied through micro-Raman spectroscopy with a precise evaluation of strain profile in the structure. In addition, surface effect — another critical parameter in understanding the role of scale — is studied by implementing the surface stress and surface

elasticity through atomistic simulations. Overall, the study presents a comprehensive approach considering large deformation, surface effects and intrinsic stresses to interpret the bending response of Si NWs.

### **3.3 Methods and Materials**

Details of the device fabrication of Si NWs co-fabricated with their supports within the same Si crystal are given in Section 3.3.1 followed by nanomechanical testing details in Section 3.3.2. Interpretation of the force-deflection results obtained from nanomechanical testing requires a nonlinear nanomechanical model including intrinsic stress and surface effects with details provided in Section 3.3.3. Raman characterization used for the measurement of intrinsic stresses and atomistic simulations used for surface stress and surface elasticity calculations are discussed in Section 3.3.4 and Section 3.3.5, respectively.

#### *3.3.1 Nanowire Fabrication*

The Si NWs for this work were fabricated using a monolithic top-down method which allows the fabrication of a NW connected to support pillars [Tasdemir et al., 2018, Tasdemir et al., 2016]. This method enables the fabrication of the NW within a thick Si crystal allowing ample space between the NW and the substrate for bending experiments [Wollschläger et al., 2016]. Furthermore, having both NWs and microscale supports fabricated from the same crystal eliminates any interface compliance, that would jeopardize the definition of boundary conditions, if NWs were attached through pick and-place assembly instead. This approach also facilitates the integration of NWs with microelectromechanical systems (MEMS) [Yilmaz et al., 2017] with implications for multiscale device fabrication [Esfahani et al., 2017b]. The process flow is developed to fabricate single-crystalline Si NWs with microscale anchors. It is a combination of a shallow and a deep etch process for the NW definition and release, respectively. The process starts with the patterning of 200-nm-thick HSQ (Hydrogen silsesquioxane) lines through e-beam lithography on a p-type  $\langle 100 \rangle$  Si wafer. Linewidths of 90 nm are patterned in  $\langle 110 \rangle$  crys-



tal orientation. This dimension directly translates into the Si NW width (in-plane dimension), as HSQ serves as an etch mask during the shallow etch, a  $\text{Cl}_2$ -based reactive ion etching (RIE) process. After the NW is thus defined on the wafer surface, a conformal low-temperature oxide (LTO) with a 80-nm thickness is coated and then removed from horizontal surfaces to protect NW sidewalls. A deep reactive ion etching (DRIE) process, the second etch step, is then carried out to produce an adequate scallop size allowing the release of Si NW at the end of the first cycle of etching. Further cycles of etching are carried out to obtain a single Si NW suspended over the desired trench depth. Further details of the process flow can be found elsewhere [Tasdemir et al., 2018, Tasdemir et al., 2016]. Figure 3.1 (a) shows the scanning electron microscopy (SEM) image of a Si NW connected to the support pillars, while the sample dimensions are shown in Figure 3.1 (b). The high-resolution transmission electron microscope (TEM) image provided after an focused ion beam (FIB) cut near the midsection (A-A') of the NW in Figure 3.1 (b) shows the NW cross-sectional dimensions.

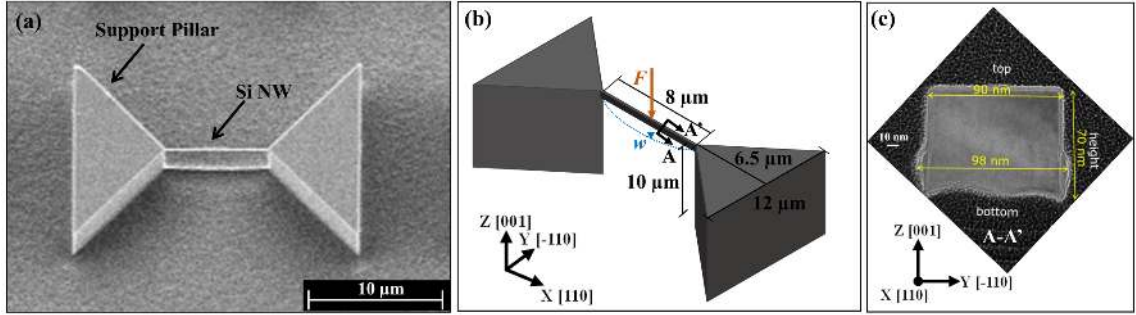


Figure 3.1: (a) Scanning electron micrograph of a suspended Si NW between support pillars. (b) A schematic demonstrating the sample dimensions and representing 3-point bending test with an applied load,  $F$ , inducing a deflection,  $w$ , at NW mid-span. (c) High-resolution TEM image of the Si NW cross-section.

### 3.3.2 Nanomechanical Testing

Double-clamped Si NWs were then tested through *in-situ* three-point bending method as explained elsewhere [Wollschläger et al., 2016], where a piezoresistive force sen-

sor attached to a probe was used to load NWs at their midspan with  $F$  as shown in Figure 3.1 (b), while resulting deflections,  $w$ , were measured through scanning electron micrographs. Upon contact with the test sample, the piezoresistive gage produces an analog voltage output, which is converted into a force value according to a former calibration step and recorded with a sampling period of 1s. The whole experiment was performed *in-situ* within the vacuum chamber of the FIB/SEM at ambient temperature. From the SEM images it was possible to extract the displacement of the nanowire with an image correlation software in pixel size precision for each force measurement. Force vs. deflection ( $F$ - $w$ ) data are obtained as a result. Tests are repeated 10 times on identical NWs for proper statistical treatment.

### 3.3.3 Nanomechanical Model

Bending is one of the well-known NW mechanical characterization techniques, where a nonlinear relation between force and deflection is commonly observed as a result of large deflection [Wang et al., 2017]. The nonlinear behavior in the elastic region of the  $F$ - $w$  curve is governed by Equation 3.1 that incorporates the effects of axial forces due to large deflection, intrinsic stresses, and surface parameters.

$$EI \frac{d^4 w}{dx^4} - T \frac{d^2 w}{dx^2} - H \frac{d^2 w}{dx^2} = F \delta(x - \frac{L}{2}) \quad (3.1)$$

where  $E$  is the modulus of elasticity,  $I$  is the second moment of area,  $x$  is the spatial coordinate along the beam length, and  $\delta$  is the Dirac delta function [Heidelberg et al., 2006]. The tension term due to large deflections,  $T$ , represents both the axial tensile force effect, which is inherently induced due to the stretching of the beam, and the residual force,  $T_0$ , as described by Equation 3.2 [Yaish et al., 2015], [Hudson et al., 2013].

$$T = \frac{EI}{2L} \int_0^L (\frac{dw}{dx})^2 dx + T_0 \quad (3.2)$$

On the other hand, surface-related parameters, surface stress,  $\tau_0$ , surface elastic

modulus,  $E_s$ , are combined into a constant surface parameter,  $H$ , as described in Equation 3.3 [Zhan and Gu, 2012].

$$H = 2hE_s\epsilon_x + 2\tau_0h \quad (3.3)$$

where  $h$  is the NW thickness and  $\epsilon_x$  is the axial strain. Solving Equation 3.1, Equation 3.2 and Equation 3.3 subjected to double-clamped boundary conditions at both ends would provide the exact analytical solution. Further details on the comprehensive solution of the governing equation with separate axial and intrinsic stresses and surface effects can be found elsewhere [Heidelberg et al., 2006, Yaish et al., 2015, Hudson et al., 2013, Zhan and Gu, 2012]. The intrinsic stress and surface parameters are key for having a sound model. In this respect, the intrinsic stress was measured using Raman spectroscopy, which will be discussed in the following section. The determination of surface parameters was carried out through atomistic simulations, which will be presented in Section 3.3.5.

#### 3.3.4 Raman Spectroscopy

Intrinsic stress,  $\sigma_0$ , represented by the residual force,  $T_0$ , above, was quantified using a home-built  $\mu$ -Raman setup equipped with Princeton Instruments SP-2500 spectrometer. A laser of 488-nm wavelength was used as an excitation source with a spot size of 1  $\mu\text{m}$  achieved through a beam splitter and microscope objective lenses. To perform a line scan along a NW, an integrated microscope with the measurement setup was used to focus the micro-spot on the NW. Raman spectroscopy can be used to quantify Si NW intrinsic stress by using the Raman shift,  $\Delta\omega$  [De Wolf, 1996]. This model links the longitudinal optical (LO) mode obtained in backscattering configuration to the sample stress components and is valid for samples with negligible shear stress components. In the case of a NW under intrinsic stress,  $\sigma_0$ ,  $\Delta\omega$  is described in Equation 3.4 as the difference between the unstrained Si peak and the LO shifted strained Si peak [Suess et al., 2014].

$$\Delta\omega = \frac{1}{2\omega_0}[pS_{12} + q(S_{11} + S_{12})]\sigma_0 \quad (3.4)$$

where  $S_{11}$  and  $S_{12}$  are the elastic constants for Si, while  $p$  and  $q$  represent the phonon deformation profiles (PDPs).  $\sigma_0$  is the stress shift coefficient with elastic constants of  $S_{11} = 7.68 \times 10^{-12} \text{ Pa}^{-1}$ ,  $S_{12} = -2.14 \times 10^{-12} \text{ Pa}^{-1}$  for Si along  $\langle 110 \rangle$  crystal orientation and PDPs of  $p = -1.85 \times \omega_0^2$  and  $q = -2.31 \times \omega_0^2$  [De Wolf, 1996]. The resulting expression is given in Equation 3.5.

$$\Delta\omega(\text{cm}^{-1}) = -2 \times 10^{-9} \times \sigma_0(\text{Pa}) \quad (3.5)$$

### 3.3.5 Atomistic Simulations

The surface parameters,  $E_s$  and  $\tau_0$ , can be quantified through various methods such as molecular dynamics, MD, [Izumi et al., 2004, Miller and Shenoy, 2000], density functional theory, DFT, [Melis et al., 2016], finite element modeling, FEM, [Quagliotti et al., 2013] and direct experimental measurement [Pennelli et al., 2012]. Surface elastic constants ( $d_{ijkl}$ ) can be calculated using the method recommended in Ref. [Izumi et al., 2004], where  $d_{ijkl}$  is defined as the second-order derivative of surface energy with respect to the strain under plane-stress condition, which represents the variation in elastic constants due to the surface formation. Elastic constants (stiffnesses) for the bulk ( $C_{ij}^{bulk}$ ) and film ( $C_{ij}^{film}$ ) can be obtained using MD simulations. The elastic constants for the bulk model should be defined under plane stress condition ( $C_{ij}^{bulk,plane}$ ) using the definitions in Equation 3.6.

$$C_{11}^{bulk,plane} = C_{11} - \frac{C_{13}^2}{C_{33}}, C_{22}^{bulk,plane} = C_{22} - \frac{C_{23}^2}{C_{33}}, C_{12}^{bulk,plane} = C_{12} - \frac{C_{12}C_{13}}{C_{33}} \quad (3.6)$$

The relationship between the plane-stress elastic constants of the bulk and film models with the surface elastic constants is represented in Equation 3.7.

$$C_{ijkl}^{film,plane} = C_{ijkl}^{bulk,plane} - 2 \times \frac{d_{ijkl}}{L_z} \quad (3.7)$$

Surface stress ( $\tau_0$ ) is defined as the variation in total surface energy per unit area with respect to the strain and by assuming the film thickness of  $Lz$ , the surface stress components denoted as  $f_{ij}$  are formulated in Equation 3.8, where  $\hat{\eta}$  represents the averaged strain due to the relaxation.

$$f_{ij}(\hat{\eta}) = f_{ij}^{film}(\hat{\eta}) - f_{ij}^{bulk}(\hat{\eta}) \quad (3.8)$$

Bulk surface stress must be estimated separately by the bulk model and surface stress for the film model can be defined by using the stress tensor definition ( $\sigma_{ij}^{film}$ ) as shown in Equation 3.9.

$$f_{ij}^{film}(\hat{\eta}) = \sigma_{ij}^{film}(\hat{\eta}) \times \frac{Lz}{2} \quad (3.9)$$

This method is applied to a nano-scale thin film of Si crystal in static states (no temperature effect) with (110)  $1 \times 1$  surface, where the Tersoff-T3 potential is used as the interatomic potential. A bulk model, as shown in Figure 3.2 (a), with a simulation box set as 8 times of Si lattice constant is defined with the crystal orientation of  $(x, y, z) = ([\bar{1}\bar{1}0], [001], [110])$  including 8192 atoms and periodic boundary conditions in all directions. To obtain elastic constants, small strains in different directions are applied to the simulation box and the variation of the energy is measured. Surface elasticity,  $E_s \epsilon_x$  can be estimated as the average of  $d_{11}$  and  $d_{22}$  surface elastic constants and is examined for Si unreconstructed surface through using a film model where periodic boundary conditions are applied in  $x$  and  $y$  directions but not in the  $z$  direction, providing an infinite size film model with limited thickness,  $Lz$ , as shown in Figure 3.2 (a). Surface stress ( $\tau_0$ ) for unreconstructed (110) Si surface is obtained by the relaxation of the film model, which was estimated by the average of  $f_{11}$  and  $f_{22}$  surface stresses due to the free surface effect upon relaxation.

### 3.4 Results

The nanomechanical model is developed for a Si NW having a width of 90 nm, a height of 70 nm, and a length of 8  $\mu\text{m}$ . In this model, the surface elasticity and

surface stress for 110 Si surface are first evaluated through MD simulations. Results demonstrate a surface elasticity,  $E_s\epsilon_x$ , and surface stress,  $\tau_0$ , of -4.3 N/m and -1.26 N/m, respectively. Raman spectroscopy is employed to measure the intrinsic stress,  $\sigma_0$ . Raman spectra obtained from the line scan measurements on support pillars and Si NWs discussed in Section 3.3.4 are shown in Figure 3.2 (b). Raman shifts of about  $520.8 \text{ cm}^{-1}$  and  $519.7 \text{ cm}^{-1}$  are obtained for the bulk Si and Si NW, respectively. This indicates an intrinsic stress of 300 MPa according to Equation 3.5. The nanomechanical model is then fitted to the bending data. Figure 3.2 (c) shows the experimental force-deflection ( $F-w$ ) data obtained for Si NW tested using the 3-point bending and fitted nanomechanical model. Results demonstrate a non-linear relationship between force-displacement as shown in Figure 3.2 (c) with a force range up to  $18 \text{ }\mu\text{N}$  and associated deflection range up to  $1.3 \text{ }\mu\text{m}$  at the middle of the NW. As a result, the modulus of elasticity,  $E$ , is estimated as 65 GPa based on the measurements on 10 identical NWs. The modulus of elasticity obtained in this work is comparable with those previously reported in the range of 70 GPa to 100 GPa for top-down fabricated Si NWs with similar size and crystal orientation [Sadeghian et al., 2009, Li et al., 2006]. A higher modulus of elasticity of 160 GPa to 230 GPa is reported for Si NWs under tensile tests [Tsuchiya et al., 2018]. This can be linked to surface elasticity, surface defects and native oxide effects [Nasr Esfahani and Alaca, 2019].

### 3.5 Conclusion

This work proposes a new technique to study the mechanical behavior of NWs through an incorporation of nanomechanical testing and modeling. Here, a nonlinear model is fitted into bending measurement of a Si NW. The nonlinear nanomechanical model incorporates intrinsic stress and surface parameters coupled with the axial tension due to large deflections. The intrinsic stress is quantified using Raman spectroscopy, while surface parameters including surface elasticity and surface stress are calculated using MD simulations. A modulus of elasticity of 65 GPa is measured for Si NWs with a size of 70 nm thickness, 90 nm width and  $8 \text{ }\mu\text{m}$  length. This

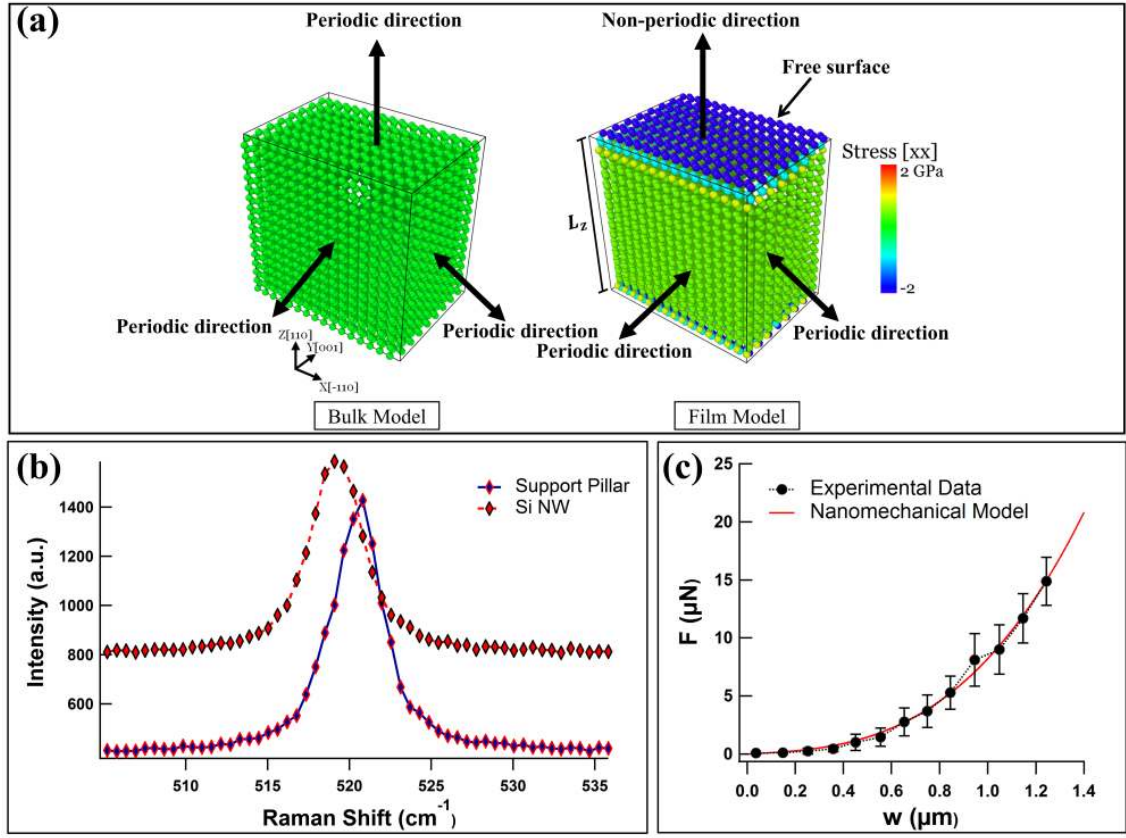


Figure 3.2: (a) Bulk and film models of Si with stress component represented in  $z$ -direction for Si(110)  $1 \times 1$  used for surface elasticity and surface stress calculations. (b) Raman spectra measured through a line represented for support pillar and Si NW locations. (c) Force vs. deflection data obtained through 3-point bending test and fitted curve using nonlinear nanomechanical model of this work.

study considered an unreconstructed surface in the nanomechanical model, while the effect of Si native oxide can be implemented into the model through introducing an oxide layer in atomic simulations. This approach can be utilized to address the contradictions on reported modulus of elasticity for Si NWs [Nasr Esfahani and Alaca, 2019].

## Chapter 4

# NANOMECHANICAL MODELING OF THE BENDING RESPONSE OF SILICON NANOWIRES

### 4.1 Overview

Understanding the mechanical behavior of silicon nanowires is essential for the implementation of advanced nanoscale devices. Although bending tests are predominantly used for this purpose, their findings should be properly interpreted through modeling. Various modeling approaches tend to ignore parts of the effective parameter set involved in the rather complex bending response. This oversimplification is the main reason behind the spread of modulus of elasticity and strength data in the literature. Addressing this challenge, a surface-based nanomechanical model is introduced in this study. The proposed model considers two important factors that have so far remained neglected despite their significance: i) intrinsic stresses composed of the initial residual stress and surface-induced residual stress, and ii) anisotropic implementation of surface stress and elasticity. The modeling study is consolidated with molecular dynamics-based study of the native oxide surface through Reactive Force Fields and a series of nanoscale characterization work through *in-situ* three-point bending test and Raman spectroscopy. The treatment of the test data through a series of models with increasing complexity demonstrates a spread of 85 GPa for the modulus of elasticity and points to the origins of ambiguity regarding silicon nanowire properties, one of the most commonly employed nanoscale building blocks. A similar conclusion is reached for strength, with variations of up to 3 GPa estimated by the aforementioned nanomechanical models. Precise consideration of the nanowire surface state is thus critical to comprehend the mechanical behavior of silicon nanowires accurately. Overall, this study highlights the need for a multiscale



theoretical framework to fully understand the size-dependent mechanical behavior of silicon nanowires with fortifying effects on the design and reliability assessment of future nanoelectromechanical systems.

## **4.2 Introduction**

Silicon (Si) nanowires (NWs) are essential building blocks in nanoelectromechanical systems (NEMS) and nanoelectronics [Nasr Esfahani and Alaca, 2019, Arjmand et al., 2022]. Thanks to their compatibility with semiconductor manufacturing, Si NWs bear potential for improving existing technologies or generating new approaches regarding mass spectroscopy [Iakab et al., 2019, Sage et al., 2018], electromechanical/biochemical sensors [Alaca and Karimzadehkhoei, 2023, Zhang et al., 2010b], field effect transistors (FETs) [Zafar et al., 2018, Sessi et al., 2020, Li et al., 2021], energy conversion, harvesting and storage media [Nehra et al., 2020]. The operation of these nanodevices, especially NEMS, relies significantly on their high surface-to-volume ratios leading to remarkable size-dependent mechanical properties [Cakirlar et al., 2022, Yang et al., 2022, Nasr Esfahani and Alaca, 2019, DelRio et al., 2015, Stassi et al., 2021]. The surface contribution to the overall mechanical behavior increases with decreasing size, thereby resulting in significant size-dependence in NW properties [Nasr Esfahani and Alaca, 2019, DelRio et al., 2015]. For example, the quality factor of Si-based nano resonators is reduced due to surface loss mechanisms such as adsorption, surface stress, surface oxidation/reconstruction, and surface defects [Nasr Esfahani and Alaca, 2019, Yang et al., 2022, Yang et al., 2002]. Fracture strength is also shown to be strongly correlated with surface-related defects [DelRio et al., 2015, Cui et al., 2003]. Therefore, a wide range of experimental and computational attempts have been carried out to explore Si NW mechanical behavior [Nasr Esfahani and Alaca, 2019, Yang et al., 2022, Espinosa et al., 2013, Wang et al., 2017, Pakzad et al., 2023b, Pakzad et al., 2021, Zare Pakzad et al., 2021, Tasdemir et al., 2018].

Among experimental techniques, bending tests are ubiquitously employed for the characterization of both elastic and strength properties of Si NWs along with other

one-dimensional nanostructures [Heidelberg et al., 2006, DelRio et al., 2015, Nasr Esfahani and Alaca, 2019, Wang et al., 2017]. Bending tests are rather straightforward, where Si NW is loaded preferentially *in-situ* with an external force-sensing probe [Zare Pakzad et al., 2021]. Similarly, Si NWs can be integrated with testing devices in the form of microelectromechanical systems (MEMS) [Elhebeary and Saif, 2018], where they are exposed to bending loads. The resulting load-displacement data have then to be interpreted through appropriate models [Wollschläger et al., 2016]. Although there are complicated experimental aspects of bending tests mainly related to nanometrology [Brand et al., 2019, Espinosa et al., 2013, DelRio et al., 2015, Zare Pakzad et al., 2021], the interpretation of test results proved to be the most challenging task, as without a reliable nanomechanical model, the quantification of even the most basic properties such as stiffness and strength becomes an enormous task [Heidelberg et al., 2006, Zare Pakzad et al., 2021, Ngo et al., 2006, Hudson et al., 2013, Zhan and Gu, 2012, Yaish et al., 2015, Calahorra et al., 2015, He and Lilley, 2008, Song et al., 2011]. The lack of such a sound modeling approach is in fact reflected by a series of conflicting observations including broad range of estimations for elastic and strength properties [Nasr Esfahani and Alaca, 2019, Yang et al., 2022] and significant differences between experimental and computational findings [Wang et al., 2017, Pakzad et al., 2023b, Yang et al., 2022, Nasr Esfahani and Alaca, 2019, Nasr Esfahani et al., 2022, Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024]. Models usually suffer from a poor description of surface-related phenomena [Wang et al., 2017, Agrawal et al., 2008, Pakzad et al., 2021] and inconsistent use of constitutive surface models as well as nonlinear elasticity [Wang et al., 2017, Agrawal et al., 2008, Nasr Esfahani and Alaca, 2019]. In this context, an effective model should involve the implementation of the following three sets of parameters:

- i) **Native oxide**, essentially amorphous silicon dioxide ( $\text{aSiO}_2$ ), is an indispensable part of the Si NW surface [Nasr Esfahani et al., 2022, Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024] and thus affects the NW structure by introducing defects or other interfaces [McDowell et al., 2011, Ohta et al.,

2007]. Although usually overlooked, a recent study has revealed tensile intrinsic stresses in Si NWs upon native oxide formation under ambient conditions [Nasr Esfahani et al., 2022]. Atomistic simulations also exhibit a reduction in the modulus of elasticity of Si NWs to be as much as 40% due to native oxide surface condition while compared to the pristine surface state [Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024]. Similar reduction in the ultimate strength is estimated to be up to 20% [Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024].

ii) Appropriate **interatomic potentials** for atomistic simulations of surface stress and surface elasticity have to be introduced [Pakzad et al., 2023b, Izumi et al., 2004, Pakzad et al., 2024]. In this regard, surface stress is defined as the reversible work per unit area needed to elastically stretch a pre-existing surface [Pakzad et al., 2021, Izumi et al., 2004]. Surface elastic constants represent the variation in bulk elastic constants due to the formation of a surface [Pakzad et al., 2021, Izumi et al., 2004]. The classical surface elasticity theory by Gurtin and Murdoch has been widely employed for NWs [Gurtin and Ian Murdoch, 1975]. Similarly, classical beam theories are extended through considering the surface flexural stiffness [Steigmann and Ogden, 1997, Chhapadia et al., 2011, Chiu and Chen, 2011] along with different surface elasticity models [He and Lilley, 2008, Chen et al., 2006b, Song et al., 2011]. However, the results employed to model the bending response [Heidelberg et al., 2006, Ngo et al., 2006, He and Lilley, 2008, Song et al., 2011, Zhan and Gu, 2012, Zare Pakzad et al., 2021, Zhang et al., 2022b] have so far delivered various degrees of success for the estimation of size-dependent NW properties.

iii) Other **structural aspects** such as finite deformation, intrinsic stresses and appropriate boundary conditions have to be modelled for mechanical consistency and relevance with respect to experimental conditions [Wang et al., 2017, Espinosa et al., 2013, Agrawal et al., 2008, Nasr Esfahani and Alaca, 2019, Izumi et al., 2004, Song and Huang, 2009, Pakzad et al., 2021]. For example, residual stress effect is embedded in nanomechanical bending models using different formulations [Song et al., 2011, Hudson et al., 2013, Zhan and Gu, 2012, Yaish et al., 2015, Zare Pakzad et al., 2021], the quantification of which is a subject of high technological demand

[Dolabella et al., 2020, Nasr Esfahani et al., 2022]. Uncertainties associated with boundary conditions can also lead to discrepancies due to their direct impact on the load-displacement relationship [Wang et al., 2017].

The first two out of the three sets of critical parameters listed above are concerned with the state of the NW surface. The effect of surface on NW flexural deformation is commonly considered via three main approaches: i) the generalized Young- Laplace linear surface elasticity model (YL) [Chen et al., 2006b], ii) modified YL [He and Lilley, 2008, Wang and Feng, 2007], and iii) extended YL [Song et al., 2011]. Meanwhile, YL has also been used for extended versions of Timoshenko nanobeams for the inclusion of surface effects [Li et al., 2014]. Recently, an ab-initio core-shell model based on surface relaxation has been proposed to evaluate the surface effect in the bending of NWs [Xiao et al., 2022]. Due to the challenges and uncertainties associated with obtaining surface properties by experiments [Massa et al., 2020, Pennelli et al., 2012], these parameters are widely studied via the first principal methods [Melis et al., 2016, Pakzad et al., 2021] and atomistic simulations [Izumi et al., 2004, Miller and Shenoy, 2000, Pakzad et al., 2021]. In this regard, the relation between the surface stress and bulk elastic modulus in NWs is revealed using molecular dynamics (MD) simulations [Diao et al., 2004, Lee and Rudd, 2007]. The surface condition and crystalline orientation of NW side surfaces can also be crucial for the precision of the nanomechanical model fitted to the experimental data [Zhan and Gu, 2012, Zare Pakzad et al., 2021, He and Lilley, 2008].

The initial core-surface model by Gurtin and Murdoch [Gurtin and Ian Murdoch, 1975] is an idealized model as it ignores the surface layer thickness and thus describes the surface as a stretchable but not a bendable structure [Xiao et al., 2022, Li et al., 2022, Yao et al., 2012, Xu et al., 2016]. This approach is further improved by a series of core-shell models [Miller and Shenoy, 2000, Yao et al., 2012, Xu et al., 2016], where the NW cross-section is considered as a composite structure composed of a bulk core and a surface layer of finite thickness, each with its distinct set of elastic constants [Agrawal et al., 2008, Stan et al., 2007]. The definition of the effective bending rigidity is another cause of further discrepancy among nanomechanical models [He

and Lilley, 2008, Song et al., 2011]. The term originates from the local geometric nonlinearity of strains through incremental deformation theory [Song et al., 2011, Song and Huang, 2009]. Ignoring its dependence on parameters such as surface induced residual stresses renders YL and modified YL models incapable of capturing surface stress effects emanating from NW side surfaces [Song et al., 2011]. These effects are significant upon large deformation of NWs leading to axial reorientations and phase transformations [Song et al., 2011, Agrawal et al., 2008]. Consequently, the effectiveness of available nanomechanical models [Heidelberg et al., 2006, Ngo et al., 2006, Hudson et al., 2013, Yaish et al., 2015, Zhan and Gu, 2012, Calahorra et al., 2015, Zare Pakzad et al., 2021] in predicting NW bending behavior is directly related to the extent of their parameter sets. Despite progress, anisotropic treatment of Si NW surface properties remains as the leading challenge in this field [Song et al., 2011, Zhang et al., 2022b, Pakzad et al., 2021].

The present work addresses this challenge through a multiscale nanomechanical model. The proposed model is based on extended YL within Euler-Bernoulli (EB) beam formulation. Addressing the first two of the three critical items mentioned above, the anisotropic implementation of surface stress and surface elasticity is carried out for a realistic native oxide surface on Si via atomistic simulations using Reactive Force Field (ReaxFF) [Pakzad et al., 2021]. Addressing the last item on structural aspects, the model also accounts for the intrinsic effects induced by both surface stresses and initial residual stresses. The discussion of the model is followed by experimental method, where bending deformation of a Si NW is examined, and its intrinsic stress state is carefully quantified through Raman spectroscopy [Nasr Esfahani et al., 2022]. Finally, findings are compared to those of prior nanomechanical models in the literature [Heidelberg et al., 2006, Ngo et al., 2006, Hudson et al., 2013, Yaish et al., 2015, Zhan and Gu, 2012, Zare Pakzad et al., 2021]. For this purpose, the force-deflection data obtained through the bending test are used in different models to compute modulus of elasticity and fracture strength. The paper is concluded with a discussion on discrepancies among models, highlighting the importance of developing a multiscale theoretical framework to address size dependence

of Si NW mechanical behavior.

### 4.3 Methods and Materials

This section introduces the nanomechanical model with its surface-, and interface-related aspects. The overall NW architecture and three-point bending test platform are described in Figure 4.1. Figure 4.1 (a) depicts a NW between support pillars and loaded at its midspan by a force sensing probe. Figure 4.1 (b) exhibits a side view with applied load,  $F$ , and resulting midspan deformation,  $w$ . A cross-sectional view showing the distinct aSiO<sub>2</sub> surface layer is provided in Figure 4.1 (c). Based on this background, the modeling approach to the Si NW bending response is introduced next, which is followed by the description of surface properties including both the unreconstructed surface and native oxide. Finally, experimental methods will be introduced.

#### 4.3.1 Modeling of Nanowire Bending Response

Modulus of elasticity ( $E$ ) and fracture strength ( $S$ ) can be predicted using analytical models based on continuum mechanics. An overview is provided in Figure 4.1 (d) with the effective parameters associated with each model including large deflection, intrinsic stress and surface properties schematically described. At the basic level, the linear bending response can be captured using EB beam theory [Bauchau and Craig, 2009], which was later revised by Heidelberg *et al* [Heidelberg et al., 2006] to include axial stresses due to large deflections, with the axial load denoted by  $T$  in Figure 4.1 (d). This model was later modified by including intrinsic stresses and surface-related parameters. One such extension regarding intrinsic stresses was introduced by Hudson *et al.* [Hudson et al., 2013] to account for the initial residual stress,  $\sigma_0$ , due to axial tension/compression loads. This treatment considers all residual stress generation mechanisms due to semiconductor manufacturing processes and manipulation operations for assembly and integration [Mills et al., 2017]. Modified YL surface model was also incorporated into the Heidelberg model by Zhan *et al.* [Zhan and Gu, 2012], where the surface parameter set is defined by  $H$  in Figure 4.1 (d).

A recent demonstration by Zare Pakzad *et al.*, SimpZP model, [Zare Pakzad *et al.*, 2021] incorporated both intrinsic stress,  $\sigma_0$ , and surface effects,  $H$ , where Raman spectroscopy provided the much needed input for the former parameter. The model proposed in the present work, ExtZP model, represents a significant multi-scale extension of SimpZP model, where the treatment of the surface is enhanced by incorporating two new sets of effective parameters as exhibited in Figure 4.1 (d): i) anisotropic surface parameters,  $H_{11}$  and  $H_{22}$ , and ii) surface-induced residual stresses,  $\sigma_{xx}$ . In the upcoming section, the computation of surface stresses and surface elastic constants will be elucidated using atomistic simulations. Hence, ExtZP represents the most general approach for the interpretation of Si NW bending response. Its governing equation for a NW of length  $L$  and of rectangular cross section loaded at its midsection by a point load  $F$  (Figure 4.1 (a) and Figure 4.1 (b)) is given in Equation 4.1.

$$(EI)^* \frac{\partial^4 w}{\partial x^4} - T \frac{\partial^2 w}{\partial x^2} - H \frac{\partial^2 w}{\partial x^2} = \frac{F}{2} \left( -\delta(x) + 2\delta\left(x - \frac{L}{2}\right) - \delta(x - L) \right) \quad (4.1)$$

where  $w$  is the transverse displacement in  $z$ -direction,  $x$  denotes NW longitudinal axis,  $E$  is the modulus of elasticity,  $I$  is the moment of inertia,  $(EI)^*$  is the effective flexural rigidity,  $T$  is the overall tension along the NW,  $\delta$  is the Dirac delta function,  $H$  is the surface parameter.  $H$  is defined as  $H = H_{11} + H_{22} + bh\sigma_{xx}$ , where,  $\sigma_{xx}$  is the surface induced residual stress,  $h$  and  $b$  are the NW thickness and width, respectively. With terms  $H_{11}$  and  $H_{22}$  defined as effective surface terms embedding the surface constants and geometrical representation of involved side surfaces [Song *et al.*, 2011, Izumi *et al.*, 2004], Equation 4.1 can be further modified (Equation 4.2). The indices 11 and 22 denote the corresponding directions for the involved planar surfaces.

$$(EI)^* \frac{\partial^4 w}{\partial x^4} - T \frac{\partial^2 w}{\partial x^2} - 2hf_{11} \frac{\partial^2 w}{\partial x^2} - 2bf_{22} \frac{\partial^2 w}{\partial x^2} - 2hd_{11} \frac{\partial^2 w}{\partial x^2} - 2bd_{22} \frac{\partial^2 w}{\partial x^2} - bh\sigma_{xx} \frac{\partial^2 w}{\partial x^2} = \frac{F}{2} \left( -\delta(x) + 2\delta\left(x - \frac{L}{2}\right) - \delta(x - L) \right) \quad (4.2)$$

The first term in Equation 4.2 with four spatial derivatives is related to bending and resulting transverse deflections, while the second term represents the effect of axial tension. The components of the overall tension term,  $T$ , are given in Equation 4.3, where  $T_0$  is the residual force due to initial tension/compression in the NW and the second term represents axial tension due to large deflections. Finally,  $A$  denotes the NW cross-sectional area. The next five terms in Equation 4.2 represent the surface effect via surface stress components ( $f_{11}$  and  $f_{22}$ ), surface elasticity constants ( $d_{11}$  and  $d_{22}$ ), and surface-induced residual stress ( $\sigma_{xx}$ ). The details and formalism regarding the treatment of surfaces and interfaces will be discussed in the next section.

$$T = T_0 + \frac{EA}{2L} \int_0^L \left( \frac{\partial w}{\partial x} \right)^2 dx \quad (4.3)$$

Equation 4.2 and Equation 4.3 are solved subject to the usual clamped boundary conditions at both ends of the NW resulting in the solution given in Equation 4.4.

$$F = \frac{192EI}{L^3} w\left(\frac{L}{2}\right) f(\alpha) \quad (4.4)$$

This equation is reduced to linear EB beam deflection approximation in the case of  $f(\alpha) = 1$ . An exact solution method results in the formulation of Equation 4.5 [Heidelberg et al., 2006].

$$f(\alpha) = \frac{\alpha}{48 - \frac{192 \tanh(\sqrt{\alpha}/4)}{\sqrt{\alpha}}} \quad (4.5)$$

To find the ultimate strength of the material ( $S$ ), the maximum stress analysis for NW at fracture results in the formulation of Equation 4.6 [Ngo et al., 2006].

$$S = \frac{FL}{2\pi R^3} g(\alpha) \quad (4.6)$$

where  $R$  is the equivalent NW radius.  $g(\alpha)$  of Equation 4.6 is given in Equation 4.7.



$$g(\alpha) = \frac{4}{\sqrt{\alpha}} \tanh\left(\frac{\sqrt{\alpha}}{4}\right) + \left(\frac{2 + \cosh\left(\frac{\sqrt{\alpha}}{2}\right) - 6\frac{\sinh\left(\frac{\sqrt{\alpha}}{2}\right)}{\sqrt{\alpha}}}{\alpha \cosh^2\left(\frac{\sqrt{\alpha}}{4}\right)}\right)^{\frac{1}{2}} \quad (4.7)$$

where  $\alpha$  is related to the maximum deflection by the following transcendental equation and is used for both  $f(\alpha)$  and  $g(\alpha)$  terms needed for  $E$  and  $S$  calculations. The exact solution for the nanomechanical model is given in Equation 4.8.

$$\begin{aligned} & \left(1 - \frac{L^2 T_0}{\alpha(EI)^*}\right) \left(\frac{(EA)^*}{T_0 + (EA)^*}\right) \left(1 - \frac{L^2 H_{11}}{\alpha(EI)^*}\right) \left(1 - \frac{L^2 H_{22}}{\alpha(EI)^*}\right) \\ & \left(\frac{\alpha \cosh^2\left(\frac{\sqrt{\alpha}}{4}\right)}{2 + \cosh\left(\frac{\sqrt{\alpha}}{2}\right) - 6\frac{\sinh\left(\frac{\sqrt{\alpha}}{2}\right)}{\sqrt{\alpha}}}\right) \left(1 - 4\frac{\tanh(\sqrt{\alpha}/4)}{\sqrt{\alpha}}\right)^2 = \\ & \Delta Z_{center}^2 \left(\frac{(EA)^* + 2hd_{11} + 2bd_{22} + bhE^*}{(EI)^*}\right) \end{aligned} \quad (4.8)$$

The formulation given in Equation 4.8 provides the solution for the calculation of effective modulus of elasticity ( $E^*$ ) and  $S$ . For  $E$  estimation, the relation between classical bending rigidity and effective bending rigidity as a function of surface properties and geometrical definitions is used. Equation 4.9 provides the formulation for the effective bending rigidity using extended YL approach implemented with ExtZP model of this work.

$$(EI)^* = EI + (E_s + \tau_0) \left(\frac{bh^2}{2} + \frac{h^3}{6}\right) \quad (4.9)$$

In this formulation, the average of surface stresses ( $f_{11}$  and  $f_{22}$ ) and surface elasticity constants ( $d_{11}$  and  $d_{22}$ ) are denoted as  $\tau_0$  and  $E_s$ , respectively. The terms  $E_s$  and  $\tau_0$  are often referred to as the surface modulus and initial surface stress, respectively, in the literature of nanomechanical models [He and Lilley, 2008]. Further details on the formulation of prior models [Heidelberg et al., 2006, Zhan and Gu, 2012, Hudson et al., 2013, Zare Pakzad et al., 2021] and related bending rigidity formulations [Song et al., 2011, He and Lilley, 2008, Wang and Feng, 2007] can be found elsewhere.

Overall, this formulation achieves an all-inclusive theoretical framework with significant improvements related to interpretation of bending deformation in Si NWs. This is achieved first due to the incorporation of the extended YL surface model [Song et al., 2011] and initial tension/compression terms into the analysis of Si NW bending test data. Second and more importantly, anisotropic treatment of NW surfaces and the resulting stiffening/softening aspects of native oxide surface are fully implemented. The technique developed for the calculation of the associated surface properties is introduced in the next subsection.

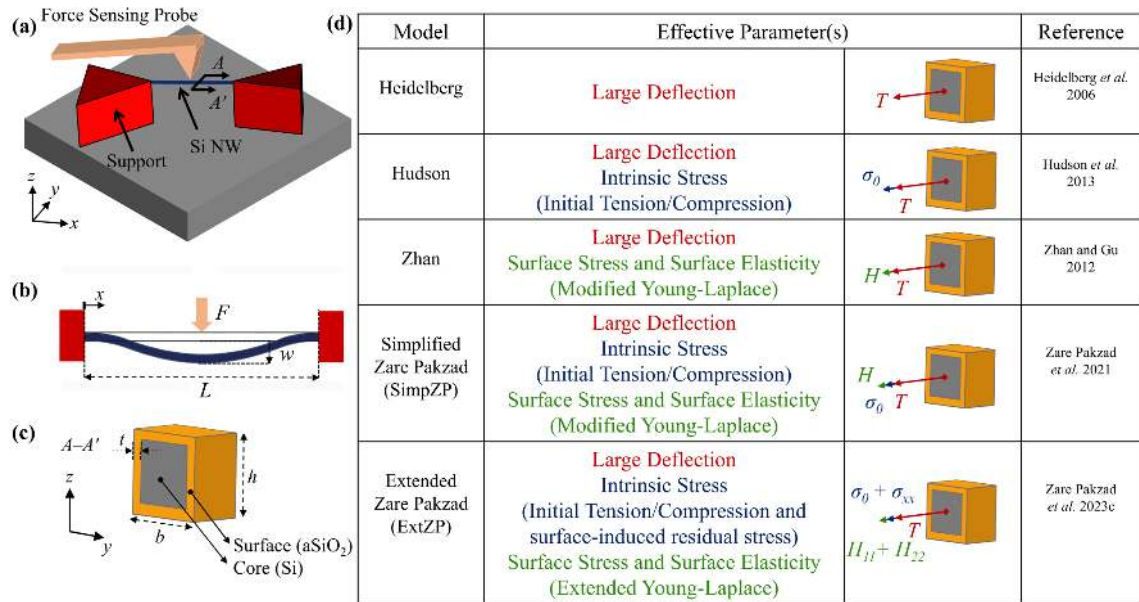


Figure 4.1: (a) Schematic representation of Si NW, clamped by monolithic support pillars and subjected to a point force applied by a force sensing probe. (b) Schematic of a NW of length  $L$  under bending test with applied load  $F$ , and subsequent deformation  $w$  at center. (c) Cross-sectional representation of the NW with associated height ( $h$ ), width ( $b$ ), and native oxide thickness ( $t$ ). (d) Effective terms of different nanomechanical models. ExtZP exhibits the model introduced in the current study. The terms  $T$  and  $H$  correspond to the axial tension due to large deflections and surface parameters, respectively, with  $H_{11}$  and  $H_{22}$  denoting anisotropic surface terms with NW side surfaces treated separately. Intrinsic stress ( $\sigma$ ) terms are shown via  $\sigma_0$  and  $\sigma_{xx}$  representing the residual terms due to initial tension/compression and surface-induced effects, respectively.

### 4.3.2 Surface and Interface Analysis

This section covers surface-, and interface-related aspects of ExtZP model. MD simulations are employed to calculate surface stresses and surface elastic constants for Si crystal surfaces that are either unreconstructed or coated with a native oxide layer. The details of generating the native oxide structures with subsequent MD approach for the calculation of surface properties are detailed next.

#### Native Oxide Model

Oxidation process is modeled at the atomic scale by using reactive MD simulations. For this purpose, ReaxFF is employed with LAMMPS [Plimpton, 1995]. The ReaxFF potential uses the concept of partial bond orders to accurately model bond breaking and bond formation, approaching quantum mechanical accuracy [Van Duin et al., 2003]. The approach was previously employed to study the effects of temperature, size, and stress on the oxidation of Si NWs [Nasr Esfahani et al., 2022, Khalilov et al., 2013a, Khalilov et al., 2013b]. A detailed description of the force field developed for the Si/SiO<sub>2</sub> system can be found elsewhere [Van Duin et al., 2003]. This approach is proven to deliver reliable process modeling as a function of temperature and defect generation [Khalilov et al., 2013b]. In this work, the force field parameters developed by Newsome *et al.* [Newsome et al., 2012] are used to model Si crystal blocks as shown in Figure 4.2. Periodic boundary conditions (B.C.s) are applied along  $x$ -, and  $y$ -directions, while a non-periodic boundary condition is applied along  $z$ -direction to mimic a two-dimensional structure, i.e. a thin film, with free surfaces. The unreconstructed Si surfaces with (100) and (110) orientations, as shown in Figure 4.2 (a) and Figure 4.2 (b), respectively, are considered as the starting point. These models are built with crystal orientations of  $(x, y, z) = ([100], [010], [001])$  and  $(x, y, z) = ([\bar{1}10], [001], [110])$  using 4096 and 4608 Si atoms, respectively. The coordinates of incident molecules of oxygen (O<sub>2</sub>) are randomly placed on both sides of Si thin films with a total number of 800 O<sub>2</sub> molecules as depicted in the middle column of Figure 4.2. A benchmark examination is carried out to determine the appropriate number and distribution of O<sub>2</sub> molecules on the upper and lower surfaces

of Si thin film models. At first, the simulation box is relaxed at a temperature of 25°C and under a pressure of 1 atm for 300 ps using isobaric ensemble (NPT) with a time step of 1 fs. The final configurations of Si structures with native oxide surface are denoted as aSiO<sub>2</sub>-Si (last column of Figure 4.2) in the remainder of this work and will be used for the calculation of surface properties as explained next.

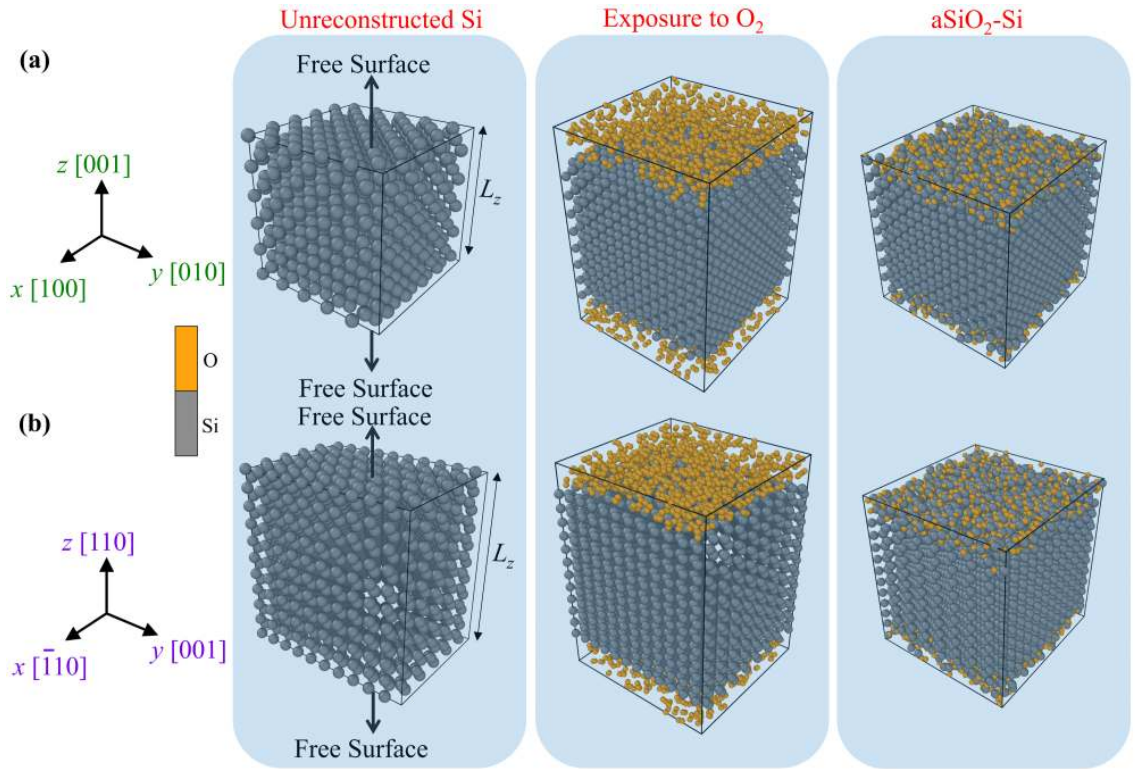


Figure 4.2: Atomic configurations for the initial unreconstructed Si thin film (left), its exposure to oxygen (middle), the oxidized Si (right) with (a) (100) and (b) (110) free surfaces in  $z$ -direction. Si and O atoms are shown with grey and orange spheres, respectively.

#### Calculation of Surface Properties

The reason behind the present spread of stiffness and strength values in the literature can mainly be traced back to the lack of a proper theoretical treatment of surface mechanics. Despite numerous atomistic [Pakzad et al., 2021, Pishkenari and Rezaei, 2017, Izumi et al., 2004, Xu and Kim, 2019, Park, 2008], DFT [Melis et al., 2015,

Table 4.1: Dimensions, number of atoms and evaluation areas of thin film structures for unreconstructed Si and aSiO<sub>2</sub>-Si structures with associated crystallographic orientations of the Si core.

| Structure                   | Si Orientation |       |       | Dimensions [nm] |      |      | # of atoms |      | $A_{film}$ [nm <sup>2</sup> ] |
|-----------------------------|----------------|-------|-------|-----------------|------|------|------------|------|-------------------------------|
|                             | $x$            | $y$   | $z$   | $x$             | $y$  | $z$  | Si         | O    |                               |
| Si (100)                    | [100]          | [010] | [001] | 4.35            | 4.35 | 4.35 | 4224       | -    | 37.8                          |
| Si (110)                    | $\bar{1}10$    | [001] | [110] | 6.15            | 4.35 | 6.15 | 8448       | -    | 53.5                          |
| aSiO <sub>2</sub> -Si (100) | [100]          | [010] | [001] | 4.35            | 4.35 | 4.50 | 4096       | 976  | 37.8                          |
| aSiO <sub>2</sub> -Si (110) | $\bar{1}10$    | [001] | [110] | 4.35            | 4.61 | 4.61 | 4096       | 1158 | 40.1                          |

Melis et al., 2016, Lee and Rudd, 2007, Jung and Shin, 2017], FE [Quagliotti et al., 2013, Delph, 2008, Payne et al., 1989, Miyamoto, 1994, Alerhand et al., 1988], and experimental [Pennelli et al., 2012] studies on Si surface constants, a consensus on surface stress profiles and subsequent calculation of constants for different crystalline orientations and surface conditions is still missing. To quantify Si NW surface stress components,  $f_{11}$  and  $f_{22}$ , and surface elastic constants,  $d_{11}$  and  $d_{22}$ , both in (100) and (110), Martin's method [Izumi et al., 2004] can be applied to the thin film structures of Figure 4.2. As periodic B.C.s are applied in  $x$ - and  $y$ -directions only, an infinite film model with finite thickness ( $L_z$ ) in  $z$ -direction is achieved as shown in Figure 4.2. The evaluation area ( $A_{film}$ ) is made up of two free surfaces that face each other, where the film must be thick enough to prevent interaction of the two free surfaces. Involved dimensions, crystallographic orientations, numbers of atoms and evaluation areas for unreconstructed Si and aSiO<sub>2</sub>-Si models are listed in Table 4.1.

To quantify surface stress components, structures are first equilibrated at 0.01 K using NPT dynamics. Subsequently, the total energy is minimized using the steepest descent and conjugate gradient techniques. By assuming a film thickness of  $L_z$ , the surface stress components are formulated as shown in Equation 4.10, where  $\eta$  represents the averaged strain due to the relaxation.

$$f_{ij}(\eta) = f_{ij}^{film}(\eta) - f_{ij}^{bulk}(\eta) \quad (4.10)$$

Bulk surface stress must be estimated separately by the bulk model and surface stress for the film model can be defined by using the stress tensor definition,  $\sigma_{ij}^{film}$ , given in Equation 4.11. Further details about the stress tensor of thin films can be found elsewhere [Izumi et al., 2004].

$$f_{ij}^{film}(\eta) = \sigma_{ij}^{film}(\eta) \frac{L_z}{2} \quad (4.11)$$

Similarly, surface elastic constants ( $d_{ijkl}$ ) are defined as second-order derivatives of surface energy with respect to strain under plane-stress conditions highlighted in Figure 4.2. The usual elastic constants for bulk ( $C_{ijkl}^{bulk}$ ) and film ( $C_{ijkl}^{film}$ ) models are calculated using MD simulations, while, for the bulk model, the elastic constants should be defined under plane-stress condition ( $C_{ijkl}^{bulk,plane}$ ) using the relations given in Equation 4.12, Equation 4.13 and Equation 4.14 [Izumi et al., 2004].

$$C_{11}^{bulk,plane} = C_{11} - \frac{C_{13}^2}{C_{33}} \quad (4.12)$$

$$C_{22}^{bulk,plane} = C_{22} - \frac{C_{12}^2}{C_{33}} \quad (4.13)$$

$$C_{12}^{bulk,plane} = C_{12} - \frac{C_{12}C_{13}}{C_{33}} \quad (4.14)$$

The relationship between the plane-stress elastic constants of the bulk and film models with the surface elastic constants is represented in Equation 4.15 [Izumi et al., 2004].

$$C_{ijkl}^{film,plane} = C_{ijkl}^{bulk,plane} - \frac{2}{L_z} d_{ijkl} \quad (4.15)$$

The Tersoff-Munetoh potential [Munetoh et al., 2007] as an empirical function composed of two-body terms depending on the local environment is used for the calculation of surface properties in this work. To obtain elastic constants, infinitesimal strains are applied to the simulation box in different directions and the resulting variation of the energy is measured. The associated thin film stress state,  $\pi_{ij}$ , is calculated using the virial theorem [Zimmerman et al., 2004], given in Equation 4.16.

$$\pi_{ij} = \frac{1}{2\Omega_0} \left[ \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \frac{1}{r^{\alpha\beta}} \frac{\partial V(r^{\alpha\beta})}{\partial r} (v_i^{\alpha\beta} v_j^{\alpha\beta}) \right] \quad (4.16)$$

where  $\Omega_0$  stands for the atomic volume in an undeformed system with  $N$  as the total number of atoms where associated atomic volumes for Si and SiO<sub>2</sub> are calculated via relaxation of related structures in each crystallographic direction with further details given in Ref. [Pakzad et al., 2021] Atomic distances between atoms  $\alpha$  and  $\beta$  are represented as  $r_{\alpha\beta}$ .  $v_j^\alpha$  stands for the position of atom  $\alpha$  along  $j$  direction, i.e.,  $v_j^{\alpha\beta} = v_j^\alpha - v_j^\beta$  and  $V$  represents the interatomic potential.

#### 4.3.3 Experimental Methods

The particular bending test approach of Figure 4.1 (a) introduces ample space between the NW specimen and the substrate, thereby allowing large out-of-plane deflections [Zare Pakzad et al., 2021, Wollschläger et al., 2016]. Si NW is thus subjected to a point force applied by a force sensing probe. As both the Si NW specimen and the microscale supports are fabricated monolithically within the same crystal, there are no interface effects, such as those encountered in pick-and-place assembly or vapor-liquid-solid (VLS)-based synthesis work that would cause ill-defined mechanical B.C.s in the present bending architecture. This structure was achieved by using a top-down fabrication technology developed specifically for Si NW integration in MEMS [Tasdemir et al., 2018, Wollschläger et al., 2016, Tasdemir et al., 2016]. The process flow is based on a combination of shallow and deep etch processes for the definition and release of Si NW, respectively, with the resulting NWs subjected to a series of structural studies [Tasdemir et al., 2018, Nasr Esfahani et al.,

2022, Wollschläger et al., 2016, Esfahani et al., 2018]. Si NWs of this work are patterned with a linewidth of 80 nm along  $\langle 110 \rangle$  direction on a p-type  $\langle 100 \rangle$  Si wafer. Further details associated with the fabrication approach can be found elsewhere [Zare Pakzad et al., 2021, Nasr Esfahani et al., 2022, Wollschläger et al., 2016, Tasdemir et al., 2016, Tasdemir et al., 2018]. A series of transmission electron microscope (TEM) images obtained through focused-ion beam (FIB) milling reveal the cross-sectional features of the Si NW [Tasdemir et al., 2018, Tasdemir et al., 2016, Wollschläger et al., 2016, Nasr Esfahani et al., 2022, Zare Pakzad et al., 2021].

The *in-situ* three-point bending test is performed within the vacuum chamber of a dual-beam FIB/SEM equipment at ambient temperature. A micromanipulator equipped with piezoresistive cantilever-based Kleindiek force sensor is used to measure the applied load,  $F$ , while the bending deflection,  $w$ , is quantified through image analysis of micrographs. Upon contact with the test sample, the piezoresistive gage produces an analog voltage output, which is converted into a force value according to a former calibration step and recorded with a sampling period of 1 s. An image correlation software (VEDDAC6) is used in pixel-level precision for each force measurement. Loading is continued until fracture. Further details related to the three-point bending method can be found elsewhere [Zare Pakzad et al., 2021, Nasr Esfahani et al., 2022, Wollschläger et al., 2016].

For the interpretation of the  $F$ - $w$  data obtained from the bending test, one needs to assess the total uniaxial intrinsic stress,  $\sigma$ , due to two residual stress components generated in the Si NW: i) the initial tension/compression force,  $T_0$ , and ii) surface induced residual stress,  $\sigma_{xx}$ .  $\sigma$  is quantified via Raman spectroscopy in a home-built  $\mu$ -Raman setup equipped with a Princeton Instrument SP-2500 spectrometer. In this measurement, a laser beam of 488-nm wavelength is used as an excitation source with a spot size of 1  $\mu\text{m}$  achieved through a beam splitter and microscope objective lenses. An integrated microscope with the measurement setup is used to focus the micro-spot on the NW. This facilitates a line scanning system to analyze the Raman shift along the entire length of suspended Si NWs with a high spatial resolution. Raman shift ( $\Delta\omega$ ) can be related to the uniaxial intrinsic stress along the



NW using the stress shift coefficient (SSC) [Spejo et al., 2020]. A broad range of SSC is reported for Si NWs, where the SSC of  $-1.93 \times 10^{-9} \text{ cm}^{-1} \text{ Pa}^{-1}$  is recommended for NWs for sub-100 nm thickness [Spejo et al., 2020]. Therefore, the relation given in Equation 4.17 is used for the intrinsic stress,  $\sigma$ , calculation, where  $S_{11}$  and  $S_{12}$  are the elastic constants and  $p$  and  $q$  are the phonon deformation profiles. Further details related to the calibration of the laser power, Raman analysis and the determination of related constants can be found elsewhere [Zare Pakzad et al., 2021, Nasr Esfahani et al., 2022, Spejo et al., 2020].

$$\Delta\omega = \frac{1}{2\omega_0} \left[ pS_{12} + q(S_{11} + S_{12}) \right] \sigma = (SSC)\sigma = -1.93 \times 10^{-9} \times (\sigma[\text{Pa}]) \quad (4.17)$$

#### 4.4 Results

This section starts with the determination of surface parameters including surface stresses and surface elasticity constants for both unreconstructed and native oxide surfaces. This is followed by the characterization of the bending response of a Si NW. The resulting force-deflection relationship is then interpreted to extract modulus of elasticity and strength of Si crystal. These results are compared and contrasted with those obtained by existing models from the literature.

##### 4.4.1 Surface Properties

The modeling of oxidation on (100) and (110) crystalline Si surfaces were already introduced in Figure 4.2, where free surfaces exposed to oxygen are defined in  $z$ -direction. The atomic snapshots in the last column, aSiO<sub>2</sub>-Si, exhibit the outcome of this process at room temperature. The oxide formation on Si surfaces is studied first through measuring the pair distribution functions (PDF) to characterize the arrangement of distances between pairs of particles within a specific volume. Figure 4.3 (a) demonstrates the magnitude of the pair distribution for Si–O bonds over the simulation time. Oxidation occurs with a high rate within the first 30 ps and then reaching a steady-state condition after 90 ps. Figure 4.3 (b) depicts the PDF

of Si–O bonds at 300 ps as a function of the bond length ( $r_{Si-O}$ ). A peak at 1.70 Å is observed for the PDF of oxide. The average Si–O bond length of 1.60 Å has been reported previous using MD simulations [Hung and Hong, 2009, Nasr Esfahani et al., 2022, Meade et al., 1992]. Similarly, the native oxide thickness is measured using the diamond crystal structure analysis while identifying Si core and native oxide regions [Maras et al., 2016]. Figure 4.3 (c) and Figure 4.3 (d) demonstrate the diamond cubic crystal in Si core in  $x - z$  and  $y - z$  cross-sections, for (100) and (110), respectively, while an amorphous native oxide layer is formed on the upper and lower surfaces. Results indicate a native oxide thickness ranging between 0.5 nm up to 0.7 nm encapsulating the Si crystal, which is comparable to previous experimental observations [Ma et al., 2003, McDowell et al., 2011], as well as MD simulations [Khalilov et al., 2013a, Nasr Esfahani et al., 2022, Ohta et al., 2007].

Once atomistic configurations for crystalline Si with and without a native oxide layer on the free surface are generated successfully, the calculation of surface constants is the subsequent step. The method for obtaining surface properties as discussed before is applied to nanoscale thin films of unreconstructed Si and aSiO<sub>2</sub>-Si depicted in Figure 4.2 and listed in Table 4.1. The surfaces are relaxed using conjugate gradient method for the calculation of surface stress and surface elastic constants. The applicability of this method was previously examined on pure Si surfaces using different interatomic potentials which provided good agreement with prior MD and density functional theory (DFT) studies on surface properties of Si thin films [Izumi et al., 2004, Pakzad et al., 2021, Xu and Kim, 2019, Pishkenari and Rezaei, 2017, Shchipalov, 2000].

Stresses obtained according to Equation 4.16 are depicted in Figure 4.4 (a) and Figure 4.4 (b) for unreconstructed Si and aSiO<sub>2</sub>-Si thin films, respectively. Stress profiles of Figure 4.4 (a) demonstrate stress variation within only 2 to 3 atomic layers in the proximity of the free unreconstructed Si surface. This finding agrees well with prior reports on unreconstructed Si surfaces [Izumi et al., 2004, Melis et al., 2015]. With the modeling approach thus validated, the objective behind the modeling of the unreconstructed Si thin film is achieved. On the other hand, for aSiO<sub>2</sub>-Si thin

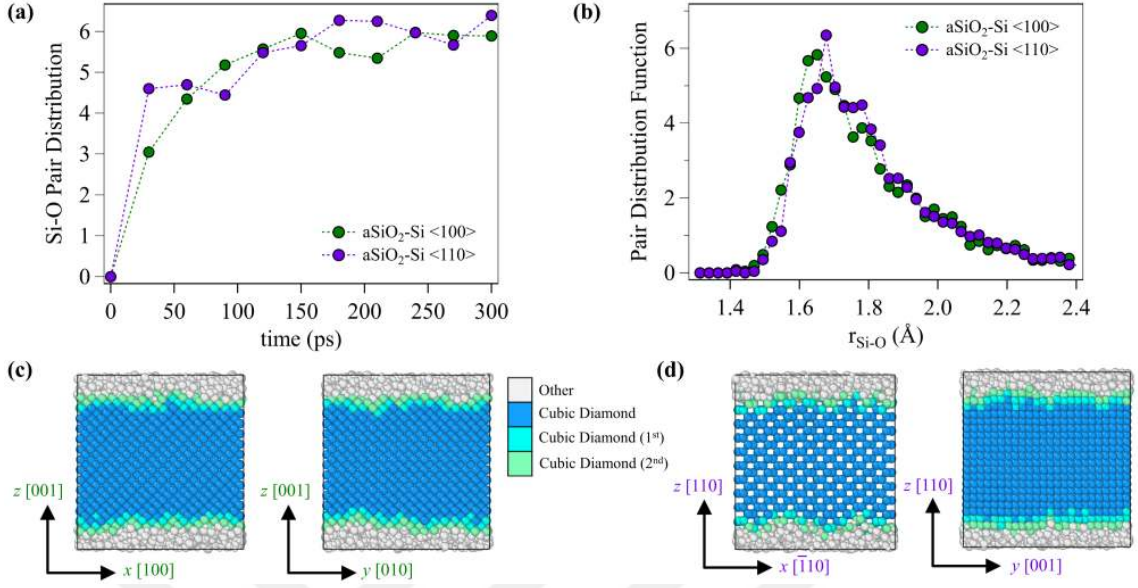


Figure 4.3: (a) The magnitude of the Si–O pair distribution as a function of time for aSiO<sub>2</sub>-Si thin films, (b) PDF of Si–O for Si NWs at 300 ps. For each aSiO<sub>2</sub>-Si structure with (c) (100) and (d) (110) free surfaces, the side surfaces are shown with associated color code representing diamond cubic structure analysis results. The color bar indicates the amorphous and cubic diamond structures with related 1st and 2nd neighbors.

films of Figure 4.4 (b), a significant stress variation is observed within 5 to 6 atomic layers colored with yellow in the plots. The distribution of stresses in the bulk crystal and free surface zones is also comparable to those in prior reports [Izumi et al., 2004, Pakzad et al., 2021, Melis et al., 2015, Melis et al., 2016]. While stress estimations range between -3 and +3 N/m for unreconstructed Si film structures, this changes from -12 to +12 N/m for aSiO<sub>2</sub>-Si films. The ability thus achieved to quantify surface stresses will provide further insight into native oxide growth [Deal and Grove, 1965, Morita et al., 1990] and associated stiffening/softening effects due to changes in surface constants [Pakzad et al., 2021, Izumi et al., 2004, Melis et al., 2016, Melis et al., 2015].

Having observed stress profiles within the immediate proximity of oxide surfaces, surface stress components,  $f_{11}$ ,  $f_{22}$ , and surface elastic constants,  $d_{11}$ ,  $d_{22}$ , are calculated using Equation 4.11 and Equation 4.15, respectively, and tabulated in

Table 4.2. The variation of surface properties are obtained with the evolution of stress and elastic components along the film thickness tracked. In this respect, calculated surface properties can be compared to those of previous studies on unreconstructed and oxidized Si thin films [Quagliotti et al., 2013, Delph, 2008, Payne et al., 1989, Pakzad et al., 2021, Pishkenari and Rezaei, 2017, Izumi et al., 2004, Miyamoto, 1994, Alerhand et al., 1988]. The surface stress and surface elastic constants calculated for unreconstructed (100) and (110) Si surfaces are in perfect agreement with prior MD [Izumi et al., 2004, Pishkenari and Rezaei, 2017, Pakzad et al., 2021, Park, 2008] and DFT [Lee and Rudd, 2007] reports modeled via different interatomic potentials. Despite the differences between the atomistic approaches, the surface elastic constants for unreconstructed (100) Si films also match well with Miller and Shenoy's constants [Miller and Shenoy, 2000]. Moreover, the surface stress constants obtained for unreconstructed (100) Si surface are in a good agreement with the predictions of prior finite element (FE) studies [Quagliotti et al., 2013, Delph, 2008, Payne et al., 1989, Miyamoto, 1994, Alerhand et al., 1988].

Similarly, aSiO<sub>2</sub>-Si surface constants are compared with those found in a limited number of reports. Prior DFT studies on oxidized (100) Si surface reported compressive surface stresses ranging between 3.2 and 4 N/m depending on the structure of native oxide [Jung and Shin, 2017]. The surface stress constants given as  $f_{11}$  and  $f_{22}$  in Table 4.2 for aSiO<sub>2</sub>-Si (100) are of the same sign and in close range. The average of surface stress components,  $f_{11}$  and  $f_{22}$ , reported as 10.3 N/m in compression by Melis *et al.* [Melis et al., 2016] agrees well with those for aSiO<sub>2</sub>-Si (110) given in Table 4.2. Considering vastly different computational approaches employed for the calculation of surface properties, the deviations observed between the predictions are quite acceptable [Quagliotti et al., 2013, Xu and Kim, 2019, Pakzad et al., 2021, Melis et al., 2016, Jung and Shin, 2017, Melis et al., 2015, Ohta et al., 2007]. The surface properties including surface stress components ( $f_{11}$  and  $f_{22}$ ) and surface elastic constants ( $d_{11}$  and  $d_{22}$ ) given in Table 4.2, are presented graphically in Figure 4.8 of the Supporting Information.

In summary, Table 4.2 demonstrates a set of significant differences in surface

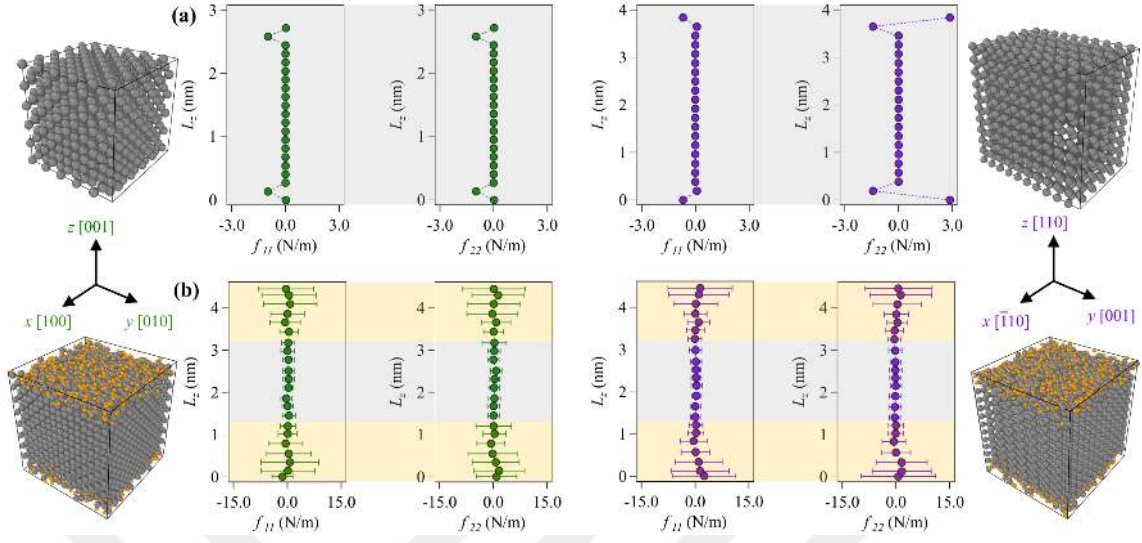


Figure 4.4: Atomic stresses for (a) unreconstructed Si and (b) aSiO<sub>2</sub>-Si film structures with (100) and (110) free surfaces of crystalline Si core. The stress components,  $f_{11}$  and  $f_{22}$ , are shown for each atomic structure studied here.

mechanics introduced by oxidation. It is interesting to see that the presence of oxide also amplifies anisotropic effects, as properties such as  $f_{22}$  and  $d_{22}$  become even more orientation sensitive compared to unreconstructed Si surfaces. Therefore it is clear that any interpretation of mechanical testing on Si NWs should incorporate the surface state with precise chemistry and crystal orientation. The constants listed in Table 4.2 are derived using the described method in this study, and the obtained results are verified through energy-based calculations. The objective of the findings presented here is to establish a standardized approach through considering different surface states or crystallographic orientations rather than providing a mere case-study. This approach aims to address the need for revisiting the previously reported scattered constants obtained using various methods and interatomic potentials. By providing a standardized framework, this study provides a guideline to characterize the surface properties of Si.

The greater surface constants obtained in this study for aSiO<sub>2</sub>-Si structures, when compared to unreconstructed Si films, provide an explanation for the findings reported by Pennelli *et al.* [Pennelli et al., 2012]. Table 4.2 shows that the surface

Table 4.2: Surface stress and surface elastic constants for unreconstructed Si and aSiO<sub>2</sub>-Si structures with associated crystallographic orientations of crystalline Si core.

| Structure                   | Surface Properties [N/m] |            |            |             |
|-----------------------------|--------------------------|------------|------------|-------------|
|                             | $f_{11}$                 | $f_{22}$   | $d_{11}$   | $d_{22}$    |
| Si (100)                    | -0.88                    | -0.88      | -8.77      | -8.77       |
| Si (110)                    | -1.57                    | -0.95      | +3.40      | -15.10      |
| aSiO <sub>2</sub> -Si (100) | -2.57±0.15               | -2.57±0.15 | -7.16±1.24 | -7.16±1.24  |
| aSiO <sub>2</sub> -Si (110) | -6.33±0.50               | -4.90±0.50 | +9.05±3.51 | +47.82±4.01 |

constants for aSiO<sub>2</sub>-Si structures are more consistent with the experimental results [Pennelli et al., 2012] than the frequently performed comparison with pure Si surfaces [Lee and Rudd, 2007, Park, 2008]. Despite the difference in Si orientation, the observed increase in surface stresses of Si structures due to oxidation as highlighted by data in Table 4.2 is also in alignment with prior experimental determination of adsorbate-induced surface stress on (111) Si surfaces [Sander and Ibach, 1991]. The significant compressive  $f_{11}$  and  $f_{22}$  components obtained for aSiO<sub>2</sub>-Si can be traced back to the mismatch between the native oxide and crystalline Si lattice constants [Melis et al., 2016]. The strong dependence of surface properties on oxidation conditions such as temperature, time, and crystallographic orientation are also consistent with previous reports in the literature [Pennelli et al., 2012, Jung and Shin, 2017, Pakzad et al., 2021].

#### 4.4.2 Si NW Bending Response

The particular  $\langle 110 \rangle$  Si NW as the test specimen of this study is shown in Figure 4.5 (a), a close-up of which is provided in Figure 4.5 (b). The close-up demonstrates the monolithic nature of the architecture with an etch depth of 10  $\mu\text{m}$  and a NW length of 8  $\mu\text{m}$ . The cross-sectional analysis of Si NW was performed using the FIB milling process, followed by TEM imaging, as reported previously in Ref. [Zare Pakzad et al., 2021]. The Si NW cross-section is found to be of a

trapezoidal shape with a height of 70 nm and a width increasing from 90 nm at the top NW surface to 98 nm at the bottom [Zare Pakzad et al., 2021]. A conformal native oxide layer with a thickness of 3-nm is also observed [Zare Pakzad et al., 2021, Wollschläger et al., 2016].

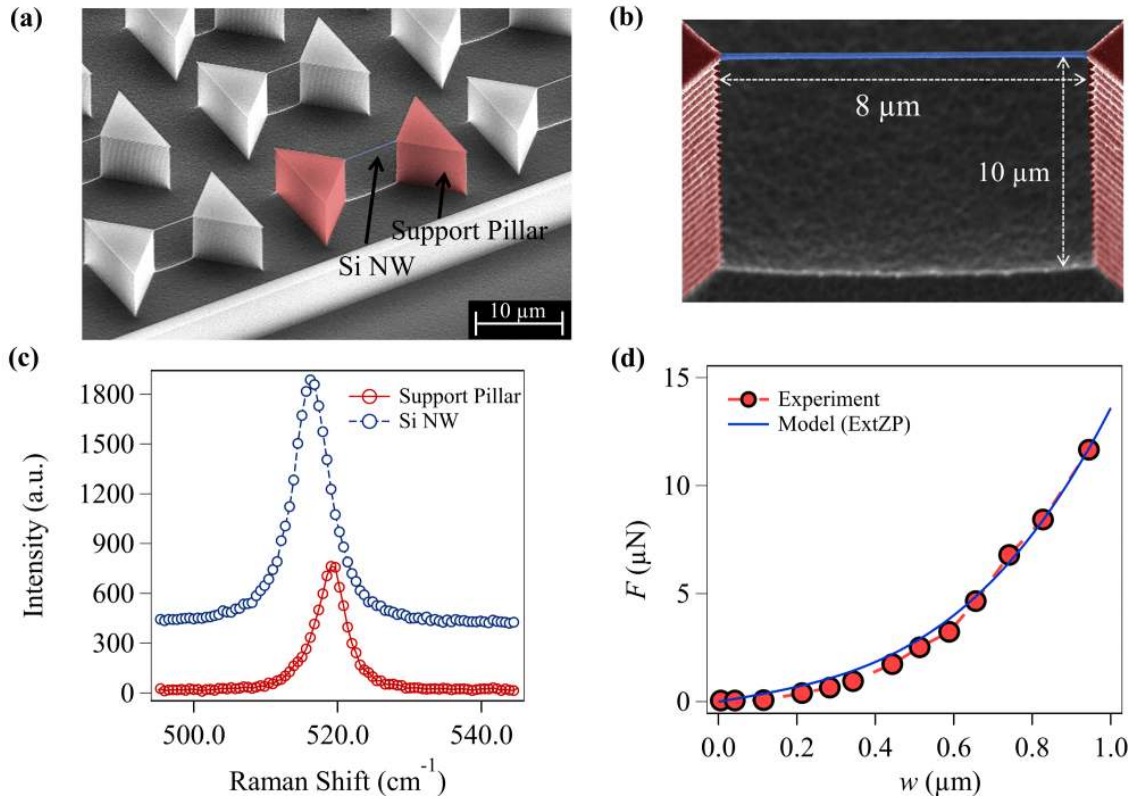


Figure 4.5: (a) Scanning electron micrograph of suspended Si NWs between support pillars. (b) A close-up micrograph showing dimensions and trench. (c) Raman spectra measured through a line on support pillar and Si NW. (d)  $F$ - $w$  data obtained through three-point bending test and fitted curve using ExtZP nanomechanical model.

After measuring NW dimensions, Raman spectroscopy is employed to measure Si NW intrinsic stress,  $\sigma$ , of Equation 4.17. For this purpose, line scans are taken both along the Si NW and support pillars, the latter representing bulk measurement. Figure 4.5 (c) shows results of such line scans, where Raman shifts of 519.0  $\text{cm}^{-1}$  and 517.5  $\text{cm}^{-1}$  are obtained for the support pillars and Si NW, respectively, resulting in a downshift of 1.5  $\text{cm}^{-1}$ . Thus, a tensile stress of 789 MPa is mea-

sured via the Raman shift formulation of Equation 4.17. Further insights into the determination of stress arising from the formation of native oxide and comparable computational investigations involving intrinsic stresses utilizing reactive MD can be found elsewhere [Nasr Esfahani et al., 2022]. Finally, the bending response of the Si NW characterized through *in-situ* three-point bending test is shown in Figure 4.5 (d) in the form of a  $F$ - $w$  curve. It exhibits a nonlinear response with a force range up to 12  $\mu\text{N}$  and associated mid-point deflection ranging up to 1  $\mu\text{m}$ . Note that this deflection is almost 15 times larger than the NW height, thereby necessitating the nonlinear formulation. ExtZP model is then fitted to the experimental data to estimate  $E$  and  $S$ . For this purpose, surface stress components ( $f_{11}$  and  $f_{22}$ ) and surface elasticity constants ( $d_{11}$  and  $d_{22}$ ) for aSiO<sub>2</sub>-Si (110) listed in Table 4.2 are used as surface constants. The resulting fit curve is also shown in Figure 4.5 (d). Force-deflection fit provided in Figure 4.5 (d) is obtained with the ExtZP model by considering the native oxide surface state, *i.e.* aSiO<sub>2</sub>-Si (110), with the corresponding parameters listed in Table 4.2. Estimated stiffness and strength values for the Si NW and their interpretation are provided next.

#### 4.4.3 Interpretation of Test Results

In addition to ExtZP model of this work,  $F$ - $w$  response of Figure 4.5 (d) is examined via a series of other models as mentioned in Figure 4.1 (d), and the predictions for  $E$  are tabulated in Figure 4.6 (a). The resulting fit curves via Heidelberg, Hudson, Zhan and SimZP models are given in Figure 4.7. First of all, considering mid-point deflections exceeding the NW height by at least one order of magnitude, large deflections (Heidelberg model [Heidelberg et al., 2006]) have to be accounted for with the resulting tensile load,  $T$ , along the NW axis. This approach yields a modulus of elasticity of 123 GPa. Incorporating an extra term for the initial tension,  $T_0$ , according to Hudson model [Hudson et al., 2013] decreases  $E$  to 95 GPa. On the contrary, if Raman results yielded a compressive intrinsic stress, the estimated modulus of elasticity would have increased. If, instead of initial tension, surface parameters,  $f_{11}$  and  $d_{11}$ , are taken into account according to Zhan model [Zhan and Gu, 2012],  $E$  is



increased to 178.9 GPa. With SimpZP model embedding both the initial tension,  $T_0$ , and surface parameters,  $f_{11}$  and  $d_{11}$ , into the formulation,  $E$  is estimated as 138.4 GPa. Finally, using ExtZP model developed in the current study,  $E$  is reduced to 113.2 GPa, as all related parameters including anisotropic surface stresses,  $f_{11}$ ,  $f_{22}$ , surface elastic constants,  $d_{11}$ ,  $d_{22}$ , and surface-induced residual stress,  $\sigma_{xx}$ , are taken into account. Findings for  $E$  along with those regarding  $E^*$  (if applicable) with all models of Figure 4.1 (d) are listed in Table 4.3. A comparison of  $E$  with other top-down studies on  $\langle 110 \rangle$ -oriented Si NWs is provided in Figure 4.6 (b). Despite similar dimensions and crystalline orientation, no clear trend is exhibited by this overview of literature. Some estimations, e.g. by Han *et al.* [Han et al., 2007] and Hsin *et al.* [Hsin et al., 2008], differ by as much as three times. The inset further depicts the distribution of modulus of elasticity estimations in close proximity of the particular NW critical dimension of this study, where predictions of all five models of Figure 4.1 (d) obtained on single test data are highlighted with 85 GPa peak-to-peak variation. This perspective shows how critical the modeling is in the interpretation of NW bending response.

Based on the same test data, a similar deviation between strength,  $S$ , estimations by different models is obtained. According to Table 4.3,  $S$  estimations range from 7.8 GPa to 10.5 GPa according to Hudson and SimpZP models, respectively, an appreciable 2.7 GPa difference. This stems from the utilization of various combinations of surface and intrinsic terms in different models, as illustrated in Figure 4.1 (d). They enter the formulation through the correction factor,  $g(\alpha)$ , of Equation 4.6. For example, implementing an initial tension,  $T_0$ , in Hudson model [Hudson et al., 2013] reduces  $S$  from 8.4 GPa, as predicted by the Heidelberg model [Heidelberg et al., 2006], to 7.8 GPa. It recovers back to 8.5 GPa, when  $H$  is considered according to the Zhan model [Zhan and Gu, 2012]. The prediction for  $S$  increases to 10.5 GPa, when SimpZP model incorporates both of the aforementioned terms of Hudson and Zhan models. Finally, the surface treatment of ExtZP model provides a fracture strength of 7.2 GPa. In this context, the ExtZP model demonstrates the lowest fracture strength compared to all other models considered in this study.

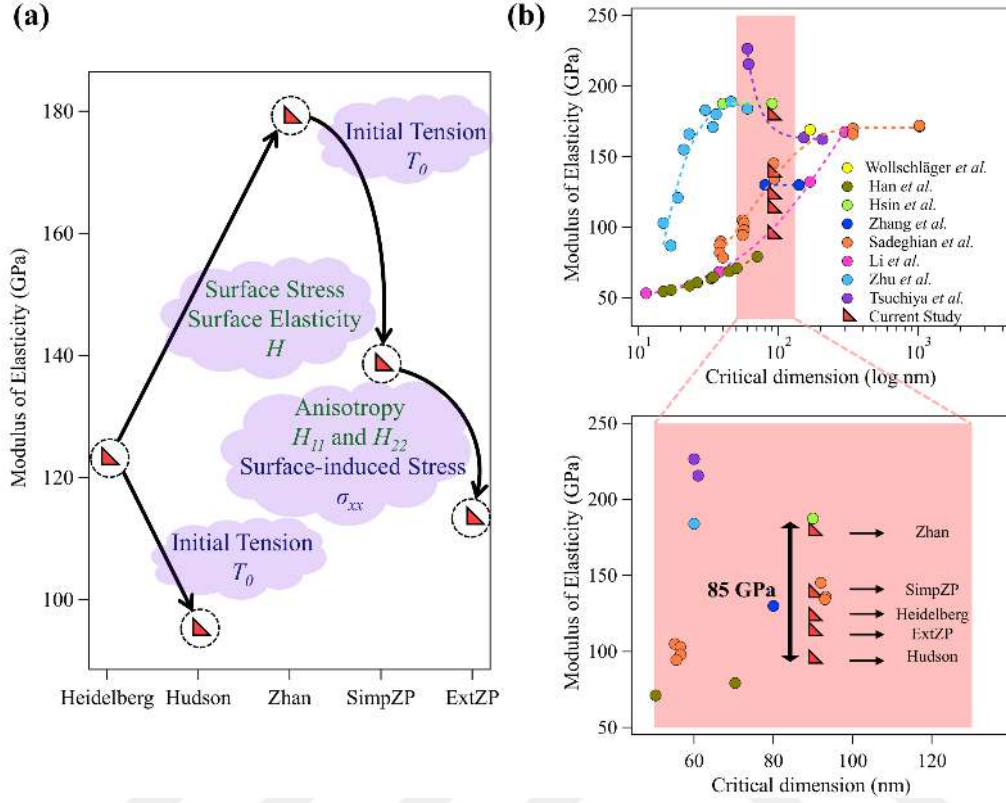


Figure 4.6: (a) Modulus of elasticity predictions by each nanomechanical model. Arrows indicating trends are accompanied by effective terms involved in each case. (b) A comparison of the predictions of panel (a) with literature reporting the modulus of elasticity for top-down  $\langle 110 \rangle$ -oriented Si NWs. The inset shows the distribution of modulus of elasticity predictions within a narrow zone between 50 nm and 130 nm of critical NW dimension. The scatter due to the use of different models for the interpretation of a single test data is 85 GPa, a significant value that questions the physical nature of the scatter reported previously.

The ExtZP model stands out as the only model that integrates the entire set of the surface properties, encompassing surface stress, surface elastic constants, and intrinsic stresses. There are other parameters, such as surface defects, influencing the fracture strength [DelRio et al., 2015], which needs further investigation in the development of nanomechanical models. Considering strength estimations for Si NWs ranging from a few MPa to 20 GPa in the literature [DelRio et al., 2015, Nasr Esfahani and Alaca, 2019], the deviation of 2.7 GPa observed here is again significant. Similar to the discussion on elasticity, this deviation highlights the necessity for an

all-inclusive model for the quantification of strength [DelRio et al., 2015, Nasr Esfahani and Alaca, 2019]. Strength levels of most Si NWs deviate from the theoretical strength of single-crystal Si estimated as 21-23 GPa [DelRio et al., 2015]. In addition to the modeling and interpretation of test data, statistical analysis is also necessary due to the brittle nature of fracture [Cheng et al., 2019, DelRio et al., 2015, Tang et al., 2012]. Hence, as long as an appropriate model is used, increasing the number of tests will further enhance the understanding in this field [Namazu et al., 2000].

The literature can be further investigated from a modeling standpoint. For example, considering studies that rely on linear modeling, one would expect no scale effect as already demonstrated in Refs. [Hsin et al., 2008, Zhang et al., 2016]. On the contrary, increasing trend for modulus of elasticity with increasing critical dimensions is often reported in Refs. [Sadeghian et al., 2009, Li et al., 2003, Han et al., 2007, Zhu et al., 2009]. The only investigation displaying a reduction in  $E$  with the increase of critical dimension, as presented in Figure 4.6, also relied on linear modeling [Tsuchiya et al., 2018]. Thus, incorporating nonlinearity into the modeling of elasticity in Si NWs appears to be highly essential. To further enhance the accuracy of interpretation, modeling efforts should take into account the influence of surface states, such as roughness, as well as the possibility of defects formation during NW fabrication [Zhang et al., 2016, Tang et al., 2012, Kim et al., 2011, Gordon et al., 2009].

By performing a benchmark analysis of the  $F$ - $w$  response of a single Si NW using various models, this paper addresses the origins of the scatter of basic Si NW properties in the literature. It is supported by a careful analysis of intrinsic stresses as well as the anisotropic modeling of all NW surfaces with the actual oxide layer. Possibility of compressive intrinsic stresses in previous bottom-up Si NW studies makes it exceedingly challenging to compare recent findings with earlier literature. However, the benchmark study presented in this work should encourage a cautious approach to the prediction of nanomechanical properties. Despite being more complex, the need for a reliable model is justified by the current fragmented state of the literature on both elastic and strength properties of Si NWs. Considering all rele-

Table 4.3: Effective modulus of elasticity ( $E^*$ ), modulus of elasticity ( $E$ ) and fracture strength ( $S$ ) estimations using different nanomechanical models for the Si NW studied here.

| Property    | Heidelberg | Hudson | Zhan  | SimpZP | ExtZP |
|-------------|------------|--------|-------|--------|-------|
| $E^*$ (GPa) | N/A        | N/A    | 126.0 | 99.0   | 85.0  |
| $E$ (GPa)   | 123.0      | 95.0   | 178.9 | 138.4  | 113.2 |
| $S$ (GPa)   | 8.4        | 7.8    | 8.5   | 10.5   | 7.2   |

vant terms that affect the mechanical behavior, ExtZP model represents a superior approach to the interpretation of test data with minimal assumptions. Simplifications such as avoiding intrinsic and surface effects have to be avoided. In addition to selecting a model, there are other requirements for refining  $E$  and  $S$  estimations for Si NWs. Increasing the number of tests along with rigorous statistical treatments is one of them. Finally, extra caution should be exercised when comparing experimental results obtained on nanostructures with computational findings on pristine crystals.

#### 4.5 Conclusion

As bending tests are the leading type of nanomechanical characterization technique applied to all types of one-dimensional nanoscale building blocks including Si NWs, its interpretation through appropriate modeling is of utmost importance. In this regard, ExtZP model introduces two critical parameters into the treatment of the bending response of Si NWs. First, intrinsic stresses are considered, that are composed of initial residual stresses and surface-induced residual stresses, and are obtained through Raman spectroscopy. In a similar fashion, surface stress and elasticity components are obtained in an anisotropic fashion, thus taking the crystalline orientation and native oxide presence on all Si NW surfaces into account. Results on pristine Si surfaces are used for validation purposes, which are then compared to those obtained on oxidized surfaces. Significant variations in surface mechanical

properties are induced by oxidation. The inclusion of oxide is found to magnify anisotropic effects, resulting in increased orientation-dependence in properties such as  $f_{22}$  and  $d_{22}$ , which may account for previous experimental observations. By demonstrating stress fluctuations ranging from -3 to +3 N/m in unreconstructed Si films and -12 to +12 N/m in aSiO<sub>2</sub>-Si films, the observed results offer a greater comprehension of the stiffening or softening effects that result from the formation of native oxide.

On the experimental side, *in situ* bending test data is obtained on a single Si NW with its intrinsic stress state quantified by Raman spectroscopy. The resulting load-deflection curve is then interpreted through a series of models with increasing complexity, including the ExtZP model as the most involved one. Findings demonstrate a spread of 85 GPa for the modulus of elasticity. The results acquired from the models are also compared and contrasted with the previous literature that focused on the modulus of elasticity of  $\langle 110 \rangle$ -oriented Si NWs. Considering the fact that Si NWs are one of the most studied and most commonly employed nanoscale building blocks, it would be reasonable to assume that other materials suffer from the same extent of oversimplification in the interpretation of bending test results. A similar conclusion is reached for strength with variations of up to 3 GPa among the aforementioned nanomechanical models. It is to be emphasized that as a single test data was analyzed through different models resulting in this significant level of variation, this approach does not exclude the statistical nature of fracture. It can similarly be improved by incorporating other surface parameters such as roughness. Precise consideration of the NW surface state is thus critical to comprehend the mechanical behavior of Si NWs accurately. Although parameters such as anisotropic treatment of NW surfaces including crystal orientation of side surfaces and the presence of native oxide have so far been excluded from the nanomechanical models, this work shows their consideration makes a significant difference. It thus highlights the need for a multiscale theoretical framework to fully understand the size-dependent mechanical behavior of Si NWs and other one-dimensional nanostructures. This understanding will be crucial for the improvement of design and reliability assessment,

and therefore the commercialization, of future nanoelectromechanical systems.

#### 4.6 Supporting Information 1

In addition to ExtZP model of this work,  $F$ - $w$  response of Figure 4.5 (d) is examined via a series of other models as mentioned in Figure 4.1 (d), and the predictions for  $E$  and  $S$  are tabulated in Figure 4.6 (a) and Table 4.3. The Supporting information includes the resulting fit curves shown in Figure 4.7 for Heidelberg [Heidelberg et al., 2006], Hudson [Hudson et al., 2013], Zhan [Zhan and Gu, 2012], and SimpZP [Zare Pakzad et al., 2021] models. The estimated stiffness and strength values for Si NW and related interpretation are provided in the main article.

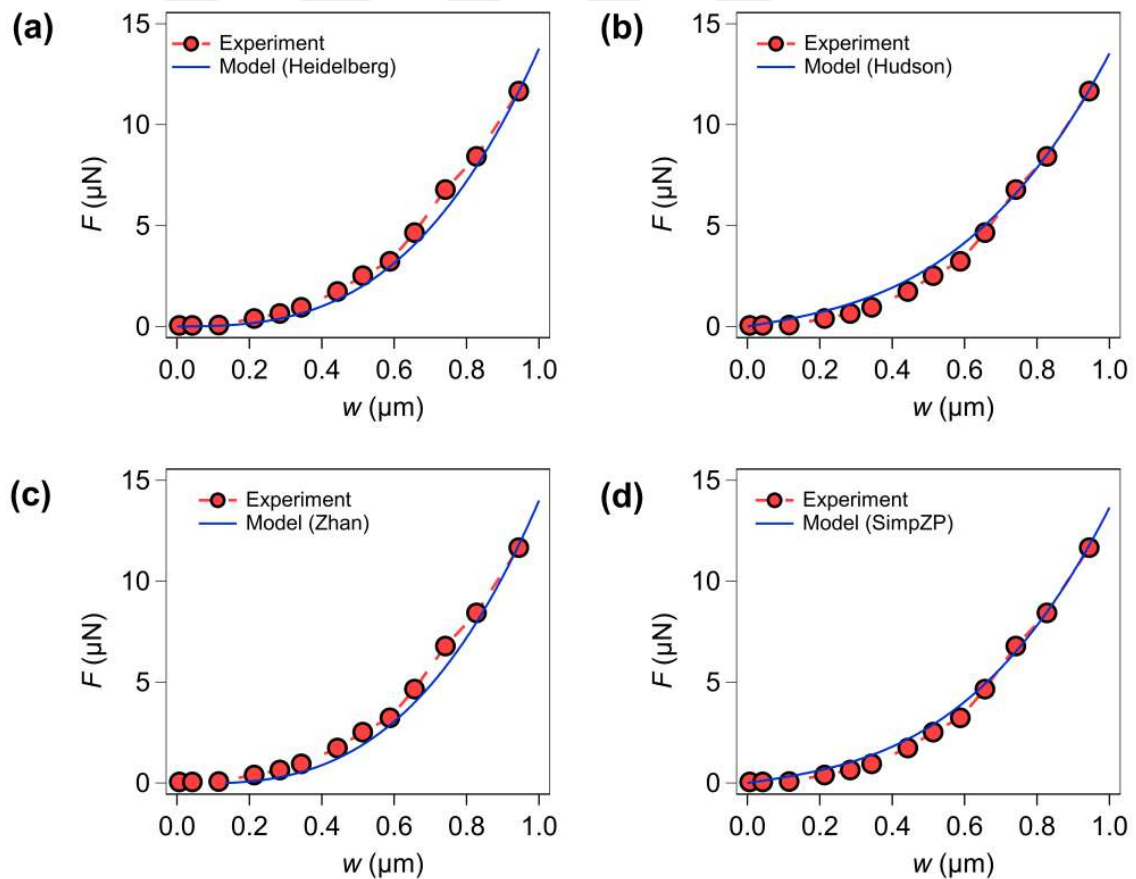


Figure 4.7:  $F$ - $w$  data obtained through three-point bending test and fitted curves using (a) Heidelberg [Heidelberg et al., 2006], (b) Hudson [Hudson et al., 2013], (c) Zhan [Zhan and Gu, 2012], and (d) SimpZP [Zare Pakzad et al., 2021] nanomechanical models.

## 4.6.1 Supporting Information 2

The surface properties including surface stress components ( $f_{11}$  and  $f_{22}$ ) and surface elastic constants ( $d_{11}$  and  $d_{22}$ ) given in Table 4.2, are presented graphically in Figure 4.8.

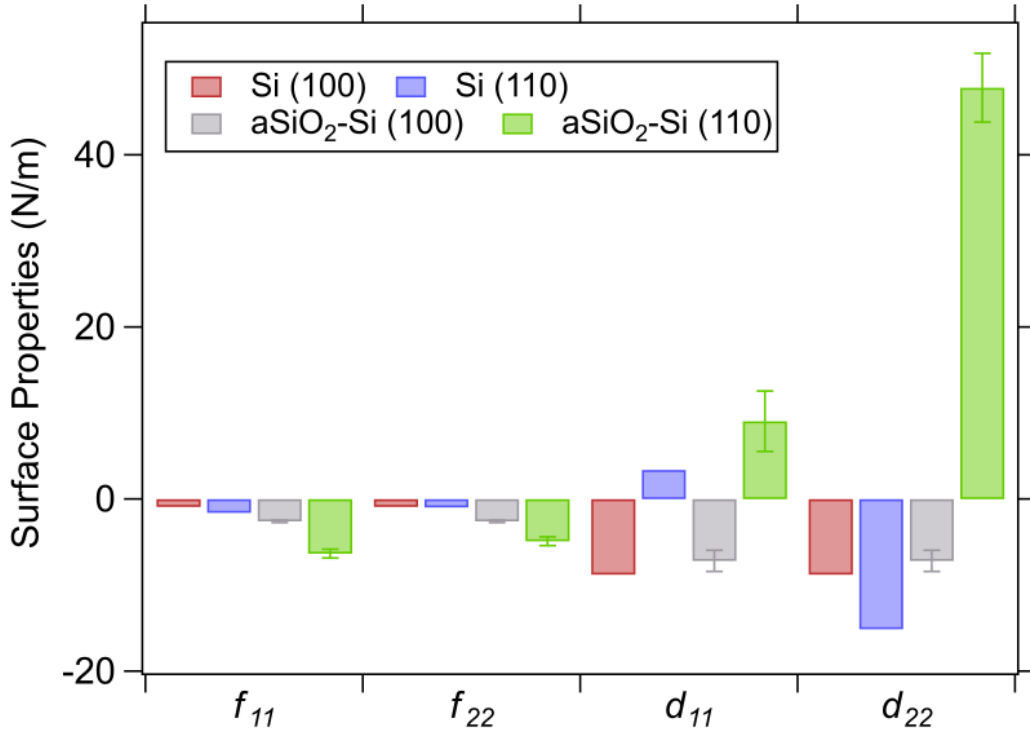


Figure 4.8: Surface stress components ( $f_{11}$  and  $f_{22}$ ) and surface elastic constants ( $d_{11}$  and  $d_{22}$ ) for unreconstructed Si and aSiO<sub>2</sub>-Si structures with associated crystallographic orientations of crystalline Si core.

## Chapter 5

## SILICON NANOMECHANICS: SIZE-DEPENDENCE REVISITED

### 5.1 Overview

In this comprehensive study, we investigate the mechanical properties of silicon nanowires (Si NWs), specifically focusing on their elasticity and fracture strength. Utilizing a detailed approach that integrates fabrication, testing, characterization, and modeling, we explore Si NWs with varying critical dimensions and lengths. The study systematically reveals the intricate influence of size variations on the elasticity of Si NWs, offering profound insights into the evolution of their elastic properties in response to dimensional changes. The results challenge conventional notions, revealing that top-down fabrication methods can yield Si NWs with high fracture strength, countering prior literature favoring bottom-up approaches. Employing advanced techniques, including Raman analysis, high-resolution imaging, atomistic modeling, and machine learning algorithms, we reveal the intricate relationship between size, surface state, and mechanical behavior in Si NWs. A thorough examination of errors illuminates both metrological and intrinsic influences, underscoring the necessity for precise statistical methodologies. The study offers a revised framework for understanding and interpreting the mechanical characteristics of Si NWs, paving the way for future advancements in nanoelectromechanical systems.

### 5.2 Introduction

Silicon nanowires (SiNWs) are crucial components for nanoelectronic and nanoelectromechanical devices due to their outstanding mechanical, electrical, and optical properties [Wang et al., 2017, Nasr Esfahani and Alaca, 2019, Bachtold et al., 2022].



These NWs possess various multifunctional characteristics, such as piezo-resistivity and thermos-electricity, making them suitable for a wide range of applications. Some notable applications include advancements in mass spectroscopy, electromechanical and biochemical sensors, field-effect transistors (FETs), energy conversion systems, and storage media [Dasgupta et al., 2014, Chen et al., 2017, Goktas et al., 2018]. A fundamental knowledge of NW mechanics is essential for designing, manufacturing, and reliably operating SiNW-based nanodevices [Wang et al., 2017, Nasr Esfahani and Alaca, 2019].

Despite the extensive research on SiNWs, particularly single-crystal-Si (SCS), the impact of size on the characteristics of this crystal material at the nanoscale is not yet comprehensively understood [Wang et al., 2017, Nasr Esfahani and Alaca, 2019, Nasr Esfahani et al., 2022, Zare Pakzad et al., 2023c]. Although the early literature [Hsin et al., 2008, Zhu et al., 2009, Gordon et al., 2009] acknowledged the considerable variability in the elastic response of Si NWs, with inconsistent trends identified in the size-dependent behavior of modulus of elasticity ( $E$ ), the matter still remains unresolved within the discipline. Even though significant discoveries have been made regarding the impact of fabrication techniques [Zhang et al., 2016], testing methods [Kim et al., 2011, Espinosa et al., 2013], atomistic modelings [Nasr Esfahani and Alaca, 2019], and theoretical interpretations [Zare Pakzad et al., 2023c] on the mechanical properties of SiNWs, a comprehensive elucidation of the size effect is not available. The uncertainty surrounding the elastic behavior of Si NWs becomes more conspicuous, especially when the prevalence of large-scale plastic deformations at room temperature is taken into account [Han et al., 2007]. In spite of  $E$  defined as a constant for material elasticity, ideally, it should remain unchanged [Nasr Esfahani and Alaca, 2019, Wang et al., 2017, Zare Pakzad et al., 2023c]. Nevertheless, the issue is not solely confined to incongruities in the elastic responses; it is further complicated by inconsistent estimations of fracture strength ( $S$ ). The assertion by Delrio *et al* [DelRio et al., 2015] that the fracture strength of SCS is expected to reach the theoretical strength limit (TSL) of 21-23 GPa at the nanoscale contradicts the findings of Zhang *et al.*, as well as a substantial body of literature reporting a range

from a few MPa to 20 GPa [DelRio et al., 2015, Wang et al., 2017, Nasr Esfahani and Alaca, 2019].

### 5.3 Methods

#### 5.3.1 Fabrication

A monolithic top-down method is employed to fabricate suspended Si NWs between microscale pillars, enabling the creation of multiscale structures with a 3-order-of-magnitude scale difference in a single batch. The fabrication process begins with an electron beam (e-beam) lithography process to pattern nanoscale features in a 200 nm-thick hydrogen silsesquioxane resist on a p-type,  $\langle 100 \rangle$  Si wafer. The substrate is then etched via reactive ion etching (RIE) in  $\text{Cl}_2$  plasma to form a Si protrusion on the surface, followed by the coating of a low-temperature oxide (LTO) film as the passivation layer via low-pressure chemical vapor deposition. After removing the LTO layer from lateral surfaces in a fluoroform plasma, the Si protrusion is protected over all of its three surfaces. Deep reactive ion etching (DRIE) is then used to release the protrusion in the form of a Si NW, which is achieved as undercuts associated with DRIE scallops from both sides are extensive enough to completely remove the Si column that extends beneath the Si surface protrusion (see Section 5.6.1 for more details). Figure 5.2 (c) shows a micrograph of a single Si NW oriented along  $\langle 110 \rangle$  direction and suspended 10  $\mu\text{m}$  above the substrate surface. The design of the architecture ensures accurate *in-situ* testing by eliminating any potential charge effects while allowing large deflections of the Si NW upon subsequent three-point bending experiments (see Section 5.6.1 and Section 5.6.6 for more details).

#### 5.3.2 Nanomechanical analytical modeling

The ExtZP nanomechanical model is used for the calculation of modulus of elasticity and fracture strength of Si NWs. The governing equation for this approach (given in Section Equation 5.1, Equation 5.2, and Equation 5.3) describes a NW of length  $L$  and rectangular cross section loaded at its midsection by a point load  $F$ .

The formulation includes terms that represent the components of the overall axial tension/compression due to large deflections combined with surface and intrinsic effects. The effective surface terms include the surface properties (surface stress and surface elastic constants) and geometrical representation of the involved side surfaces. Moreover, the intrinsic terms include the residual stresses induced due to surface and initial tension/compression effects. The clamped boundary conditions at both ends of the NW are used, resulting in the solution and correction factor given by Equation 5.4 and Equation 5.5, respectively. In this respect, to find the ultimate strength of the SCS, the maximum stress analysis for the NW at fracture results in the formulation of Equation 5.6 with correction factor given in Equation 5.7. The exact solution for ExtZP nanomechanical model is given in Equation 5.8. The relationship between classical bending rigidity and effective bending rigidity (modulus of elasticity and effective modulus of elasticity) formulated in Equation 5.9 is used for the prediction of the modulus of elasticity. For this study, the ExtZP model is utilized to calculate the elastic response of Si NWs using two distinct approaches. These approaches involve considering surface parameters and disregarding surface contribution formulated within ExtZP model. This enables obtaining the separate results for the modulus of elasticity of the Si core and the Si NW covered with its native oxide. In this context, it becomes achievable to acquire results for the modulus of elasticity of both SCS and the Si NW by considering the oxide surface condition. Figure 5.1 (a) and Figure 5.2 (h) visually illustrate the details associated with employing these different methods. In this respect, Figure 5.1 (a) and Figure 5.1 (b) show the computation of elastic properties and strength for Si NWs, employing different combinations of critical dimensions and lengths (see Section 5.6.2 and Section 5.6.7 for more details).

### 5.3.3 Raman characterization

The Raman shift ( $\Delta\omega$ ) is analyzed along the entire length of suspended Si NWs with a high spatial resolution using a line scanning system facilitated by an integrated microscope with the measurement setup. The intrinsic stress in suspended Si

NWs is quantified using a home-built  $\mu$ -Raman setup, which employs a Princeton Instruments SP-2500 spectrometer and a laser with a 488 nm wavelength as the excitation source. A beam splitter and microscope objective lens are used to create a spot size of 1  $\mu\text{m}$ , and the scattered light is collected through a focusing lens and passed into a notch filter before being guided to the spectrometer. The Raman shift is used to measure stress by linking the longitudinal optical (LO) mode obtained in backscattering configuration with stress components in the Si NW. The intrinsic stress,  $\sigma$ , can be calculated using the relation given in Equation 5.10 and Equation 5.11 with a stress shift coefficient (SSC) of  $-1.93 \times 10^{-9} \text{ cm}^{-1} \text{ Pa}^{-1}$  formulated in Equation 5.12. The intrinsic stresses ( $\sigma$ ) are considered, that are composed of initial residual stresses ( $\sigma_0$ ) and surface-induced residual stresses ( $\sigma_{xx}$ ) (see Section 5.6.2 and Section 5.6.3 for more details).

#### 5.3.4 Atomistic surface analysis

To model the oxidation process at the atomic level, reactive MD simulations are employed using the reactive molecular dynamics (ReaxFF Potential). The starting point for the model is the unreconstructed Si surface with (110) orientation of free surfaces, built with crystal orientations of  $(x, y, z) = ([\bar{1}10], [001], [110])$ . The model contains 4608 Si atoms and 800  $\text{O}_2$  molecules randomly placed on both sides of the Si thin film (see Figure 5.7 (a)). Initially, the simulation box is relaxed at 25°C and under 1 atm pressure for 300 ps using an isobaric ensemble (NPT) with a time step of 1 fs with details given in Figure 5.7 (b) and Figure 5.7 (c)). The final configuration of the Si structure with a native oxide surface is shown in Figure 5.7 (d). Martin's method is employed to quantify surface stress stresses and surface elastic constants of oxidized Si structure with periodic boundary conditions applied along the  $x$ - and  $y$ -directions and a non-periodic boundary condition along the  $z$ -direction. The structure is equilibrated using NPT dynamics at 0.01 K, and the total energy is minimized using the steepest descent and conjugate gradient techniques. The Tersoff-Munetoh potential is used to calculate surface properties, while the atomic volumes for Si and  $\text{aSiO}_2$  are obtained separately. Surface properties are then calcu-

lated using Equations 5.13-5.18. Thin film stress state is calculated using the virial theorem, given in Equation 5.19, by applying infinitesimal strains to the simulation box in different directions and measuring the resulting variation in energy. Ultimately, the surface properties including  $f_{11}$ ,  $f_{22}$ ,  $d_{11}$ , and  $d_{22}$  for aSiO<sub>2</sub>-Si thin film structure is listed in Table 5.1. Further details associated with the oxidation process, inspection of diamond cubic crystal structure, and other surface stress components ( $f_{33}$ ,  $f_{12}$ ,  $f_{13}$ , and  $f_{23}$ ) are available in Section 5.6.4 and Figure 5.7 (e-j)).

### 5.3.5 FIB/HR-TEM cross-sectional imaging

Si NWs are known to gradually oxidize, resulting in a uniform native oxide layer around the Si core. This phenomenon is confirmed by cross-sectional HR-TEM studies, including images obtained through FIB milling. Cross-sectional HR-TEM images of Si NWs with different nominal widths, including 20 nm and 80 nm (see Figure 5.8 (a) and Figure 5.8 (b) for Si NW sets), have revealed the dimensions of the Si core as well as the native oxide envelope (see Figure 5.8 (c-g) for the HR-TEM images). The HR-TEM imaging attempt is conducted on Si NWs with different combinations of critical dimension and length (see Section 5.6.5 for more details).

### 5.3.6 Bending test

The *in-situ* three-point bending test is performed within the vacuum chamber of a dual-beam FIB/SEM equipment at ambient temperature using a micromanipulator equipped with a piezoresistive cantilever-based Kleindiek force sensor to measure the applied load and image analysis of micrographs to quantify the bending deflection. The piezoresistive gage produces an analog voltage output upon contact with the test sample, which is converted into a force value according to a former calibration step and recorded with a sampling period of 1 s. Loading is continued until fracture, and an image correlation software (VEDDAC6) is used in pixel size precision for each force measurement. Double-clamped Si NWs are then tested through the same method, shown in Figure 5.9, using a piezoresistive force sensor attached to a probe to load NWs at their midspan with  $F$  while measuring resulting deflections,  $w$ ,

through scanning electron micrographs. The whole experiment is performed *in-situ* within the vacuum chamber of the FIB/SEM at ambient temperature. Force vs. deflection ( $F - w$ ) data are obtained as a result (see Section 5.6.6 for more details), and tests are repeated on 10 identical Si NWs for proper statistical treatment (see Section 5.6.6, Section 5.6.7, and Section 5.6.12 for more details).

### 5.3.7 Atomistic modeling of Si NWs with native oxide

MD simulations are employed to examine the modulus of elasticity of  $\langle 110 \rangle$ -oriented Si NWs with native oxide surface condition using LAMMPS code. The cross-section and perspective views of an aSiO<sub>2</sub>-Si NW are shown in Figure 5.11 (a) and Figure 5.11 (b), respectively. The non-periodic B.C.s are applied along all directions. The dimensions of the NWs are determined by the length ( $L$ ), and native oxide thickness ( $t$ ) where diameter ( $D$ ) is used as the critical dimension indicator. The length-to-diameter ( $L/D$ ) ratio of 10 is used for all NWs studied here. The simulations are repeated with square cross-sections given in Figure 5.11 (c) to compare the impact of shape and subsequent effects on the elastic properties of Si NWs. Figure 5.11 (b) shows an aSiO<sub>2</sub>-Si NW with the associated  $L$  while support and movable boundaries are labeled as  $L_s$  and  $L_m$ , respectively. The interaction between atoms in NWs are described by the Tersoff-Munetoh and modified Stillinger-Weber potentials. The details of the corresponding expressions and coefficients of the formulations for the potentials can be found in the related references given in Section 5.6.8. The tensile simulation is performed by anchoring one side of the NW ( $L_s$ ) while having the other end as the moveable boundary ( $L_m$ ). The  $L_s$  and  $L_m$  are set to the  $1/8^{th}$  of  $L$ . An initial velocity with the Gaussian distribution at a finite temperature of 300 K was assigned to atoms followed by the energy minimization using the conjugate gradient method. Then, all NWs are relaxed at 300 K for 50 ps with a time step of 1 fs using a canonical NVT ensemble. The support and moveable regions attached to the NWs are defined in a fixed configuration for both sides during initialization and relaxation steps. To mitigate the shock wave from the high loading rate, a constant velocity that varies linearly from zero at the

support to a finite maximum at the free end with a constant finite velocity to the movable boundary along the tensile direction of the NW ( $x$ -direction) is applied. For the tensile simulations, finite velocity value of  $1.0 \text{ \AA/ps}$  at a finite temperature of  $300 \text{ K}$  is used. Assignment of  $1.0 \text{ \AA/ps}$  finite velocity corresponds to the strain rates of  $\dot{\epsilon} \approx 1.0 \times 10^9 \text{ s}^{-1}$ . The atomic stress based on the virial theorem given in Equation 5.19 is used for the stress calculations. Critical dimensions ranging from  $4 \text{ nm}$  to  $8 \text{ nm}$  are assigned to Si NWs with a native oxide surface state. In this respect, two oxide thicknesses,  $t = 0.5 \text{ nm}$  and  $t = 1.0 \text{ nm}$ , are investigated (see Section 5.6.8 for more details).

### 5.3.8 Modified core-shell model

The analytical interpretation of the elastic properties of Si NWs, involving the modified core-shell (M-CS) model, incorporates the definition of surface elasticity. In this respect, the surface elasticity is represented as an exponential function that either increases or decreases within the interface region between the core and surface regions. Si NWs with circular cross-sections having an inner core (bulk) and an outer shell (surface) are considered. Figure 5.12 illustrates the schematic representation of the M-CS model for a surface layer thickness of  $t$  and a core Si radius of  $R_0$ . The surface elasticity is formulated using Equation 5.20. The surface factor parameter  $\alpha$  relates the oxide thickness  $t$  to a dimensionless constant,  $\tilde{\alpha}$ . The value of  $\tilde{\alpha}$  indicates the degree of inhomogeneity in the elasticity during the transition from the bulk region to the surface layer. The sign of  $\tilde{\alpha}$  indicates whether the surface layer is stiffening (positive) or softening (negative). The estimation of the combination of critical dimension and oxide thickness for Si NWs with native oxide, examined both computationally and experimentally in this study, is performed using the M-CS model described by Equation 5.21. Figure 5.12 (b) illustrates the trendlines that exhibit the size-dependent elastic properties of Si NWs using the M-CS model (see Section 5.6.8 and Section 5.6.9 for more details).

### 5.3.9 Atomistic modeling of unreconstructed Si NWs

Si NWs featuring unreconstructed surface states undergo modeling using three distinct testing methods: i) non-periodic tensile, ii) periodic tensile, and iii) bending simulations, as elaborated here with further details given in Section 5.6.10. The non-periodic tensile modeling of Si NWs involve critical dimensions ranging from 2 nm to 10 nm and length-to-critical-dimension aspect ratios spanning from 7 to 20. Two distinct interatomic potentials, Tersoff-T3 and Stillinger-Weber, are employed. Modeling efforts are conducted at three different temperatures: 10 K, 300 K, and 600 K. To consider finite size effects, non-periodic boundary conditions are applied in all three directions. The simulation process involves an energy minimization step using the conjugate gradient method, followed by assigning initial velocities based on a finite temperature distribution for all atoms. Subsequently, a relaxation process lasting 60 ps is carried out at a constant temperature in the canonical NVT ensemble with a 1 fs time step. Throughout the relaxation phase, the fixed and movable regions connected to the NW remain in fixed configurations. The subsequent tensile test involves fixing one end of the NW while allowing the other end to move. To prevent shock wave generation due to rapid loading, a linearly increasing constant velocity is applied along the longitudinal direction, starting from zero at the support and gradually reaching its maximum at the movable boundary. This results in a velocity of 1.0 Å/ps at a constant temperature, corresponding to a strain rate of approximately  $\dot{\epsilon} \approx 1.0 \times 10^9 \text{ s}^{-1}$  (see Section 5.6.10 for more details). The periodic tensile simulations follow a similar procedure, incorporating identical critical dimensions, aspect ratios, temperatures, and interatomic potentials as outlined for the non-periodic simulations. In contrast to the Si NWs discussed earlier, this modeling involves applying periodic boundary conditions along the longitudinal direction, while the other directions are constrained to simulate an infinitely long NW segment. MD simulations starts with an initial energy minimization step using the conjugate gradient method, followed by assigning initial velocities based on a Gaussian distribution at the specified temperature. Subsequently, a dynamic equilibration process at the designated temperature is conducted for 60 ps, utilizing the



Nose-Hoover isobaric-isothermal (NPT) ensemble with a time step of 1 fs. After the equilibration process, the simulation cell undergoes longitudinal deformation at a strain rate of  $\dot{\epsilon} = 1 \times 10^9 s^{-1}$ , maintaining compatibility with the strain rate utilized in non-periodic tensile simulations (see Section 5.6.10 for more details). The parameters outlined for the tensile simulations are replicated in the bending simulations of Si NWs, with the primary distinction being a focus on critical dimensions ranging from 2 nm to 5 nm. Using the MD method, three-point bending simulations are conducted on double-clamped Si NWs. In this respect, the fixed support regions correspond to one-eighth of the NW length are constrained in all three dimensions. Non-periodic shrink-wrapped boundary conditions are implemented in the opposing directions, while periodicity is enforced along the longitudinal direction. Si NWs undergo a relaxation process using the conjugate gradient method to achieve a local minimum configuration. Subsequently, a 60 ps relaxation process at a specified finite temperature is conducted, employing a 1 fs time step within a canonical NVT ensemble with a Nose-Hoover thermostat. The force-deflection ratio is determined by analyzing the slope of the initial linear section of the force-deflection response. In this context, the ExtZP nanomechanical model given in Section 5.6.2 is utilized to estimate the modulus of elasticity for Si NWs with different configurations. Accurate interpretation of the elastic response involves extracting necessary surface properties for unreconstructed Si surfaces from the provided references, with further details discussed in Section 5.6.10. A total of 1242 Si NWs modeled with an unreconstructed surface state, along with 72 Si NWs with native oxide previously published by the authors, are tabulated in Appendix, resulting in a combined total of 1314 Si NWs.

### 5.3.10 Machine learning

Machine learning (ML) is utilized as a facilitating tool to predict the size-dependent elastic properties of Si NWs acquired through atomistic modeling. Section 5.6.11 outlines the methodology associated with data preparation (Section 5.6.11), feature selection (Section 5.6.11), and ML algorithms (Section 5.6.11). In this context, a

comprehensive dataset comprising 1314 Si NWs is modeled, where each data point corresponds to the modulus of elasticity. The data preprocessing step incorporates z-score normalization to standardize feature scales. The handling of important features involves identifying and excluding correlated parameters through the utilization of Pearson's correlation coefficient (PCC) and the random forest (RF) method. ML algorithms including RF, K-Nearest Neighbors (KNN), Linear Regression (LR), Decision Trees (DT), Multi-Layer Perceptron (MLP), and Support Vector Machines (SVM), are employed to assess the accuracy of various ML models on the acquired data and explore the possible nonlinearity in the elasticity of Si NWs. The predictive accuracy of models is evaluated using root mean squared error, mean absolute error, and coefficient of efficiency formulated in Equation 5.22, Equation 5.23, and Equation 5.24, respectively. The scikit-learn library in Python facilitates computations, and identified effective models undergo further optimization, including hyperparameter tuning, to enhance training efficacy and mitigate overfitting risks. After assessing the accuracy of the models, 70% of the dataset is allocated for training, and 30% is reserved for validation, utilizing a 10-fold cross-validation approach. This dedicated split is crucial for the final evaluation of models aimed at predicting the relationship between elasticity and size. The complete MLprocess is intricately outlined in Section 5.6.11, providing insights into the mechanical behavior of Si NWs shown in Figure 5.7 (b) with sophisticated computational findings provided in Section 5.6.11.

### 5.3.11 Statistical error analysis

The accuracy of the measured variables and parameters with subsequent effects on prediction of modulus of elasticity and fracture strength for Si NWs are conducted through a multiple-sample uncertainty analysis. Although individual parameter uncertainties may be small, using several parameters in a calculation can lead to uncertainty propagation. To calculate this propagation of error, each result is described using three parameters: the overall systematic error, overall random error, and overall uncertainty. The overall fixed error is determined by taking the root sum square of all residual fixed errors in the bending experiments, HR-TEM cross-

sectional imaging and Raman characterizations. Up to 6% errors are obtained for displacement analysis in bending tests via SEM images. The uncertainty in force calibration of bending experiment is found to be up to 10%. The cross-sectional HR-TEM images are used for the prediction of systematic errors of fabrication of Si NWs with a total of 8 samples used. For Raman measurements, the error analysis is obtained through prediction of deviations in intrinsic stress calculations with a total of 33 samples used for Raman analysis. The overall random error is calculated from the observed data set of multiple samples. It is determined by conducting nanomechanical estimations for the modulus of elasticity and fracture strength on 10 identical Si NWs with different combinations of sizes (70 NWs in total). The overall uncertainty is calculated as the root sum square of the fixed and random error terms, while also considering the number of degrees of freedom in the data set. This is achieved by overall systematic and overall random error calculations (see Section 5.6.7 and Section 5.6.12 for more details).

#### 5.4 Results

In this work, we employ a synchronized approach encompassing fabrication, testing, characterization, and modeling to exploit the mechanical properties of SiNWs, whose precise interpretation has remained unresolved. To ensure consistency with the existing literature, a key criterion for categorizing distinct geometrical sets involves employing SiNWs with cross-sectional areas ranging beyond and below  $1 \mu\text{m}^2$ . SiNWs possess a nominal width ( $W$ ) of either 20 nm or 80 nm, and their length-to-width ( $L/W$ ) ratio, denoted as the aspect ratio (AR), is utilized for classification. In this respect, SiNWs in sets A, B, and C have a 20 nm  $W$  with ARs of 75, 100, and 150, while sets E, F, G, and H feature SiNWs with an 80 nm  $W$  and ARs of 50, 75, 100, and 150, respectively. In this respect, sets A, B, and C display Si NWs with surface areas below  $1 \mu\text{m}^2$ , whereas sets E, F, G, and H signify surface areas exceeding  $1 \mu\text{m}^2$ .

The present study investigates the elastic properties and strength of distinct sets of Si NWs. In this regard, the developed methodology enables a unique in-

terpretation of elasticity in Si NWs, offering insights that contribute to a better understanding compared to the existing literature domain illustrated in Figure 5.1. Considering the influence of significant parameters (given schematically in Figure 5.1 (a)) including large deformation ( $T$ ), surface effects ( $H$ ), and intrinsic effects ( $\sigma$ ), this study employs the newly developed ExtZP nanomechanical model to decode the associated effective parameters with special attention given to the surface state of SiNWs. In particular, when examining the elasticity of Si NWs as a comprehensive nano-scale structure, which encompasses surface states, intrinsic effects involving surface-induced residual stresses, and residual stresses induced during fabrication or assembly, in addition to anticipated large deformations, a unique methodology developed herein becomes essential.

Considering the substantial body of literature presented in Figure 5.1 (a), which displays contrasting trends and scattered moduli of elasticity based on size, represented here by surface area, the ExtZP model used in this analysis reveals the modulus of elasticity of Si NWs, represented by the red color-code. Notably, the bulk modulus of elasticity for  $\langle 110 \rangle$ -oriented SCS is depicted as a constant line. The ExtZP model provides a unique approach for calculating the modulus of elasticity for Si NWs as an intact nanostructure, taking into account intrinsic, surface, and structural details. Figure 5.1 (a) also presents the extraction of the modulus of elasticity in different sets for the central region of Si NWs from a cross-sectional perspective, recognized as the SCS core. It is crucial to emphasize that, considering the related uncertainties, the successful retrieval of the modulus of elasticity for bulk SCS with a crystallographic orientation aligned with the bulk elastic modulus represents a distinctive outcome of the methodology developed in this study.

More precisely, the literature on the elastic properties of Si NWs often presents diverse interpretations. While a substantial body of research supports the notion that the modulus of elasticity for Si NWs is equivalent to the bulk modulus without significant size effects, opposing perspectives primarily argue for increasing, decreasing, or scattered elasticity trends with decreasing critical dimensions or other representative dimensional parameters. Consequently, the existence of an unclear

size effect is evident, with a recent study highlighting that the choice of a specific model alone could result in a difference of up to 85 GPa in the interpretation of the modulus for an identical Si NW. Given such discrepancies in the literature, the concept associated with the ExtZP model, empowered by detailed testing and characterization techniques, allows for the precise differentiation of the commonly recognized effective modulus of elasticity. Figure 5.1 (a) resolves a longstanding dispute regarding the size-dependent elasticity of Si NWs. Nevertheless, findings in this study indicate consistent deviations from available assumption, attributed to intrinsic and surface effects. Additionally, it has been observed that employing unreliable modeling approaches can result in the misinterpretation of the effective modulus of elasticity. Regarding this matter, when examining a Si NW as a cohesive and intact structure, the accurate interpretation, substantiated by additional modeling efforts presented in the subsequent sections of this article, is that elasticity increases with an increase in size. This indicates that the diverse and conflicting prior literature lacks precision in its theoretical, characterization, modeling and interpretative aspects. Concerning the frequently observed relationship between size and elasticity in Si NWs, this study will examine the experimental findings in a more detailed perspective, incorporating computational efforts. This approach enables a thorough consideration of the critical dimension effect when comparing the Si NWs in this work to the existing literature, providing supporting evidence for the validation of the findings.

The literature focusing on the strength of Si NWs, especially in the context of SCS, reveals substantial variability with indistinct trends during the transition between scales. In this perspective, the shift from the milli-scale in SCS to the micro-scale yields comparable observations regarding increased strength. This pattern persists into the nanoscale domain, while introducing uncertainties attributed to the interplay of *processing-structure-property* relations in the calculation of fracture strength. More precisely, it appears that the differentiation between fabrication techniques for drawing a reliable conclusion on the strength of SCS presented by Zhang *et al.* [Zhang et al., 2016] is no longer applicable. Moreover, Delrio *et*

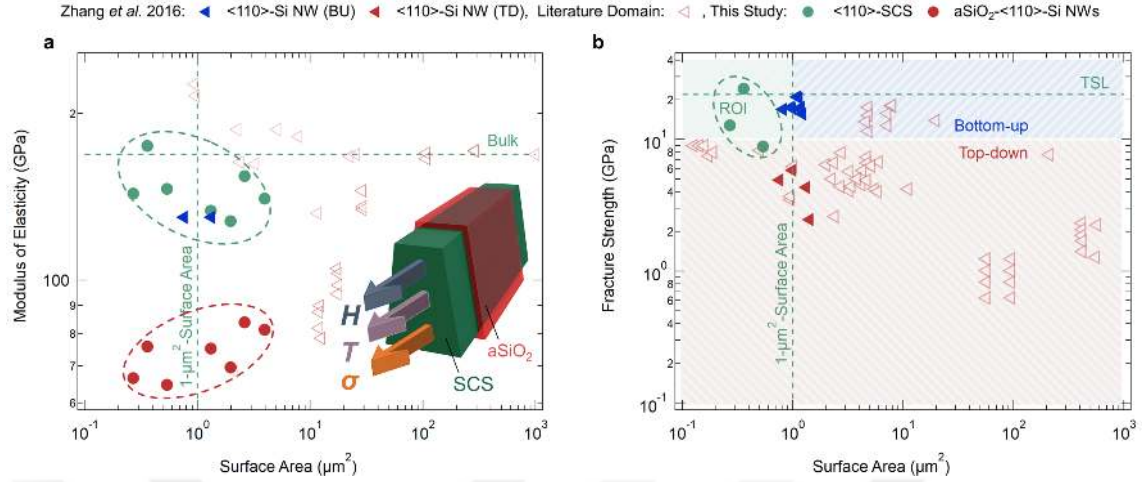


Figure 5.1: (a) Modulus of elasticity for different sets of Si NWs, with the corresponding elastic modulus estimated for SCS, are displayed against the literature domain. The schematic illustrates the key parameters within the ExtZP nanomechanical model, encompassing large deformation ( $T$ ), surface effects ( $H$ ), and intrinsic effects ( $\sigma$ ). (b) Fracture strength of SCS for sets A, B, C is given with the literature domain, emphasizing insights into the transition between top-down and bottom-up estimations in the literature. The theoretical strength limit (TSL) is presented as a constant line for SCS, with a region of interest (ROI) delineated. Given the nano-scale surface area regime for Si NWs with a 20 nm nominal width examined in this study, the calculated fracture strength are given within the ROI. In particular, data points from Zhang *et al.* [Zhang *et al.*, 2016] are presented within two separate domains, differentiating between Si NWs fabricated via top-down and bottom-up methods.

*al.*'s speculation that Si NWs with diminishing dimensions will continue to exhibit fracture strength proximate to the theoretical strength limit (TSL) appears to be substantiated [DelRio *et al.*, 2015].

In an effort to enhance the comprehension of this phenomenon, the current study scrutinizes single-crystalline Si NWs, with a particular focus on interpreting the fracture strength within a defined surface area given as the region of interest (ROI). Within this context, there is an absence of conclusive evidence regarding strength for top-down Si NWs. The data points highlighted in Figure 5.1 (b), representing the fracture strengths of Si NWs labeled as A, B, C in this study, provide support for the conjecture proposed by DelRio *et al.* [DelRio *et al.*, 2015] and the extensive body of literature [Nasr Esfahani and Alaca, 2019] suggesting such an outcome,

despite the lack of proven studies to date. This observation is closely tied to the previously discussed size-dependent fracture strength, where the transition between scales becomes evident. As previously emphasized, viewing the transition between bottom-up and top-down as an artificial barrier in terms of fabrication technologies, leading to a permanent loss in fracture strength, appears to be unfounded. Further details regarding the exclusion of fracture strength analysis for sets E, F, G, and H from this graph are discussed later in this article. Thus, this fresh insight into the fracture strength of SCS within the ROI can be characterized as a revisitation of the size dependence in Si NWs. With respect to this, the study exhibits that top-down fabrication holds the potential to generate the smallest Si NWs with high fracture strength. The findings challenge Zhang *et al.*'s assertion [Zhang et al., 2016] that bottom-up Si NWs can exclusively achieve high strength compared to top-down approaches. This achievement is attributed to the application of precise modeling and interpretation techniques, representing the highest strength ever reported for sub-1- $\mu\text{m}^2$  surface area of Si NWs. These results underscore the need for a comprehensive framework outlining the steps in fabrication, testing, characterization, modeling, and interpretation, serving as a valuable resource for future studies in this field.

Building upon the principal findings depicted in Figure 5.1, which illustrate the modulus of elasticity and fracture strength using the developed methodology, this article proceeds with an elaborate discussion of the methods employed. The process involves a sequential approach starting with fabrication, followed by *in-situ* mechanical testing, Raman characterization, and the utilization of focused-ion-beam (FIB), followed by high-resolution transmission electron microscopy (HR-TEM) imaging for intricate structural characterization. The subsequent analysis delve into the specifics of stress analysis, particularly examining intrinsic and surface effects. Si NWs are fabricated through the monolithic top-down method, as described in Section 5.6.1. Figure 5.2 (a) presents a micro Raman analysis setup specifically designed for characterizing the intrinsic stresses of Si NWs. Additionally, a scanning electron micrograph (SEM) is included, depicting a suspended Si NW positioned between support pillars. Additional details on the Raman characterization are provided in Section

5.6.3. The schematics below the micrograph illustrate the deployment of FIB, SEM, and gas injection system (GIS) during FIB/HR-TEM imaging of Si NWs. This facilitates the cross-sectional imaging of Si NWs at the midsection. The cross-sectional characterization of Si NWs, obtained through the process of FIB milling and subsequent HR-TEM imaging, is repeated across multiple sets of Si NWs with further details given in Section 5.6.5.

Through high-resolution imaging and the use of the reactive ion etching (RIE) process upon fabrication, the cross-section of Si NWs exhibit a trapezoidal shape. This configuration allows for the observation of the thickness associated with the native oxide layer, with SCS forming the core of the Si NWs. Within this framework, Figure 5.2 (b) illustrates the atomistic model utilized to calculate surface properties, including surface stresses and surface elastic constants. This analysis pertains to the native oxide surface state and the crystallographic orientation of Si NWs ( $\langle 110 \rangle$ ) in this study. As an illustrative instance among multiple cross-sectional imaging results, the cross-section of a Si NW with a height of 63.0 nm is provided in Figure 5.2 (c). The thickness gradually increases from 22.0 nm at the top surface of the NW to 26.8 nm at the bottom. Additionally, an adherent native oxide layer with a uniform thickness of 3.6 nm is observed, conformally covering the Si NW.

In the context of this study, the ExtZP nanomechanical model [Zare Pakzad et al., 2023c] is applied to interpret the nonlinear deformation exhibited by Si NWs. The ExtZP model schematically given in Figure 5.2 (d) is a comprehensive and intricate framework specifically crafted for the analysis of Si NWs considering large deflections in three-point bending experiments. It takes into consideration intrinsic effects and surface properties. Within this model, the governing equation, as elucidated in Equation 5.1 and Equation 5.2, integrates distinct terms for intrinsic stresses induced by surface formation (such as the native oxide layer) and effects arising from fabrication processes. Furthermore, anisotropic surface stresses represented by  $f_{11}$  and  $f_{22}$ , along with surface elastic constants denoted as  $d_{11}$  and  $d_{22}$ , are defined within the ExtZP model to accurately incorporate surface parameters into the interpretation. For a more comprehensive understanding of the nanomechanical



approach employed in this study, that encompasses the determination of modulus of elasticity ( $E$ ) and fracture strength ( $S$ ) of Si NWs, the set of equations offered in Section 5.6.2 is recommended for further details.

Through the use of a Raman characterization setup and atomistic methodology, the quantification of stresses related to intrinsic and surface effects is achieved. Figure 5.2 (e) presents the results of Raman shift analysis performed along a line scan on the support pillars and a Si NW. A total of 33 samples are analyzed, and the intrinsic stresses ( $\sigma$ ) for sets A to G are depicted in Figure 5.2 (f). Deviations associated with multiple samples of the same size are included in the characterization. The total intrinsic stress incorporates both the surface-induced residual stress ( $\sigma_{xx}$ ) and potential residual stresses resulting from the fabrication process ( $\sigma_0$ ). The findings in Figure 5.2 (f) indicate that, owing to the adoption of a low-temperature process with minimal stress generation during fabrication, the majority of the stresses arise from the formation of the native oxide layer on the surface. Remarkably, the tensile stress exhibited by the Si NWs in this study ranges from 272 MPa to 940 GPa. This stress range corresponds to an intrinsic strain of up to 0.5-0.2%. The largest standard deviations of 384 MPa and 302 MPa are observed for  $W$  of 80 nm and 20 nm, respectively. For detailed information regarding the Raman analysis, as well as the calculations pertaining to intrinsic stress using related constants, one can refer to Section 5.6.3 [Nasr Esfahani et al., 2022].

The subsequent components of the ExtZP model involve the anisotropic effects of the surface, represented by the constants  $f_{11}$ ,  $f_{22}$ ,  $d_{11}$ , and  $d_{22}$ , acquired through the developed atomistic methodology based on reactive molecular dynamics. The creation of a native oxide layer with an amorphous structure on two sides of the crystalline Si structure, referred to as the aSiO<sub>2</sub>-Si thin film model, and the follow-up computations for surface properties are discussed in Section 5.6.4. In this regard, The relevant details and surface constants provided for the aSiO<sub>2</sub>-Si thin film with  $\langle 110 \rangle$ -free surfaces of Si are given in Table 5.1, found in the Section 5.6.4. The planar surface constants  $f_{11}$  and  $f_{22}$ , describing the anisotropic effects along the thickness of the aSiO<sub>2</sub>-Si thin film structure with a (110) free surface definition for

the crystalline Si core, are illustrated in Figure 5.2 (g) and Figure 5.2 (h), respectively. In Figure 5.2 (i), a schematic depiction is presented, illustrating a Si NW clamped between monolithic support pillars and exposed to a point force applied through a force-sensing probe. In this context, the acquired force  $F$  and deflection ( $w$ ) at the mid-segment of Si NWs are recorded, with additional details provided in Section 5.6.6.

Figure 5.2 (j) showcases a representative lateral force-deflection ( $F$ - $w$ ) curve acquired for a Si NW during a three-point bending test. To obtain the modulus of elasticity for Si NWs, the ExtZP model is utilized, incorporating the intrinsic and surface constants discussed earlier. The methodology is reiterated for Si NWs from different sets, as detailed in Section 5.6.7, wherein the ExtZP model is adjusted to the obtained  $F$ - $w$  responses through two distinct approaches. The observed variations in  $F$ - $w$  responses stem from the repeated testing of 10 identical samples for each set (A to G). The specifics of the fitting process involve both the inclusion and exclusion of surface effects, rendering the methodology suitable for quantifying the modulus of elasticity for Si NWs and SCS separately.

In the discussion regarding the size-dependent elasticity of Si NWs depicted in Figure 5.1 (a), the critical dimension, along with surface area, emerges as a crucial geometric parameter to consider when addressing the transition between scales. The variability in Si NWs' elasticity, as indicated in Figure 5.2 with critical dimension as the scale parameter, demonstrates the size effect. Notably, the broad range of moduli of elasticity in the literature domain, exhibiting contrasting trends while navigating towards larger one-dimensional Si structures, raises significant questions. Additionally, the transition to critical dimension analysis allows for the examination of multiple sets of Si NWs within the current study, considering the length effect. Addressing and scrutinizing the anticipated outcomes of the current study on elasticity compared to the literature domain pose a noteworthy challenge. This can be characterized as a computational-experimental barrier observed at the nano-scale level, with previous studies identifying it as a 10-nm scale barrier where computations and experiments converge. Therefore, expanding on the earlier discussion

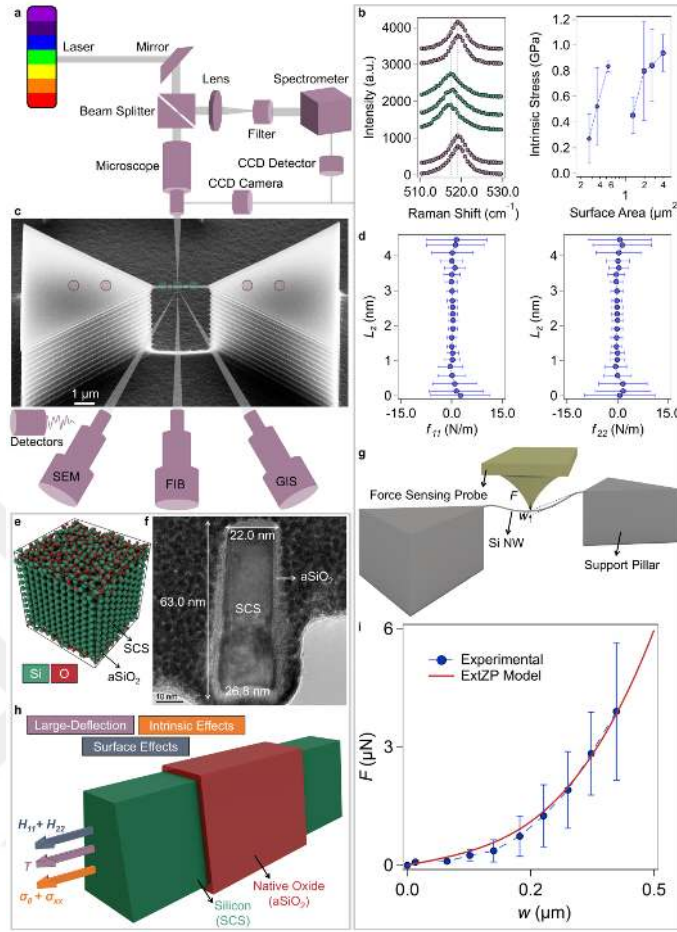


Figure 5.2: (a) The micro Raman analysis setup for characterizing intrinsic stresses, and an SEM image shows a suspended Si NW between support pillars. The schematics below the micrograph depict the deployment of FIB, SEM, and a gas injection system (GIS) during FIB/HR-TEM imaging for cross-sectional imaging of Si NWs. (b) The atomistic model used for calculating surface properties including surface stresses and elastic constants for Si thin film with native oxide layers. (c) The cross-section of a Si NW, obtained through HR-TEM imaging exhibits a trapezoidal shape enabling observation of the native oxide layer covering the SCS. (d) The ExtZP nanomechanical model [Zare Pakzad et al., 2023c] is employed to interpret nonlinear deformation in Si NWs, considering large deflections in three-point bending experiments. The schematic represents the ExtZP model, integrating large deflection, intrinsic effects and surface properties. (e) Raman shift along a line scan on support pillars and a Si NW is shown. (f) Intrinsic stresses obtained for Si NWs of sets A to G with associated deviations. The planar surface stresses given as (g)  $f_{11}$  and (h)  $f_{22}$  describing anisotropic effects along the thickness of the aSiO<sub>2</sub>-Si thin film structure are shown. (i) Schematic demonstration of a Si NW clamped between support pillars and subjected to a point force, with force ( $F$ ) and deflection ( $w$ ) recorded at the mid-segment. (j) The representative lateral force-deflection ( $F$ - $w$ ) curve obtained upon conducting a three-point bending test on a Si NW. The ExtZP model is utilized to determine the modulus of elasticity and fracture strength of the Si NW, incorporating intrinsic and surface constants.

of size-dependent elasticity, particularly emphasizing the synchronized methodology in the current research context, it becomes apparent that a reliable agreement between different methodologies (experimental, analytical, atomistic) and extensions facilitated by approaches like machine learning algorithms is crucial. Within this framework, a thorough examination of Figure 5.3 is essential to achieve a comprehensive understanding, often associated with discrepancies between experimental and computational results.

The micrograph in Figure 5.3 (a) exhibits three sets of Si NWs with a  $W$  of 20 nm, each characterized by a distinctive color code (A, B, C). In this context, Figure 5.3 (b) illustrates the moduli of elasticity obtained for Si NW sets in the current study, with distinct data points assigned to each set characterized by a common critical dimension but different lengths. Building upon the earlier discussion on the elasticity of the SCS for the studied Si NW sets, the corresponding data points are also included here. A parallel observation can be made regarding the determination of the bulk elastic modulus for  $\langle 110 \rangle$ -oriented Si. Notably, in this specific figure, the literature domain extends beyond experiments. Below the 10-nm scale barrier, a diverse range of moduli of elasticity is reported for Si NWs, modeled through atomistic simulations, particularly molecular dynamics (MD). The discussion surrounding the 10-nm scale barrier prompts the authors to argue for the effective modulus of elasticity, represented by red spheres for distinct experimental sets. Specifically, in the sub-10 nm scale, the literature is confined to unreconstructed surface conditions when modeling Si NWs via MD. Providing detailed information on the computational methodology, Si NWs with a native oxide surface state and critical dimensions ranging from 4 nm to 8 nm, along with two different native oxide layer thicknesses (0.5 nm and 1.0 nm), are modeled using two reliable interatomic potentials namely modified Stillinger-Weber (m-SW) and Tersoff-Munetoh (TM). The data points associated with these Si NWs are represented in Figure 5.3 (b) by triangular red symbols. Additional information on atomistic modeling, including MD parameters and shape effects, is discussed in Section 5.6.8.

Encompassing a significant dimensional range below 10 nm, and prioritizing cru-

cial parameters such as surface thickness and interatomic potential, a consistent increasing trend in effective modulus of elasticity with increasing critical dimension for Si NWs is observed. In this regard, Figure 5.3 (b) showcases the literature domain represented by blue triangles, while experimental and atomistic data (circular and triangular) regarding the effective modulus of elasticity for Si NWs are presented in red. Furthermore, the data presented as part of the literature domain is accompanied by references in Section 5.6.13. Upon digesting the data derived from experiments and atomistic modeling, the authors employed two distinct developed methodologies to delve deeper into this scale transition. The first methodology is grounded in an analytical-atomistic approach, leveraging insights from the modified core-shell (M-CS) model. A detailed explanation of this developed method is provided in Section 5.6.9. This approach enables the utilization of geometric parameters, specifically critical dimension and native oxide thickness, alongside the appropriate bulk modulus of elasticity associated with the crystallographic orientation of Si. The M-CS method predicts the effective modulus by incorporating a dimensionless constant describing the level of inhomogeneity in elasticity. This approach facilitates a proper consideration of the transition in elasticity between the core and shell regions, denoted as SCS and aSiO<sub>2</sub> in this study. Figure 5.3 (b) displays the outcomes of applying M-CS method to predict size-dependent elasticity for experimental and computational Si NWs in this work. The M-CS methodology is represented by black dashed lines, and three distinct oxide thicknesses are explored: 0.5 nm and 1.0 nm based on MD analysis, and 3.65 nm as observed in experiments, representing the average native oxide layer. Considering the critical dimension effect and the similarity in bulk modulus of elasticity, one can observe the significant role played by the native oxide from a thickness perspective, altering the angle of size-dependency observed upon transitioning to the bulk state. Nevertheless, the key insight derived from the M-CS method lies in its effectiveness for revealing the size effect within the context of Si NWs.

Considering the observed trends and data gathered within the framework of the current study, when compared to the extensive literature, the surface state emerges

as the most crucial parameter in resolving the longstanding debate on the size effect in the elasticity of Si NWs. Specifically, the insights gained into the role played by the native oxide extend beyond defining a distinct layer in terms of geometrical and structural aspects, such as thickness and specific modulus of elasticity different from the core. It involves inducing intrinsic stresses to the core SCS, modifications to the surface stresses with anisotropic effects, necessitating further analysis on this topic. At this stage, MD simulations on unreconstructed Si NWs are conducted across a broad set of parameters, including dimensions, thermodynamic states, types of testing (tensile and bending), and interatomic potentials. Detailed information on the simulation parameterization is available in Section 5.6.10. Enabled by unreconstructed Si NWs and the inclusion of Si NWs with a native oxide surface state, a total of 1314 data points on atomistic modeling of Si NWs are generated. Building upon the previous efforts in developing machine learning (ML)-based atomistic analysis of the mechanical behavior of Si NWs, ML algorithms are employed to interpret the scale effect. Further details on dataset preparation, ML algorithms, feature selections, along with the importance of parameters and hyperparameter tuning, are discussed in Section 5.6.11. In this context, the ML trendline depicted in Figure 5.3 (b) enables an examination of the predictions made by the tuned KNN algorithm within the conceptual framework of the current study, predicting the modulus of elasticity of Si NWs within the transitional range between scales. Despite variations from M-CS, experimental, and atomistic trendlines, ML appears to be another viable method for investigating the size effect in Si NWs.

Considering the ongoing scientific inquiries surrounding the elastic properties and strength of Si NWs, the current study aims to comprehensively address this matter. Beyond the significant impact of experimental and modeling intricacies on the calculated characteristics of Si NWs, a significant challenge in nanoscale mechanics is error analysis. Specifically, the challenges include experimental aspects involving the sequential processes of fabrication, testing, characterization, and modeling of identical Si NWs. Computational costs on the other end pose limiting factors, contributing to the current state of the literature. Furthermore, to the best of our

knowledge, nearly all studies on elasticity, and the majority of studies on strength, excluding those incorporating Weibull analysis, do not extensively report statistical treatments on experimental efforts. This underscores the explanation behind the current study's focus, which aims to dedicate attention to finite sets of Si NWs with multiple identical samples. This approach allows for a detailed error analysis within the framework of chained testing and characterization schemes, involving systematic error calculations and addressing sample-to-sample errors through randomness error analysis.

In this context, the color-coded representation of Si NWs in Figure 5.3 (a) is employed for executing a systematic error analysis on the elasticity and strength of sets A, B, and C as detailed in this article. The sources of error are classified into two subcategories: metrology and intrinsic effects. The latter is directly linked to the deviations as previously illustrated in the Raman analysis shown in Figure 5.2 (f). The errors linked to *in-situ* bending tests, encompassing deformation measurements based on SEM images, are approximated to be within 6%. The error assessment for force measurements experiences a deviation of about 10% due to uncertainties inherent in the calibration procedure. In the case of FIB/HR-TEM characterization, an error analysis is performed through multi-sample tests detailed in Section 5.6.5. The deviations arising from fabrication and subsequent measurements are taken into account under metrology, particularly for the resulting width and height measurements of Si NWs obtained from HR-TEM images. A comparable error analysis is conducted for measurements of oxide thickness, along with deviations noted in surface properties such as surface stress and surface elastic constants. This analysis reveals an impact of less than a GPa on the modulus of elasticity of Si NWs. In Figure 5.3 (c), the errors resulting from metrological considerations and intrinsic effects are presented, showcasing deviations arising from various error sources as part of a systematic methodology within the scope of this study.

The analysis will now shift its focus to the perspective of fracture strength. Acknowledging the substantial impact of fabrication techniques and their subsequent effects in establishing diverse trendlines across milli-, micro-, and nano-levels, Fig-

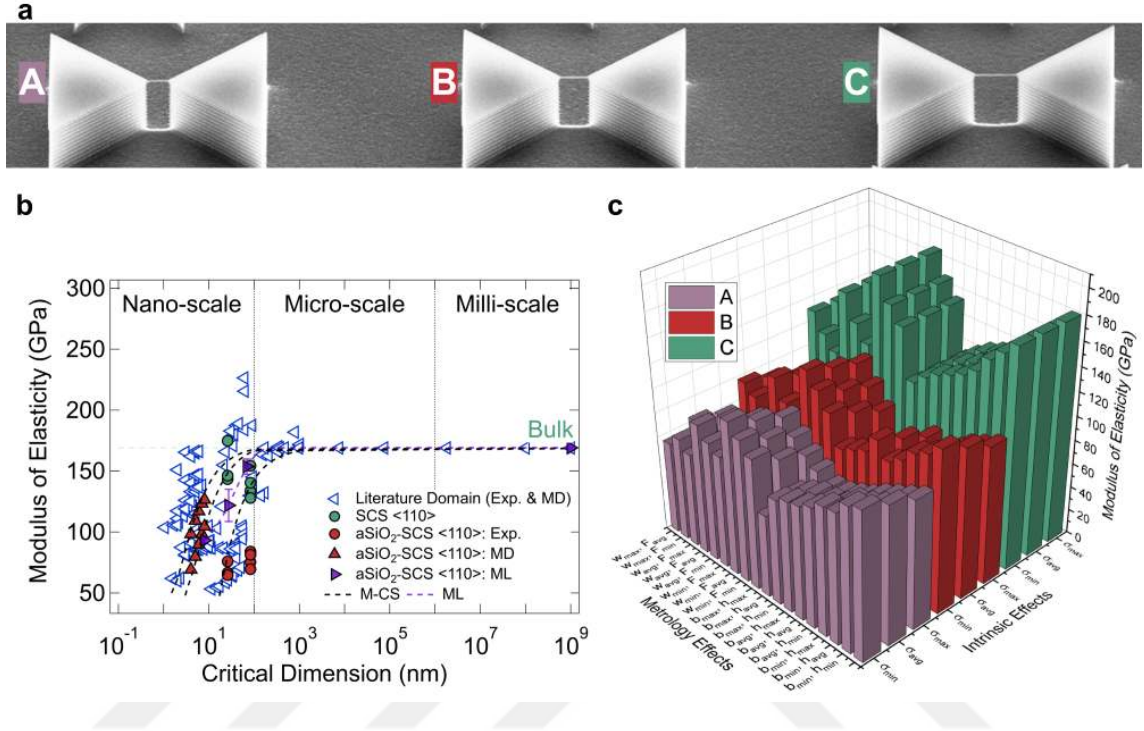


Figure 5.3: (a) The SEM micrograph featuring three sets of Si NWs, each with a width ( $W$ ) of 20 nm, distinguished by distinct color codes (A, B, C). (b) The elastic moduli obtained for Si NW sets in the current study are illustrated. Each set, characterized by a common critical dimension but different lengths, is represented by distinct data points. This figure builds upon the earlier discussion on the elasticity of the SCS for the studied Si NW sets, incorporating the bulk elastic modulus for  $\langle 110 \rangle$ -oriented Si. The literature domain in this figure extends beyond experimental findings, encompassing a diverse range of moduli of elasticity reported for Si NWs below the 10-nm scale barrier. The red spheres denote the effective modulus of elasticity for distinct experimental sets, emphasizing the discussion around the 10-nm scale barrier. Si NWs with native oxide surface states, critical dimensions ranging from 4 nm to 8 nm, and two different native oxide layer thicknesses (0.5 nm and 1.0 nm) are modeled using the m-SW and TM interatomic potentials and are shown via triangular red symbols. The graph presents an ML trendline, utilizing the tuned KNN algorithm, to predict elastic properties of Si NWs within the transitional range between scales. Additionally, the trendline associated with the analytical methodology based on the M-CS model is included. (c) A systematic error analysis is conducted for the modulus of elasticity calculation of Si NWs within sets A, B, and C, considering separate metrological and intrinsic effects.



ure 5.4 (a) provides an extensive literature survey of fracture strength reported for SCS using different methods, categorized as grown, dry etch, wet etch, and mechanical approaches. Aligned with the dry etch fabrication technology employed in this study, the fracture strength obtained for sets A, B, and C present a notable representation within the existing literature. It is important to highlight that, with the exception of grown Si NWs, there are limited high-strength Si NWs within such a small surface area at the nanoscale in the literature. This addition also enables the observation of the highest fracture strength, surpassing 10 GPa, as reported for dry-etched Si NWs. It is important to emphasize that the authors do not assert that the Si NWs examined in this study possess the highest fracture strength ever reported. However, we firmly believe that with meticulous characterization and modeling, it is possible to attain fracture strength matching the TSL of SCS, as demonstrated in this study.

Analyzing the fracture strain in Si NWs is a crucial aspect of the insights presented in Figure 5.4 (b), particularly in the context of strain engineering, with ultra-high strain notably reported for bottom-up Si NWs. The fracture strain analysis for sets A, B, and C closely aligns with previous top-down Si NWs reported in the literature, thereby enhancing the reliability and confirming the validity of the strength analysis presented in this study. Similar to the systematic error analysis conducted on the elasticity of sets A, B, and C, an assessment of metrology and intrinsic effects is performed on the fracture strength of Si NWs. In this context, the error analysis depicted in Figure 5.4 (c) highlight a vital aspect on the metrology effects which can lead to estimations deviating by up to 10 GPa, depending on the specific combinations derived from Raman characterization. Additionally, the calculations for fracture strength resulting in values as low as 9 GPa, provides further insight into the significance of systematic error analysis. This clarifies the inconsistent literature on bottom-up strength in Si NWs, where substantial deviations are observed, particularly around  $1 \mu\text{m}^2$ . Employing appropriate statistical treatment and employing accurate error calculations is essential for a thorough uncertainty analysis of the findings.

Accordingly, the credibility of the reported properties can be evaluated through uncertainty analysis. Random error calculations, outlined in Section 5.6.12, are conducted with data from 10 Si NWs per set. These computations are complemented by the systematic error analysis illustrated in Figure 5.4 (c). These assessments confer a confidence level exceeding 95% for fracture strength and over 85% for modulus of elasticity estimations. Additional details on the confidence calculations can be found in Section 5.6.12. Moreover, this analysis illuminates the interconnected scheme of fabrication, testing, characterization, and modeling that has been employed for the precise interpretation of Si NW properties in this study. In this regard, the fracture of Si NWs is classified into three subcategories based on the fracture locations, similar to a prior study in the literature set by Tang *et al.* [Tang et al., 2012]. Hence, type 1 fracture refers to rupture at the clamping, and type 2 signifies the fracture at the mid-segment of the NW, while type 3 represents the fracture type between them. Thus, type 2 fracture exhibits the most anticipated type of fracture without any additional side effects such as clamping or assembly involvement. This necessitates statistical analysis to perform the calculations of fracture strengths for Si NWs with type 2 fractures, which corresponds to sets A, B, and C in this study. As per the statistics presented in Figure 5.4 (d), 90% of Si NWs with a 20-nm critical dimension undergo type 2 fractures during bending experiments. Consequently, the fracture strength analysis conducted on 80-nm Si NWs is excluded upon the strength analysis due to such fracture statistics. Hence, sets D, E, F, and G, characterized by a high occurrence of type 1 and type 3 fractures, are excluded from the analysis of fracture strength.

## 5.5 Conclusion

In conclusion, the comprehensive investigation into the mechanical properties of Si NWs has yielded valuable insights into their size-dependent elasticity and fracture strength. Through a meticulous integration of fabrication, testing, characterization, and modeling, we systematically explored Si NWs with different critical dimensions and lengths, challenging available assumptions and shedding light on the relation-

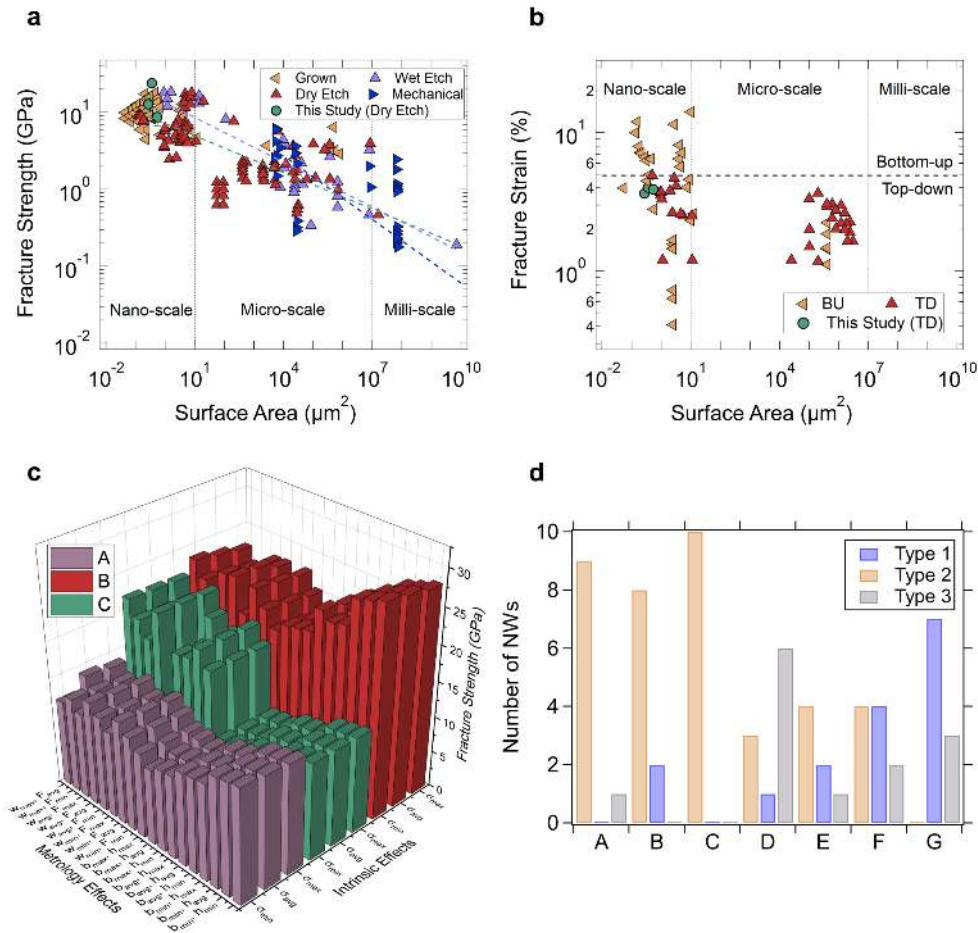


Figure 5.4: (a) Fracture strength is plotted against surface area for SCS reported in the literature, considering different etching technologies during fabrication. The data points from the current study illustrate fracture strength for sets A, B, and C using the developed methodology. (b) Fracture strain associated with SCS, obtained through top-down (TD) and bottom-up (BU) techniques, is presented. The dashed line presents the separation between the range of fracture strain reported via the two fabrication approaches. Data points from this study align with the common range observed in TD literature. (c) A systematic error analysis is conducted for the fracture strength calculation of Si NWs within sets A, B, and C, considering separate metrological and intrinsic effects. (d) The type of fracture observed in statistical analysis for Si NWs of sets A to G is presented, with type 1 indicating clamping fracture, type 2 signifying midsegment fracture, and type 3 representing rupture between. Statistical data reveals that sets A, B, C predominantly experience midsegment fractures (type 2), while sets D, E, F, and G exhibit different fracture types.

ship between size and mechanical behavior. Advanced techniques, including Raman analysis, high-resolution imaging, atomistic modeling, and machine learning algorithms, were instrumental in studying the interplay between size, surface state, and mechanical properties in Si NWs. This study emphasizes the importance of a precise statistical methodology, showcased through a detailed examination of errors encompassing both metrological and intrinsic influences. This work not only contributes to a refined understanding of Si NWs but also provides a robust framework for future advancements in nanoelectromechanical systems, underscoring the potential of top-down fabrication in producing Si NWs with exceptional mechanical characteristics.

## 5.6 Supporting Information

### 5.6.1 Fabrication process flow

The process flow used in this study to create suspended Si NWs between two support micropillars is based on a recently developed monolithic fabrication method [Tasdemir et al., 2016, Tasdemir et al., 2018, Wollschläger et al., 2016]. The process flow steps are outlined here, with details provided in the Methods section. Here, a schematic description of the fabrication process is presented (Figure 5.5 (a-f)), along with an SEM image of a suspended Si NW as the resulting outcome aligned with a schematic description from a cross-sectional perspective (Figure 5.5 (g)). The process begins with a p-type,  $\langle 100 \rangle$  silicon wafer of 100 mm diameter, 525  $\mu\text{m}$  thickness, and a resistivity range of 0.1-100  $\Omega\text{cm}$ . Using e-beam lithography, nanoscale features are patterned in a 200 nm-thick hydrogen silsesquioxane (HSQ) resist (Figure 5.5 (a)). The expected Si NWs with a linewidth of 20 nm and 80 nm have been patterned along the  $\langle 110 \rangle$  direction. The substrate is then etched via RIE in  $\text{Cl}_2$  plasma to create a Si protrusion on the surface (Figure 5.5 (b)). The NW width is defined by e-beam lithography, while the RIE process ensures that all patterned nanoscale features have the same thickness regardless of their in-plane dimension. Deposition of a low temperature oxide (LTO) film is carried out as the passivation layer via low-pressure chemical vapor deposition (Figure 5.5 (c)), fol-

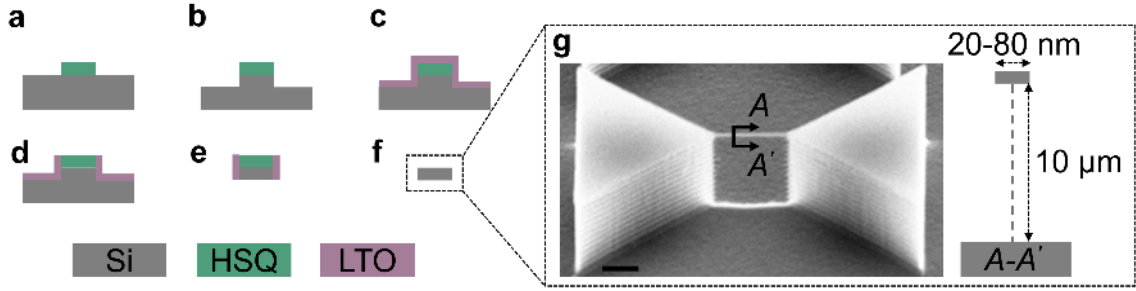


Figure 5.5: (a) High-resolution patterning through electron beam lithography. b, Anisotropic etching step forming the surface protrusion, the precursor line for the future Si NW. c, Conformal coating of LTO. d, LTO removal from horizontal surfaces. e, DRIE with adequate undercut to release the Si NW. f, Etching of protective layers via HF etch. g, Electron micrograph of a Si NW anchored between two 10  $\mu\text{m}$ -thick triangular supports along with a schematic – not drawn to scale – showing the multi architecture in the  $A - A'$  cross section. The scale bar in the micrograph corresponds to 4  $\mu\text{m}$ .

lowed by removal of the LTO layer from lateral surfaces using inductively coupled plasma-based etching (Figure 5.5 (d)). The Si protrusion is protected over all three surfaces, and then released through deep reactive ion etching (DRIE) to form a Si NW, with pillars serving as microscale support columns (Figure 5.5 (e)). The e-beam resist and LTO film encapsulating the NWs are removed by hydrofluoric (HF) vapor etching (Figure 5.5 (f)), resulting in a multiscale structure with a 3-order-of-magnitude scale difference. Figure 5.5 (g) shows a micrograph of a single Si NW suspended 10  $\mu\text{m}$  above the substrate surface with a schematic – not drawn to scale – illustrating the multi-architecture in the cross-sectional view along the  $A - A'$  axis. The current architecture with the Si NWs anchored on support pillars promotes the departure of incident charge during *in-situ* testing, which helps to alleviate potential charging issues [B Spejo et al., 2023]. For further information regarding the fabrication of Si NWs, the readers are encouraged to consult additional sources or relevant literature on this subject [Karimzadehkhoei et al., 2023, Nasr Esfahani and Alaca, 2019, Alaca and Karimzadehkhoei, 2023, Dasgupta et al., 2014, Chen et al., 2017, Zare Pakzad et al., 2023c, Zare Pakzad et al., 2021].

### 5.6.2 ExtZP nanomechanical model

A detailed description of the ExtZP nanomechanical model employed in this study for calculating the mechanical properties of Si NWs is presented in this section [Zare Pakzad et al., 2023c]. The terms and equations utilized for determining the modulus of elasticity and strength of Si NWs are discussed here. In this respect, the ExtZP model includes effective parameters representing the surface effect within anisotropic surface parameters,  $H_{11}$ , and  $H_{22}$ , and the surface-induced residual stress,  $\sigma_{xx}$ . The total intrinsic stress,  $\sigma$ , determined via Raman characterization, with analysis discussed in Section 5.6.3, includes the combined effects of  $\sigma_{xx}$  and initial tension/compression effect,  $\sigma_0$ , representing the fabrication or assembly induced residual stress. The computation of surface constants using atomistic simulations given as surface stresses ( $f_{11}$  and  $f_{22}$ ) and surface elasticity constants ( $d_{11}$  and  $d_{22}$ ) will be explained in Section 5.6.4. The ExtZP model provides a comprehensive approach to calculate the elastic properties and strength of Si core given as SCS and Si NWs with native oxide while combined with bending rigidity formulations. Elaborating on the ExtZP model, Equation 5.1 provides the governing equation for a Si NW of rectangular cross section and length  $L$ , subjected to a point load  $F$  at its midsection, as shown in Figure 5.5 (g). Equation 5.1 relates the transverse displacement  $w$  in the  $z$ -direction to the longitudinal axis  $x$ .

$$(EI)^* \frac{\partial^4 w}{\partial x^4} - T \frac{\partial^2 w}{\partial x^2} - H \frac{\partial^2 w}{\partial x^2} = \frac{F}{2} \left( -\delta(x) + 2\delta\left(x - \frac{L}{2}\right) - \delta(x - L) \right) \quad (5.1)$$

The terms in Equation 5.1 including the modulus of elasticity ( $E$ ), moment of inertia ( $I$ ), effective flexural rigidity  $(EI)^*$ , overall tension ( $T$ ) along the NW, Dirac delta function ( $\delta$ ), and total surface parameter ( $H$ ), are all explicitly defined. The surface parameter  $H$  is stated as the sum of the effective surface terms  $H_{11}$  and  $H_{22}$ , as well as the product of the surface-induced residual stress  $\sigma_{xx}$ . The effective surface terms, represented by the indices 11 and 22, incorporate the surface constants and geometrical representation of the involved side surfaces. Here, the NW thickness and width are represented as  $h$  and  $b$ , respectively. In this respect, Equation 5.1 can

be further modified to Equation 5.2.

$$(EI)^* \frac{\partial^4 w}{\partial x^4} - T \frac{\partial^2 w}{\partial x^2} - 2bf_{11} \frac{\partial^2 w}{\partial x^2} - 2hf_{22} \frac{\partial^2 w}{\partial x^2} - 2bd_{11} \frac{\partial^2 w}{\partial x^2} - 2hd_{22} \frac{\partial^2 w}{\partial x^2} - bh\sigma_{xx} \frac{\partial^2 w}{\partial x^2} = \frac{F}{2} \left( -\delta(x) + 2\delta\left(x - \frac{L}{2}\right) - \delta(x - L) \right) \quad (5.2)$$

The term with four spatial derivatives in Equation 5.2 is associated with bending and resulting transverse deflections, while the second term accounts for the effect of axial tension. The total tension term  $T$  is expressed in Equation 5.2, where  $T_0$  is the residual force due to initial tension or compression in the NW, and the second term represents axial tension due to large deflections. The cross-sectional area of the NW is denoted by  $A$ . The following five terms in Equation 5.2 consider the surface effect via surface stress components ( $f_{11}$  and  $f_{22}$ ), surface elasticity constants ( $d_{11}$  and  $d_{22}$ ), and surface-induced residual stress ( $\sigma_{xx}$ ). The details and methodology regarding the treatment of surfaces and interfaces via atomistic simulations will be discussed in Section 5.6.4.

$$T = T_0 + \frac{EA}{2L} \int_0^L \left( \frac{\partial w}{\partial x} \right)^2 dx \quad (5.3)$$

The solution to Equation 5.2 and Equation 5.3 is obtained by applying the standard clamped boundary conditions at both ends of the NW, leading to the expression provided in Equation 5.4.

$$F = \frac{192EI}{L^3} w\left(\frac{L}{2}\right) f(\alpha) \quad (5.4)$$

If  $f(\alpha)$  is equal to 1, Equation 5.4 can be simplified to the linear Euler-Bernoulli beam deflection approximation. However, an exact solution method leads to the development of Equation 5.5.

$$f(\alpha) = \frac{\alpha}{48 - \frac{192 \tanh(\sqrt{\alpha}/4)}{\sqrt{\alpha}}} \quad (5.5)$$

In order to determine the ultimate strength ( $S$ ), a maximum stress analysis is conducted on the NW at the point of fracture, which yields the expression given by Equation 5.6.

$$S = \frac{FL}{2\pi R^3} g(\alpha) \quad (5.6)$$

Here, the equivalent radius of the NW is denoted by  $R$ . Equation 5.6 represents the maximum stress analysis for the NW at fracture. The function  $g(\alpha)$ , which appears in Equation 5.6, is defined by Equation 5.7.

$$g(\alpha) = \frac{4}{\sqrt{\alpha}} \tanh\left(\frac{\sqrt{\alpha}}{4}\right) + \left( \frac{2 + \cosh\left(\frac{\sqrt{\alpha}}{2}\right) - 6 \frac{\sinh\left(\frac{\sqrt{\alpha}}{2}\right)}{\sqrt{\alpha}}}{\alpha \cosh^2\left(\frac{\sqrt{\alpha}}{4}\right)} \right)^{\frac{1}{2}} \quad (5.7)$$

The transcendental equation related to the maximum deflection is denoted by  $\alpha$  and is utilized for both  $f(\alpha)$  and  $g(\alpha)$  terms in the calculation of modulus of elasticity ( $E$ ) and fracture strength ( $S$ ). Equation 5.8 presents the exact solution for the ExtZP nanomechanical model.

$$\begin{aligned} & \left(1 - \frac{L^2 T_0}{\alpha(EI)^*}\right) \left(\frac{(EA)^*}{T_0 + (EA)^*}\right) \left(1 - \frac{L^2 H_{11}}{\alpha(EI)^*}\right) \left(1 - \frac{L^2 H_{22}}{\alpha(EI)^*}\right) \\ & \left(\frac{\alpha \cosh^2\left(\frac{\sqrt{\alpha}}{4}\right)}{2 + \cosh\left(\frac{\sqrt{\alpha}}{2}\right) - 6 \frac{\sinh\left(\frac{\sqrt{\alpha}}{2}\right)}{\sqrt{\alpha}}}\right) \left(1 - 4 \frac{\tanh\left(\frac{\sqrt{\alpha}}{4}\right)}{\sqrt{\alpha}}\right)^2 = \\ & \Delta Z_{center}^2 \left(\frac{(EA)^* + 2d_{11}b + 2d_{22}h + bhE^*}{(EI)^*}\right) \end{aligned} \quad (5.8)$$

The solution given in Equation 5.8 enables the calculation of the effective modulus of elasticity ( $E^*$ ) and ultimate strength ( $S$ ). To calculate the modulus of elasticity,  $E$ , the relation between the classical bending rigidity and effective bending rigidity is utilized as a function of surface properties and geometrical definitions. Equation 5.9 presents the formulation for the effective bending rigidity, employing the extended Young-Laplace approach implemented along with the ExtZP model.

$$(EI)^* = EI + (E_s + \tau_0) \left(\frac{bh^2}{2} + \frac{h^3}{6}\right) \quad (5.9)$$



In this formulation, the average of surface stresses ( $f_{11}$  and  $f_{22}$ ) and surface elasticity constants ( $d_{11}$  and  $d_{22}$ ) are represented by  $\tau_0$  and  $E_s$ , respectively. These terms are commonly known as the surface modulus and initial surface stress in the field of nanomechanical models. More information on prior alternative models [Heidelberg et al., 2006, Ngo et al., 2006, Hudson et al., 2013, Zhan and Gu, 2012, Zare Pakzad et al., 2021] and related bending rigidity formulations [Wang and Feng, 2007, He and Lilley, 2008, Song et al., 2011] can be found elsewhere. The ExtZP model's potential effectiveness in revealing the influence of surface and intrinsic effects on the size-dependent modulus of elasticity and strength of Si NWs has been demonstrated in a recent study [Zare Pakzad et al., 2023c]. In the present study, the ExtZP model is employed using two different approaches to calculate the elastic response of Si NWs, while i) considering and ii) disregarding the surface effect. This enables obtaining the separate results for the modulus of elasticity of the Si core (SCS) and the Si NW covered with its native oxide. Further details about the nanomechanical models can be found in the related references [Zare Pakzad et al., 2023c, Zare Pakzad et al., 2021].

### 5.6.3 Raman characterization

To measure the intrinsic stress ( $\sigma$ ) in suspended Si NWs, a custom micro-Raman setup depicted in Figure 5.6 (a) is used. The measurement setup comprises a Princeton Instruments SP-2500 spectrometer and a 488 nm laser for excitation. The laser beam is divided by a beam splitter and directed through a microscope objective lens, producing a 1  $\mu\text{m}$  spot size. A focusing lens collects the scattered light, which is then filtered with a notch filter and directed to the spectrometer. The microscope, which is integrated into the measurement setup, allows for precise focusing of the microspot on the NWs and features a line scanning system that permits the high-resolution analysis of Raman shift along the entire length of the suspended Si NWs. Then, stress can be measured using the Raman shift,  $\Delta\omega$ , which relates the longitudinal optical (LO) mode obtained in backscattering configuration to the stress components in the Si NW. This is achieved by calculating the shift between the unstrained

Si peak,  $\omega_0$ , and the LO shifted strained Si peak,  $\omega_i$  given in Equation 5.10.

$$\Delta\omega = \omega_i - \omega_0 = \frac{1}{2\omega_0} \left[ [pS_{12} + q(S_{11} + S_{12})](\sigma'_{xx} + \sigma'_{yy}) + (pS_{11} + 2qS_{12})\sigma'_{zz} \right] \quad (5.10)$$

The equation includes elastic constants  $S_{11}$  and  $S_{12}$ , and phonon deformation profiles  $p$  and  $q$ , which are used to model stress in samples with minimal shear stress. Normal stress components along  $x$ ,  $y$ , and  $z$  directions are represented by  $\sigma'_{xx}$ ,  $\sigma'_{yy}$ , and  $\sigma'_{zz}$ , respectively. With the NW aligned along the  $x$  axis,  $\sigma'_{yy}$  and  $\sigma'_{zz}$  can be disregarded and Equation 5.10 can be simplified as Equation 5.11.

$$\Delta\omega = \frac{1}{2\omega_0} \left[ [pS_{12} + q(S_{11} + S_{12})] \right] \sigma'_{xx} = (SSC)\sigma \quad (5.11)$$

The stress shift coefficient (SSC) given in Equation 5.11 is an important parameter that relates the Raman shift to the uniaxial stress along the NW. The SSC has a wide range of reported values for Si NWs, and a value of  $-1.93 \times 10^{-9} \text{ cm}^{-1} \text{ Pa}^{-1}$  is recommended for NWs with a thickness of less than 100 nm [Spejo et al., 2020]. Thus, Equation 5.11 can be written as Equation 5.12 and is used for the calculation of intrinsic stress ( $\sigma$ ) in this study.

$$\Delta\omega = -1.93 \times 10^{-9} \times (\sigma[\text{Pa}]) \quad (5.12)$$

Further details related to the calibration of the laser power, Raman analysis and the determination of related constants can be found elsewhere [Zare Pakzad et al., 2021, Nasr Esfahani et al., 2022, Spejo et al., 2020]. In this respect, the intrinsic stress ( $\sigma$ ) is composed of initial residual stress ( $\sigma_0$ ) and surface-induced residual stress ( $\sigma_{xx}$ ) components. The statistical treatment is followed while 33 samples of different dimensions are subjected to Raman measurements. The Raman shifts are depicted along the longitudinal axis ( $x$ -direction) of the NW in Figure 5.6 (a), using the same color scheme as shown in Figure 5.6 (b). In this respect, Figure 5.6 (b) illustrates the Raman shifts in Si NWs and supports as a function of surface area.

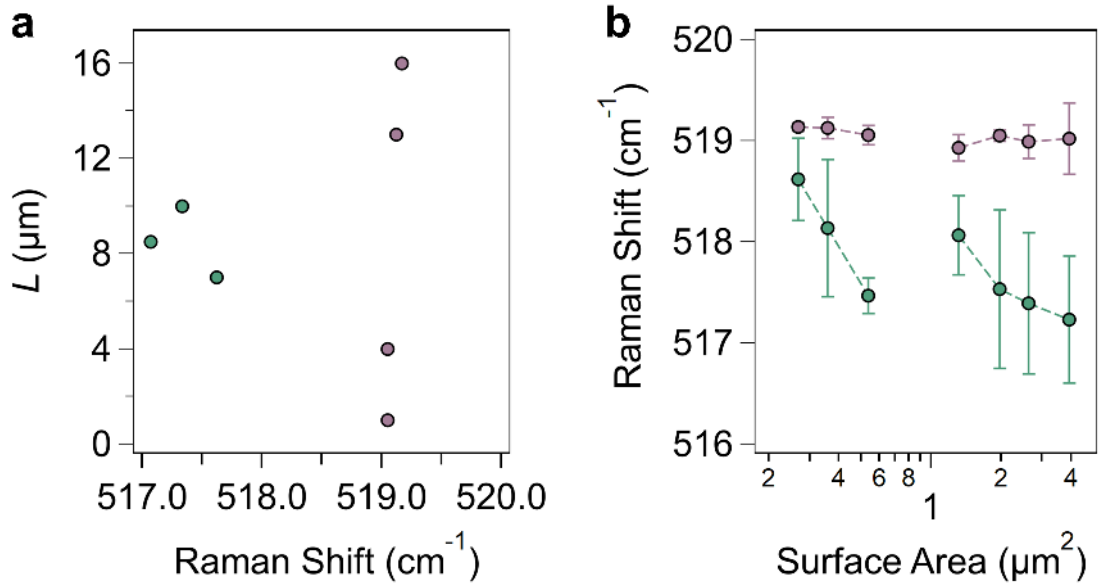


Figure 5.6: (a) Raman shifts, extracted from Figure 5.2 (b) and presented along the NW, are provided with the corresponding color code. (b) Raman peak shifts obtained in line scans as a function of surface area for micropillar supports and suspended Si NWs.

#### 5.6.4 Surface properties

This section presents the specifics of the Si thin film oxidation process and subsequent modeling of anisotropic surface properties, including surface stresses ( $f_{11}$  and  $f_{22}$ ) and surface elastic constants ( $d_{11}$  and  $d_{22}$ ). The oxidation process is simulated at the atomic level using reactive molecular dynamics (MD) simulations. To achieve this, the ReaxFF potential with LAMMPS code [Thompson et al., 2022] is utilized. This potential uses the notion of partial bond orders to effectively model bond breaking and bond formation, approaching accuracy comparable to quantum mechanics, as described in Ref. [Van Duin et al., 2003]. The method has been employed to investigate the influence of temperature, size, and stress on the oxidation of Si NWs, as documented in Refs. [Zare Pakzad et al., 2023c, Khalilov et al., 2013b, Khalilov et al., 2013a]. Additional information on the force field suitable for the modeling of Si/SiO<sub>2</sub> system can be found in relevant reference [Van Duin et al., 2003]. The force field parameters developed by Newsome *et al* [Newsome et al.,

2012] are used to model Si crystal blocks upon oxidation via oxygen (O) molecules as shown in Figure 5.7 (a). The initial part of the discussion covers the specifics of the oxidation of Si thin film, followed by an explanation of the procedure for the calculation of surface stresses ( $f_{11}$  and  $f_{22}$ ) and surface elastic constants ( $d_{11}$  and  $d_{22}$ ). To simulate a two-dimensional structure, specifically a thin film with free surfaces, periodic boundary conditions (B.C.s) are implemented in the 1- and 2-directions, while a non-periodic B.C. is utilized in the 3-direction. A Si model comprising 4608 atoms is constructed with a crystal orientation of  $(1, 2, 3) = ([\bar{1}10], [001], [110])$ . A total of 800 O<sub>2</sub> molecules are distributed on either side of Si thin film as incident molecules, with their coordinates being determined randomly as shown in Figure 5.7 (a). The simulation box is initially relaxed for 300 ps at a temperature of 25°C and a pressure of 1 atm using the isobaric ensemble (NPT) with a time step of 1 fs. The oxidation initiates with a rapid rate during the initial 30 ps and achieves a stable state after 90 ps following the calculation of Si-O pair distribution given in Figure 5.7 (b). Figure 5.7 (c) displays the probability density function (PDF) of Si-O bonds at 300 ps, correlating with the bond length ( $r_{Si-O}$ ). In this respect, the PDF of the oxide reveals a prominent peak at 1.7 Å. Previous MD simulations reported an average Si-O bond length of 1.60 Å [Hung and Hong, 2009, Nasr Esfahani et al., 2022], while bond length measurements for various SiO<sub>2</sub> polymorphs range between 1.55 Å and 1.75 Å [Meade et al., 1992]. The resulting configuration of Si structure featuring a native oxide surface is identified as aSiO<sub>2</sub>-Si and is depicted in Figure 5.7 (d) with associated side views in the 1 – 3 and 2 – 3 planes depicted in Figure 5.7 (e). Similarly, the thickness of the native oxide is determined using analysis of the diamond crystal structure, where the Si core and native oxide regions are identified [Maras et al., 2016]. Figure 5.7 (f) illustrates the cross-sections of the diamond cubic crystal in the 1 – 3 and 2 – 3 planes, with an amorphous native oxide layer formed on the upper and lower surfaces. The results indicate a native oxide thickness ranging from 0.5 nm to 0.7 nm enveloping the Si crystal, which aligns with previous experimental observations [Ma et al., 2003, McDowell et al., 2011] as well as MD simulations [Khalilov et al., 2013a, Nasr Esfahani et al., 2022, Ohta et al.,

2007].

Throughout the remainder of this section, the aSiO<sub>2</sub>-Si model will be utilized to compute surface properties including surface stresses ( $f_{11}$  and  $f_{22}$ ) and surface elastic constants ( $d_{11}$  and  $d_{22}$ ). In order to measure the surface stress components, the aSiO<sub>2</sub>-Si structure is initially equilibrated at 0.01 K through NPT dynamics. Next, the total energy is minimized using both the steepest descent and conjugate gradient methods. The surface stress components are then determined by assuming a film thickness of  $L_z$ , as expressed in Equation 5.13. Here,  $\eta$  denotes the average strain resulting from relaxation.

$$f_{ij}(\eta) = f_{ij}^{film}(\eta) - f_{ij}^{bulk}(\eta) \quad (5.13)$$

The determination of bulk surface stress requires a separate estimation using the bulk model. Moreover, the surface stress for the film model can be defined by utilizing the stress tensor definition,  $\sigma_{ij}^{film}$ , as provided in Equation 5.14. For more comprehensive information regarding the stress tensor of thin films, additional details can be found elsewhere [Izumi et al., 2004, Zare Pakzad et al., 2023c, Pakzad et al., 2021].

$$f_{ij}^{film}(\eta) = \sigma_{ij}^{film}(\eta) \frac{L_z}{2} \quad (5.14)$$

Similarly, the surface elastic constants ( $d_{ijkl}$ ) are determined as the second-order derivatives of surface energy concerning strain under plane-stress conditions. The conventional elastic constants for bulk ( $C_{ijkl}^{bulk}$ ) and film ( $C_{ijkl}^{film}$ ) models are computed using MD simulations. However, for the bulk model, the elastic constants need to be defined under plane-stress conditions ( $C_{ijkl}^{bulk,plane}$ ) using the relationships provided in Equation 5.15, Equation 5.16, and Equation 5.17 [Izumi et al., 2004, Zare Pakzad et al., 2023c].

$$C_{11}^{bulk,plane} = C_{11} - \frac{C_{13}^2}{C_{33}} \quad (5.15)$$

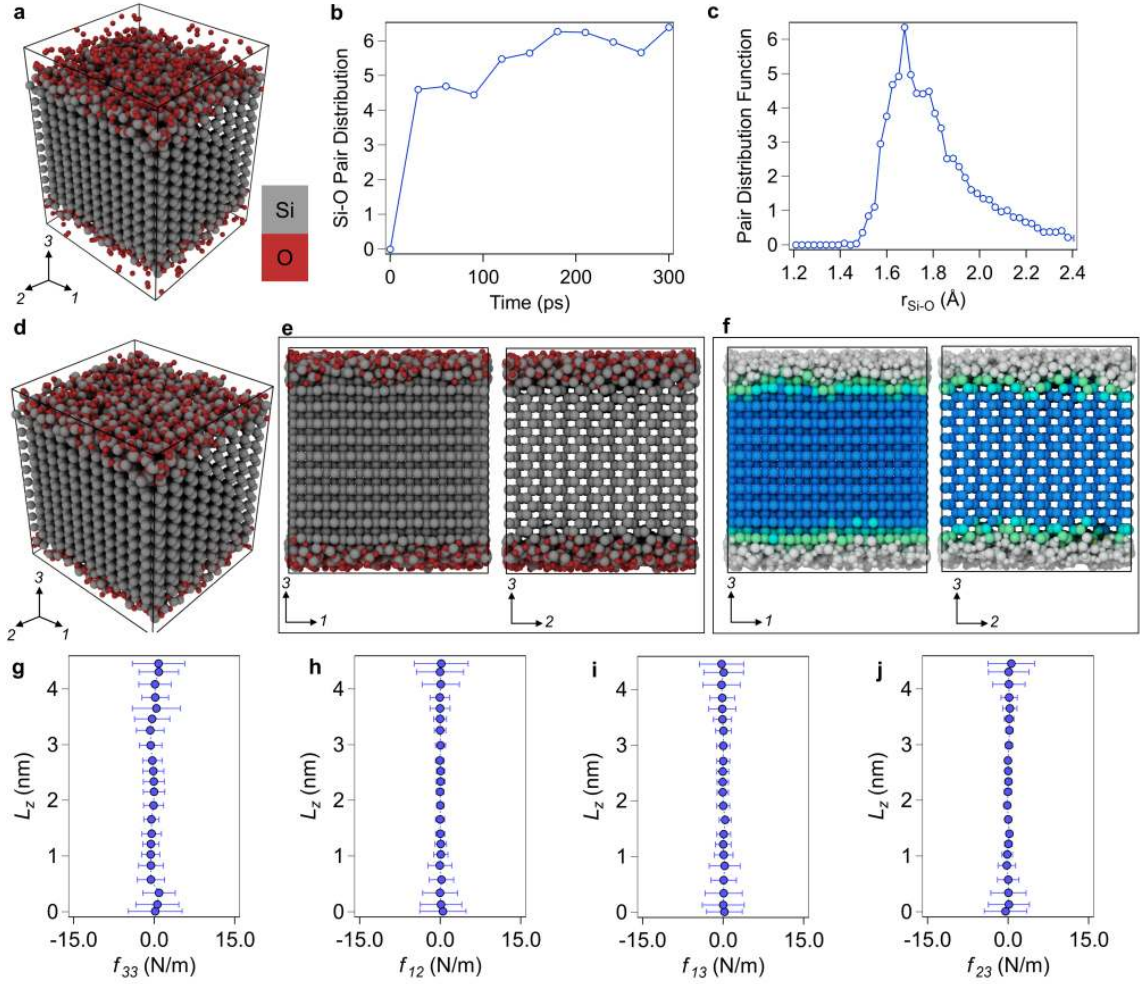


Figure 5.7: (a) Atomic configurations for the initial unreconstructed Si thin film and its exposure to oxygen (O) molecules with (110) free surface in the 3-direction. Si and O atoms are shown with grey and red spheres, respectively. (b) Magnitude of the Si-O pair distribution as a function of time for aSiO<sub>2</sub>-Si thin film. (c) PDF of Si-O for aSiO<sub>2</sub>-Si thin film at 300 ps. (d) The oxidized Si structure with free surface in the 3-direction given as aSiO<sub>2</sub>-Si thin film. (e) The side views of aSiO<sub>2</sub>-Si thin film in the 1 – 3 and 2 – 3 planes. (f) The side surfaces in the 1 – 3 and 2 – 3 planes, with an amorphous native oxide layer formed on the upper and lower surfaces. The color bar indicates the amorphous and cubic diamond structures with related first and second neighbors obtained via diamond cubic structure analysis. The stress components, (g)  $f_{33}$ , (h)  $f_{12}$ , (i)  $f_{13}$ , and (j)  $f_{23}$ , are shown for the aSiO<sub>2</sub>-Si thin film structure.

$$C_{22}^{bulk,plane} = C_{22} - \frac{C_{12}^2}{C_{33}} \quad (5.16)$$

$$C_{12}^{bulk,plane} = C_{12} - \frac{C_{12}C_{13}}{C_{33}} \quad (5.17)$$

Equation 5.18 [Izumi et al., 2004, Zare Pakzad et al., 2023c] presents the correlation between the plane-stress elastic constants of the bulk and film models and the surface elastic constants.

$$C_{ijkl}^{film,plane} = C_{ijkl}^{bulk,plane} - \frac{2}{L_z} d_{ijkl} \quad (5.18)$$

The Tersoff-Munetoh potential [Munetoh et al., 2007], which is an empirical function comprising two-body terms that depend on the local environment, is used for the calculation of surface properties. To determine the elastic constants, infinitesimal strains are applied to the simulation box in different directions, and the resulting energy variation is measured. The corresponding stress state of the thin film, denoted as  $\pi_{ij}$ , is calculated using the virial theorem [Zimmerman et al., 2004], as expressed in Equation 5.19.

$$\pi_{ij} = \frac{1}{2\Omega_0} \left[ \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \frac{1}{r^{\alpha\beta}} \frac{\partial V(r^{\alpha\beta})}{\partial r} (v_i^{\alpha\beta} v_j^{\alpha\beta}) \right] \quad (5.19)$$

In the equation,  $\Omega_0$  represents the atomic volume in an undeformed system, with  $N$  being the total number of atoms. The atomic volumes for Si and aSiO<sub>2</sub> are obtained through the relaxation of related structures in each crystallographic direction. The atomic distances between atoms  $\alpha$  and  $\beta$  are denoted as  $r^{\alpha\beta}$ , while  $v_j^\alpha$  denotes the position of atom  $\alpha$  along the  $j$  direction, such that  $v_j^{\alpha\beta} = v_j^\alpha - v_j^\beta$ . The interatomic potential is represented by  $V$ . Readers are advised to refer to existing literature on this topic for further information [Pakzad et al., 2021, Zare Pakzad et al., 2023c].

Table 5.1: Surface stresses and surface elastic constants for aSiO<sub>2</sub>-Si thin film model.

| Structure                   | Surface Properties(N/m) |            |            |             |
|-----------------------------|-------------------------|------------|------------|-------------|
|                             | $f_{11}$                | $f_{22}$   | $d_{11}$   | $d_{22}$    |
| aSiO <sub>2</sub> -Si (110) | -6.33±0.50              | -4.90±0.50 | +9.05±3.51 | +47.82±4.01 |

Stresses, as determined by Equation 5.19, are illustrated in Figure 5.2 (d), revealing a significant variation in stress within 5 to 6 atomic layers at the outer bounds of the aSiO<sub>2</sub>-Si structure. In this respect, Equation 5.13 is used for the calculation of surface stress components ( $f_{11}$  and  $f_{22}$ ) given in Figure 5.2 (d), as well as the remaining surface stresses ( $f_{33}$ ,  $f_{12}$ ,  $f_{13}$ , and  $f_{23}$ ) provided in Figure 5.7 (g-j). Similarly, the surface elastic constants ( $d_{11}$  and  $d_{22}$ ) are determined using Equation 5.18. The changes in surface properties are determined by examining the evolution of stress and elastic components throughout the thickness of the film. The surface stress components,  $f_{11}$  and  $f_{22}$ , and surface elastic constants,  $d_{11}$  and  $d_{22}$ , are tabulated in Table 5.1. In this regard, the computed surface properties can be compared to those reported in prior studies concerning unreconstructed and oxidized Si thin films [Zare Pakzad et al., 2023c, Quagliotti et al., 2013, Delph, 2008, Payne et al., 1989, Pakzad et al., 2021, Pishkenari and Rezaei, 2017, Izumi et al., 2004, Miyamoto, 1994, Alerhand et al., 1988]. The average surface stress components,  $f_{11}$  and  $f_{22}$ , as reported by Melis et al. [Melis et al., 2016], equal to 10.3 N/m in compression, closely align with the values for aSiO<sub>2</sub>-Si (110) presented in Table 5.1. Considering the significantly different computational approaches employed to calculate surface properties, the observed deviations between the predictions fall within an acceptable range [Quagliotti et al., 2013, Xu and Kim, 2019, Pakzad et al., 2021, Melis et al., 2016, Jung and Shin, 2017, Melis et al., 2015, Ohta et al., 2007].

#### 5.6.5 FIB/HR-TEM cross-sectional imaging

Si NWs are known to undergo a gradual oxidation process, leading to the formation of a uniform native oxide layer surrounding the Si core as single crystal silicon



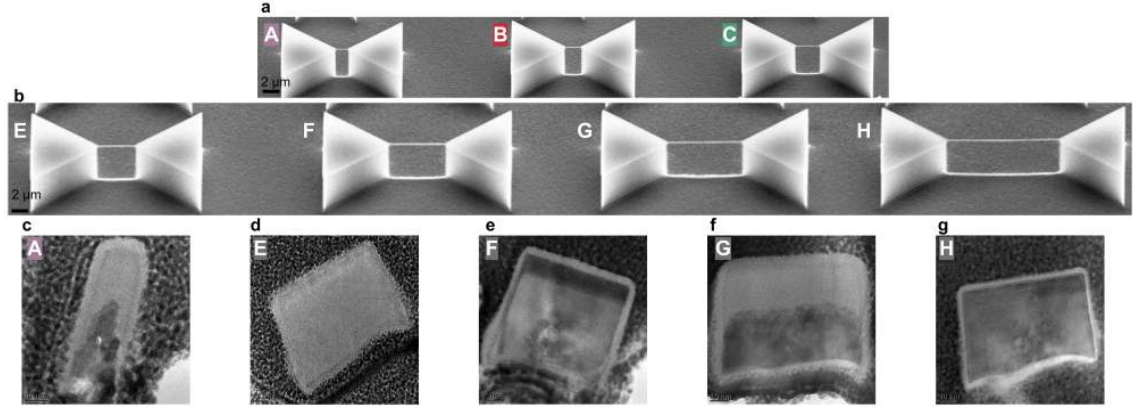


Figure 5.8: SEM images of Si NWs with (a) a nominal width of 20 nm and (b) a nominal width of 80 nm suspended between triangular micropillars. (c-g) Cross-sectional HR-TEM images of Si NWs reveal the dimensions of the SCS core as well as the aSiO<sub>2</sub> native oxide envelope. The label provided next to each HR-TEM image corresponds to the specific combination of width and length to which the respective Si NW belongs.

(SCS) [Nasr Esfahani et al., 2022, Zare Pakzad et al., 2023c]. This phenomenon has been verified through cross-sectional high-resolution transmission electron microscopy (HR-TEM) studies, which involved acquiring images via focused ion beam (FIB) milling. The process includes HR-TEM imaging of Si NWs with nominal widths of 20 nm and 80 nm shown in Figure 5.8 (a) and Figure 5.8 (b), respectively. The analysis is conducted for the determination of the dimensions of the Si core (SCS) and the native oxide (aSiO<sub>2</sub>) layer. Cross-sectional HR-TEM images are presented in Figure 5.8 (c-g). A total of six Si NWs are imaged during this study (One HR-TEM image is given in Figure 5.2 (f) and the remaining five are presented in Figure 5.8 (c-g)). As an integral component of the statistical analysis, two cross-sectional images from prior study [Nasr Esfahani et al., 2022] by the authors are included to assess the width, height, and oxide thickness of Si NWs exhibiting different dimensionalities. In this regard, a total of eight HR-TEM images are employed for the dimensional analysis.

### 5.6.6 *in-situ* Bending experiment

The *in-situ* three-point bending test is conducted at ambient temperature within the vacuum chamber of a dual-beam focused ion beam/scanning electron microscope (FIB/SEM) equipment. A micromanipulator equipped with a piezoresistive cantilever-based Kleindiek force sensor is used to apply and measure the force, while image analysis of micrographs is utilized to determine the bending deflection. Upon contact with the test sample, the piezoresistive gage produces an analog voltage output, which is converted into a force value. The start of the three-point bending experiment is shown in Figure 5.9 (a), which shows the SEM image of the force sensor making contact with the Si NW. Figure 5.9 (b) illustrates Si NW during the testing process with its associated deflection at the midsection. The test continues until the NW experiences a complete fracture. The results of bending tests are given in 5.6.7 with detailed elaboration of the ExtZP nanomechanical model fits. To gain additional insights into the nanomechanical testing of Si NWs, the following relevant literature are suggested [Wollschläger et al., 2016, Zare Pakzad et al., 2021, Espinosa et al., 2013, Dasgupta et al., 2014, Elhebeary and Saif, 2017b].

### 5.6.7 Interpretation of bending test results

The three-point bending test results of Si NWs, given as  $F - w$  data, with nominal widths of 20 nm and 80 nm and different lengths are presented in Figure 5.10. Section 5.6.2 already discussed the details associated with the ExtZP nanomechanical model's formulation and related parameters for the calculation of modulus of elasticity and strength of Si NWs. This section provides the fitting procedure via ExtZP nanomechanical model for the interpretation of elastic properties and strength of Si NWs and SCS. For this purpose, the ExtZP model is used with and without considering the contribution from the surface-related effects. This would allow one to capture and distinguish the elasticity of core SCS and Si NWs with native oxide surface condition studied in this work. In this regard, the obtained  $F - w$  responses for the Si NWs with nominal widths of 20 nm, 80 nm and follow-up fits conducted via the ExtZP model incorporating the surface effects for decoding the SCS elastic-

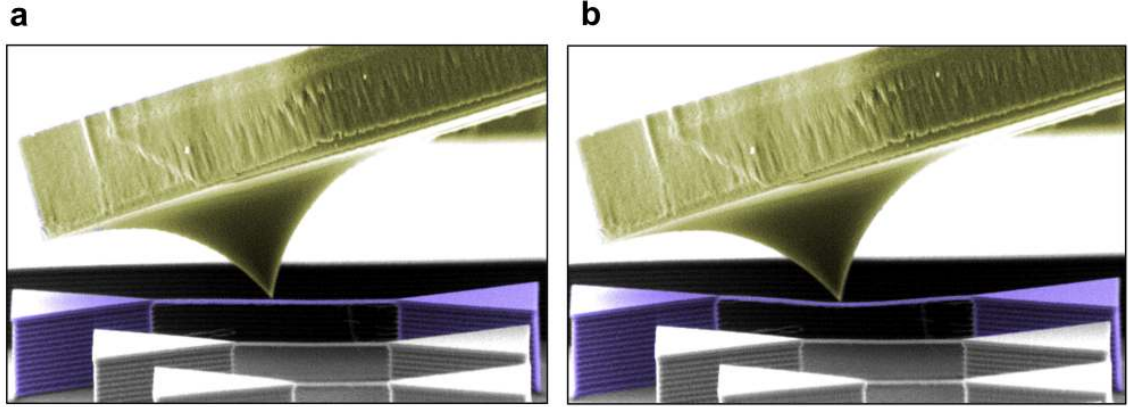


Figure 5.9: (a) The SEM image captures the initiation of the three-point bending experiment, showcasing the force sensor making contact with the Si NW within the vacuum chamber of a dual-beam FIB/SEM setup. (b) The SEM image shows the Si NW in the midst of the three-point bending test, providing a visual representation of its deflection at the midsection. The micromanipulator, equipped with a piezoresistive cantilever-based Kleindiek force sensor, applies and measures the force, while image analysis of micrographs aids in determining the bending deflection.

ity are shown in Figure 5.10 (a) and Figure 5.10 (b), respectively. Similarly, fitting curves for the ExtZP model without considering surface properties are illustrated in Figure 5.10 (c) and Figure 5.10 (d) for Si NWs with nominal widths of 20 nm and 80 nm, respectively. Thus, the elastic response obtained here is considered as the effective modulus of elasticity for Si NWs with native oxide effect.

To interpret the  $F$ - $w$  data obtained from the bending test, it is necessary to evaluate the total uniaxial intrinsic stress,  $\sigma$ , resulting from two residual stress components generated in the Si NW: i) the initial tension/compression force,  $T_0$ , and ii) surface-induced residual stress,  $\sigma_{xx}$ . The quantification of  $\sigma$  is accomplished through Raman spectroscopy using a custom-built  $\mu$ -Raman setup, with detailed information provided in Section 5.6.3. In this respect, Raman spectroscopy is utilized to measure the intrinsic stress,  $\sigma$ , as given in Equation 5.12. The Raman shift of the support pillars and the NW is measured by conducting line scans along the Si NW, as shown in Figure 5.2 (b). Thus, the intrinsic stress obtained for different dimensions of Si NWs are presented in Figure 5.2 (c). As a byproduct of the RIE process, Si NW cross-sections are found to be of a trapezoidal shape with length,

width, height, and oxide thickness details discussed in Section 5.6.5. The  $F$ - $w$  results obtained for Si NWs with 20-nm nominal widths and different lengths labeled as A, B, and C given in Figure 5.10 (a) and Figure 5.10 (c) exhibit nonlinear responses with a force range up to  $2.92 \mu\text{N}$ ,  $5.95 \mu\text{N}$ , and  $3.90 \mu\text{N}$ , respectively. In this respect, the associated mid-point deflections,  $w$ , ranging up to  $0.23 \mu\text{m}$ ,  $0.38 \mu\text{m}$ , and  $0.42 \mu\text{m}$  are obtained for Si NW sets of A, B, and C, respectively. Similarly, for Si NWs with nominal width of 80 nm and length-to-nominal width of 50, 75, 100, and 150 denoted as set E, F, G, and H, nonlinear  $F - w$  responses are achieved. For sets of E, F, G, and H, the force ranges up to  $16.08 \mu\text{N}$ ,  $18.03 \mu\text{N}$ ,  $15.10 \mu\text{N}$ , and  $18.09 \mu\text{N}$  and resultant deflections of  $0.67 \mu\text{m}$ ,  $1.02 \mu\text{m}$ ,  $1.27 \mu\text{m}$ , and  $1.98 \mu\text{m}$  are obtained, respectively.

Note that such deflection is almost 15-20 times larger than the NW height, thereby necessitating the nonlinear formulation given in the ExtZP model. In this respect, the model is then fitted to the experimental data to estimate the elastic properties given as  $E$  and  $E^*$  as well as the fracture strength,  $S$ . To address the  $E$  for SCS, ExtZP model is used with inclusion of surface properties, where surface stress components ( $f_{11}$  and  $f_{22}$ ) and surface elasticity constants ( $d_{11}$  and  $d_{22}$ ) for aSiO<sub>2</sub>-Si listed in Table 5.1 are used. To address the  $E^*$  for Si NWs with native oxide, ExtZP model is conducted while surface properties are disregarded. Further details about the interpretation of bending deformation via ExtZP nanomechanical model can be found in the relevant references [Zare Pakzad et al., 2023c, Zare Pakzad et al., 2021]. In this respect, Figure 5.1 (a) displays the obtained modulus of elasticity for core SCS and Si NWs with native oxide for different sets of NWs. Figure 5.1 (b) displays the fracture strength obtained for SCS using the ExtZP nanomechanical mode.

#### 5.6.8 Atomistic Modeling of Si NWs with native oxide

The modulus of elasticity in  $\langle 110 \rangle$ -oriented Si NWs with a native oxide surface condition is examined using MD simulations. The NWs are denoted as aSiO<sub>2</sub>-Si NWs, with Figure 5.11 (a) presenting the circular cross-section, and Figure 5.11 (b) providing perspective views of an aSiO<sub>2</sub>-Si NW. Moreover, to investigate the cross-

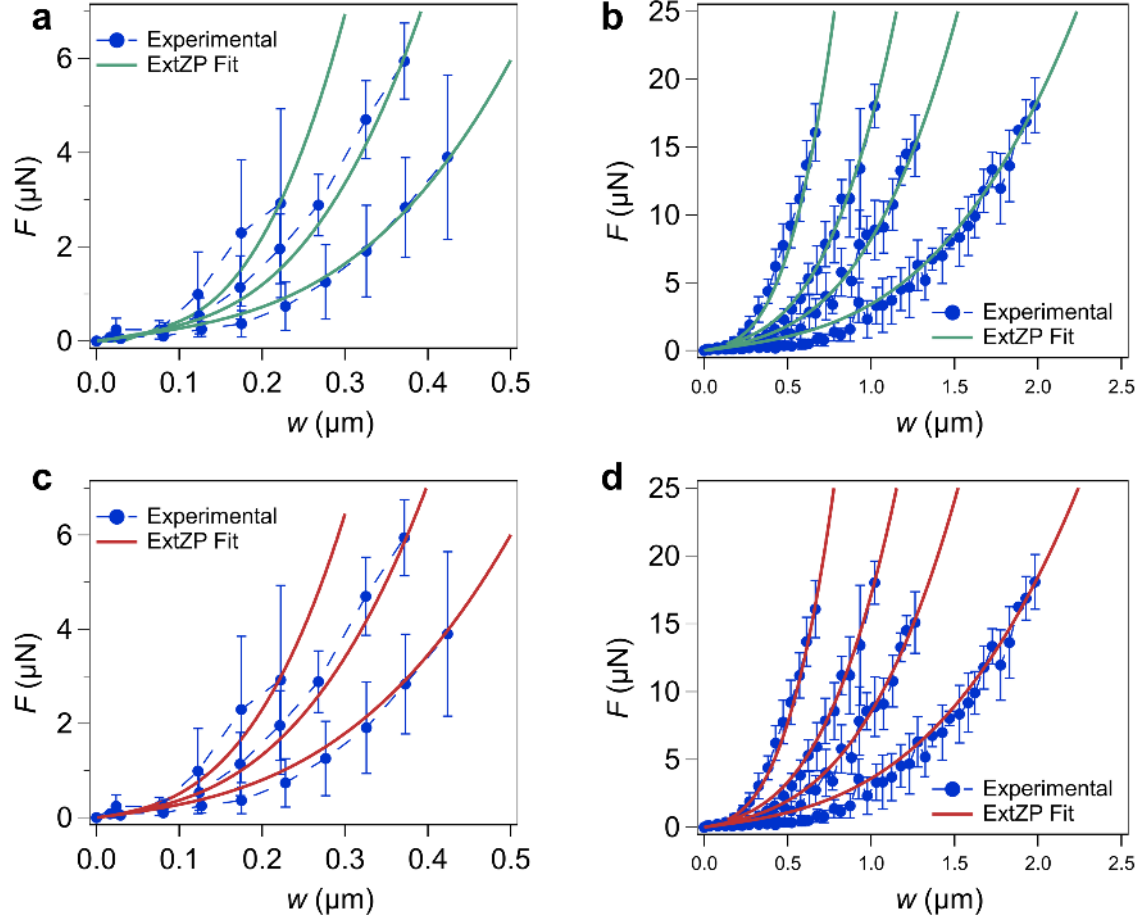


Figure 5.10: (a)  $F - w$  data obtained through a three-point bending test on Si NWs with 20 nm nominal width and different lengths given as sets A, B, and C. The fitted curve using the ExtZP nanomechanical model is with inclusion of surface effects for the interpretation of elasticity for core SCS. (b)  $F - w$  data obtained through a three-point bending test on Si NWs with 80 nm nominal width and different lengths given as sets E, F, G, and H. The fitted curve using the ExtZP nanomechanical model is with inclusion of surface effects for the interpretation of elasticity for core SCS. (c)  $F - w$  data obtained through a three-point bending test on Si NWs with 20 nm nominal width and different lengths given as sets A, B, and C. The fitted curve using the ExtZP nanomechanical model is with exclusion of surface effects for the interpretation of elasticity for Si NWs with native oxide. (d)  $F - w$  data obtained through a three-point bending test on Si NWs with 80 nm nominal width and different lengths given as sets E, F, G, and H. The fitted curve using the ExtZP nanomechanical model is with exclusion of surface effects for the interpretation of elasticity for Si NWs with native oxide.

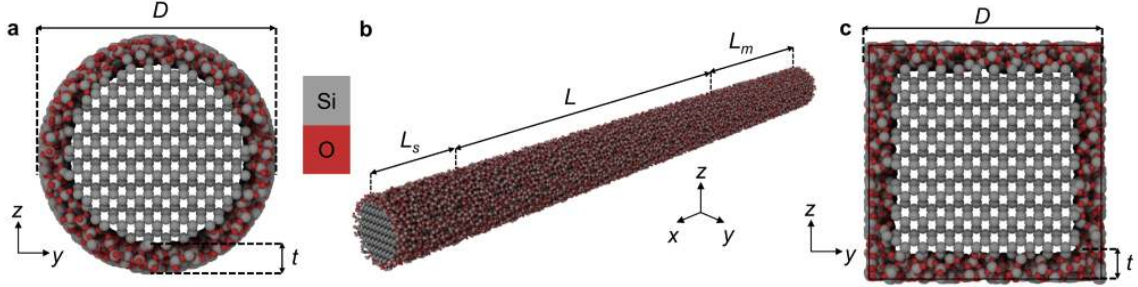


Figure 5.11: (a) Cross-sectional atomic configuration of an aSiO<sub>2</sub>-Si NW with circular shape. (b) Representative view of an aSiO<sub>2</sub>-Si NW, illustrating the lengths: NW length ( $L$ ), support region length ( $L_s$ ), and movable region length ( $L_m$ ). (c) Square cross-section of an aSiO<sub>2</sub>-Si NW. The critical dimension,  $D$ , and native oxide thickness,  $t$ , are indicated for both cross-sectional representations. Si and O atoms are depicted by grey and red spheres, respectively.

sectional shape effect on modulus of elasticity of Si NWs, comparable simulations are conducted using square cross-sections given in Figure 5.11 (c). In this respect, the MD simulations involve similar combinations of critical dimension, oxide thickness, and length assignments. The tensile simulation of Si NWs with native oxide surface state is performed via LAMMPS code [Thompson et al., 2022]. The non-periodic B.C.s are applied along all directions. The dimensions of the NWs are determined by the length ( $L$ ), and native oxide thickness ( $t$ ) where diameter or width ( $D$ ) is used as the critical dimension (CD) indicator. The length-to-CD ( $L/D$ ) ratio of 10 is used for all Si NWs studied here. Figure 5.11 (b) shows an aSiO<sub>2</sub>-Si NW with the associated  $L$ , while support and movable boundaries are labeled as  $L_s$  and  $L_m$ , respectively. The interaction between atoms in NWs are described by the Tersoff-Munetoh (TM) and modified Stillinger-Weber (m-SW) potentials [Munetoh et al., 2007, Ganster et al., 2010]. The details of the corresponding expressions and coefficients of the formulations for the potentials can be found in the related references [Munetoh et al., 2007, Ganster et al., 2010, Pakzad et al., 2023b].

The tensile simulation is performed by anchoring one side of the NW ( $L_s$ ) while having the other end as the moveable boundary ( $L_m$ ). The  $L_s$  and  $L_m$  are set to the  $1/8^{th}$  of  $L$ . An initial velocity with the Gaussian distribution at a finite

temperature of 300 K is assigned to atoms followed by the energy minimization using the conjugate gradient method. Then, the NWs are relaxed at 300 K for 50 ps with a time step of 1 fs using a canonical NVT ensemble. The support and moveable regions attached to the NWs are defined in a fixed configuration for both sides during initialization and relaxation steps. In order to reduce the impact of the high loading rate, a uniform velocity is employed along the tensile direction of the NW ( $x$ -direction), starting from zero at the support and gradually increasing to a maximum value at the free end. The velocity remains constant towards the movable boundary. For the tensile simulations, finite velocity value of  $1.0 \text{ \AA/ps}$  at a finite temperature of 300 K is used. Assignment of  $1.0 \text{ \AA/ps}$  finite velocity corresponds to the strain rates of  $\dot{\epsilon} \approx 1.0 \times 10^9 \text{ s}^{-1}$ . Such strain rate is in the range of suitable strain rates for tensile tests of NWs via MD [Kang and Cai, 2007, Kang and Cai, 2007, Pakzad et al., 2023b, Pakzad et al., 2021]. The atomic stress based on the virial theorem [Cormier et al., 2001] given in Equation 5.19 is used for the stress calculations. The examination of the cross-sectional shape effect involves repeating modeling efforts on aSiO<sub>2</sub>-Si NWs with both circular and square cross-sections. A range of CDs for aSiO<sub>2</sub>-Si NWs spanning from 4 to 8 nm is considered. The investigated SiO<sub>2</sub>-Si NWs are designed with two distinct oxide thicknesses given as  $t = 0.5 \text{ nm}$  and  $t = 1.0 \text{ nm}$ . The stress-strain relationship for aSiO<sub>2</sub>-Si NWs is linear in the elastic range at small strains, allowing for the direct prediction of the modulus of elasticity for Si NWs with native oxide surface state. Utilizing the stress-strain curves, the modulus of elasticity for the aSiO<sub>2</sub>-Si NWs with circular and square cross-sections is calculated and tabulated in Table 5.2.

The comparable moduli of elasticity presented in the table allow for an assessment of the shape effect. In particular, the results given in Table 5.2 indicate a significant dependence of the modulus of elasticity on size for aSiO<sub>2</sub>-Si NWs when the  $D$  is less than 10 nm. Within this range,  $E$  experiences a variation of up to 28% as  $D$  increases from 4 nm to 8 nm, considering a native oxide thickness of 0.5 nm. With the change of  $t$  to 1.0 nm, the size effect becomes more pronounced, leading to a 51% change in  $E$  when  $D$  increases from 4 nm to 8 nm. Furthermore, the

Table 5.2: Modulus of elasticity ( $E$ ) estimations for aSiO<sub>2</sub>-Si NWs with different critical dimension (CD) given as  $D$  and oxide thickness ( $t$ ) combinations modeled via TM and m-SW interatomic potentials.

| Cross-section Shape | $D$ (nm) | $E$ (GPa)    |              |              |              |
|---------------------|----------|--------------|--------------|--------------|--------------|
|                     |          | $t = 0.5$ nm | $t = 1.0$ nm | $t = 0.5$ nm | $t = 1.0$ nm |
|                     |          | m-SW         | m-SW         | TM           | TM           |
| Circular            | 4        | 89.7         | 75.9         | 98.3         | 69.1         |
|                     | 5        | 98.6         | 85.4         | 109.3        | 79.7         |
|                     | 6        | 105.6        | 95.2         | 117.0        | 89.8         |
|                     | 7        | 111.2        | 100.8        | 123.4        | 98.4         |
|                     | 8        | 115.5        | 105.0        | 126.4        | 104.6        |
| Square              | 4        | 91.3         | 76.0         | 103.7        | 68.7         |
|                     | 5        | 99.9         | 84.6         | 110.9        | 82.7         |
|                     | 6        | 105.8        | 93.7         | 117.4        | 91.0         |
|                     | 7        | 111.3        | 98.3         | 126.1        | 98.8         |
|                     | 8        | 115.3        | 103.6        | 129.8        | 106.1        |



size-dependence of the TM potential is observed to be more significant compared to the m-SW potential, although the disparities between the predictions are not substantial. Additional insights into the distinctions between these two potentials can be found in other sources, as detailed in Ref. [Pakzad et al., 2023b]. In this context, Figure 5.4 (b) in Article exhibits the estimated modulus of elasticity of aSiO<sub>2</sub>-Si NWs with different combinations of CDs and oxide thicknesses modeled via m-SW and TM potentials. To facilitate interpretation, the follow-up analysis is performed on aSiO<sub>2</sub>-Si NWs with circular cross-sections. This choice facilitates the application of the M-CS model, adopting a circular perspective. Furthermore, choosing circular cross-sections over square ones is justified by the minimal shape discrepancy, with variations of up to 5 GPa. Additional information about the follow-up analytical calculations via M-CS model is available in Section 5.6.9. Additional information regarding the modeling of Si NWs with native oxide can be found in the relevant references [Zare Pakzad et al., 2023c, Nasr Esfahani et al., 2022, Pakzad et al., 2021, Pakzad et al., 2023b]. Further information about the role of inter-atomic potential in modeling efforts for Si NWs can be acquired from the provided sources [Bartók et al., 2018, Esfahani, 2022, Pakzad et al., 2023b]. More details on atomistic modeling of Si NWs can be found elsewhere [Justo et al., 2007, Yang et al., 2009, Zhuo and Beom, 2019, Godet et al., 2015, Yao et al., 2012, Chen et al., 2018, Ilinov and Kuronen, 2014, Park, 2008, Zhuo and Beom, 2018].

#### 5.6.9 Modified core-shell model

Si NWs with circular cross-sections composed of an inner core (bulk) and an external shell (surface), shown in Figure 5.12, are considered as core Si (SCS) with a native oxide surface layer (aSiO<sub>2</sub>), respectively. The M-CS model defines the surface elasticity with an increasing or decreasing exponential expression at the interface region between the core and surface regions [Yao et al., 2012, Xu et al., 2016, Li et al., 2022]. For the surface layer thickness of  $t$  and the core Si radius of  $R_0$ , Figure 5.12 provides the schematic representation of the M-CS model where  $E_{aSiO_2}$  is defined a function of the surface radius,  $r$ , ranging between  $R_0$  and  $R_0 + t$ . Equation 5.20

describes the surface elasticity via the M-CS model where  $E_{aSiO_2}(r)$  represents the variable elasticity in the surface shell region. The modulus of elasticity at the core Si is denoted by  $E_{Si}$  in the M-CS method. The surface factor parameter,  $\alpha$ , relates  $t$  to a dimensionless constant,  $\tilde{\alpha}$  with  $\alpha = \tilde{\alpha}/t$ . The magnitude of  $\tilde{\alpha}$  describes the inhomogeneity degree in the elasticity upon transition from the bulk region as of SCS to the surface layer as aSiO<sub>2</sub>. In such context, the sign of  $\tilde{\alpha}$  describes the stiffening (positive) or softening (negative) of the surface layer.

$$E_{aSiO_2}(r) = E_{Si}e^{\alpha(r-R_0)} \quad R_0 \leq r \leq R_0 + t \quad (5.20)$$

The formulation for modulus of elasticity of aSiO<sub>2</sub>-Si NW based on the M-CS model is given in Equation 5.21. The analytical M-CS model is utilized in this study to estimate the modulus of elasticity for different combinations of critical dimension ( $D$ ) and oxide thickness ( $t$ ), using the elastic moduli obtained via MD simulations given in Section 5.6.8. In addition to MD results, the experimentally determined elastic moduli for the Si NWs are integrated into the M-CS model. The resulting M-CS trendlines are presented in Figure 5.3 (b) in Article. Further details associated with the M-CS models can be found elsewhere [Yao et al., 2012, Xu et al., 2016, Li et al., 2022].

$$E = E_{Si} \left[ \left(1 - \frac{2t}{D}\right)^2 + \frac{4t}{\tilde{\alpha}D} (e^{\tilde{\alpha}} - (1 - \frac{2t}{D})) - \frac{8t^2}{\tilde{\alpha}^2 D^2} (e^{\tilde{\alpha}} - 1) \right] \quad (5.21)$$

#### 5.6.10 Atomistic modeling of unreconstructed Si NWs

This section presents an overview of the tensile and bending modeling for Si NWs with unreconstructed surface state using MD simulations. The modeling efforts explore the two common approaches for modeling the tensile behavior: non-periodic and periodic tensile tests, as well as three-point bending simulations for Si NWs. Sections 5.6.10 and 5.6.10 are specifically allocated to the individual discussion of the two tensile modeling approaches. Section 5.6.10 provides detailed information

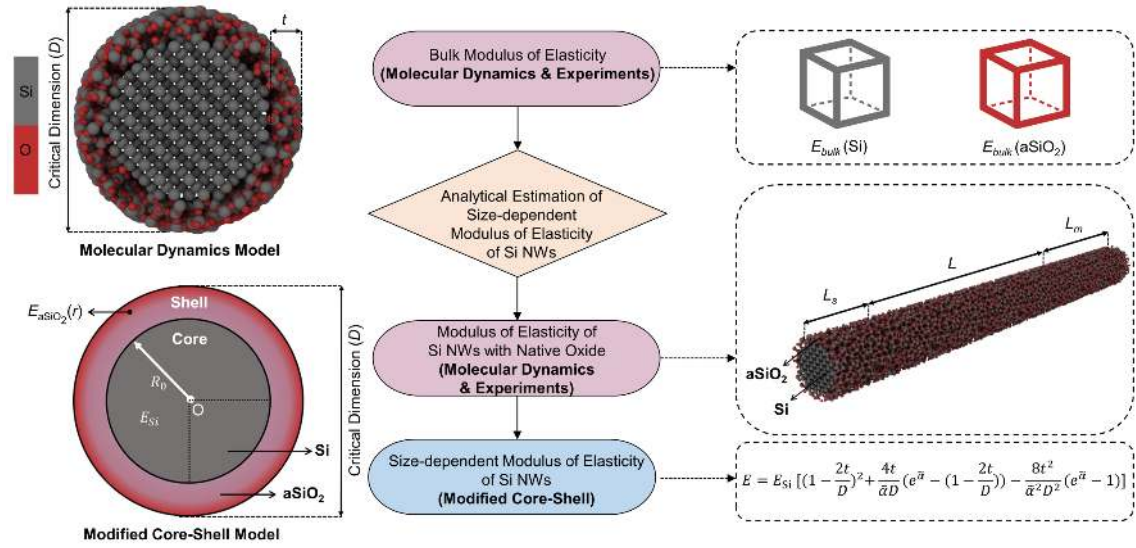


Figure 5.12: Flowchart depicting the methodology for the combination of Modified Core-Shell (M-CS) model with Molecular Dynamics (MD) and experiments to implement the native oxide surface state in the calculation of the Si NW elastic properties. For the M-CS model, the native oxide modulus, ( $E_{aSiO_2}(r)$ ), is evolving as a function of  $r$ . Si core and native oxide surface are depicted by grey and red colors, respectively, with a shaded grey layer in between indicating the transition between bulk and surface. The atomic configuration in MD simulations is represented over a circular cross-section of  $aSiO_2$ -Si NWs with a critical dimension, CD, of  $D$  and a native oxide thickness,  $t$ . Dimensional parameters associated with MD model include NW length ( $L$ ), support region length ( $L_s$ ), and movable region length ( $L_m$ ). The grey and red spheres represent Si and O atoms, respectively. The elastic moduli obtained experimentally for the studied Si NWs in this study are utilized and integrated with the M-CS method.

regarding the modeling of bending behavior. Moreover, each subsection covers the specifics of different computational details, including the preparation of atomic configurations, utilization of interatomic potentials, and other relevant parameters.

#### *Non-periodic tensile simulation*

In this subsection, the atomistic methodology employed for the exploration of the tensile behavior of Si NWs utilizing a non-periodic boundary condition along the NW is explained. Tensile tests are conducted on Si NWs with unreconstructed surface states, utilizing the MD method via LAMMPS code [Thompson et al., 2022]. Figure 5.13 (a) illustrates the initial atomic configuration of Si NWs, emphasizing the geometric characteristics of the NW, which exhibits a square cross-sectional shape. This representation includes the width, which serves as a representation of the critical dimension (CD) in Si NWs. Figure 5.13 (b) schematically describes the non-periodic tensile modeling approach where the length ( $L$ ) of Si NW and the support and movable boundaries are labeled as  $L_s$  and  $L_m$ , respectively. The lengths  $L_s$  and  $L_m$  correspond to one-eighth of the NW length ( $L$ ). In this respect, the length to CD ratio ( $L/CD$ ) is termed as the aspect ratio (AR). Regarding the geometrical and computational details, Table 5.3 provides a complete description of input parameters. In this respect, the CD spans from 2 nm to 10 nm, while the predefined ARs are assigned as 7, 8, 9, 10, 12, 14, 16, 18, and 20. The Si NWs are oriented along  $\langle 110 \rangle$  crystal orientation ( $[110]-x$   $[001]-y$   $[\bar{1}10]-z$ ) and are subjected to tensile test where the interactions between Si atoms are modeled using the Tersoff-T3 (TT3) [Tersoff, 1988] and Stillinger-Weber (SW) [Stillinger and Weber, 1985] potentials. Comprehensive details of the potential expressions and coefficients are available in the respective references [Tersoff, 1988, Stillinger and Weber, 1985].

Non-periodic boundary conditions are imposed in all directions ( $x$ ,  $y$ , and  $z$ ) to account for a finite size. An energy minimization step is executed using the conjugate gradient method, followed by assigning an initial velocity distribution based on a finite temperature to all atoms. Subsequently, a relaxation process is carried out

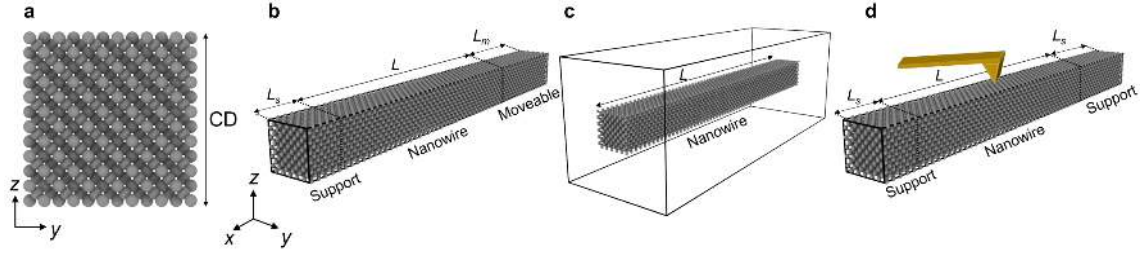


Figure 5.13: (a) Cross-section of a Si NW with dimensional parameter defined as CD, representing the NW width. (b) Non-periodic tensile simulation of Si NWs is exhibited with the associated atomic configuration. The NW length ( $L$ ) and B.C. regions are referred as support ( $L_s$ ) and movable boundaries ( $L_m$ ). (c) Periodic tensile simulation of Si NWs is shown with related atomic configuration. The associated NW length ( $L$ ) and simulation box are given. (d) Bending simulation with the perspective view of a double-clamped Si NW showing the atomic configuration under 3-point bending simulation using a spherical indenter with associated support regions. The NW length ( $L$ ) and support region lengths ( $L_s$ ) are shown here.

for 60 ps at a constant temperature, employing a 1 fs time step in the canonical NVT ensemble. During relaxation, the support and movable regions connected to the NW remain in fixed configurations. The subsequent tensile test involves fixing one end of the NW ( $L_s$ ) while allowing the other end ( $L_m$ ) to move. To mitigate shock wave generation due to rapid loading, a linearly increasing constant velocity is applied along the longitudinal direction ( $x$ ). The velocity starts from zero at the support and gradually increases to its maximum at the movable boundary. A velocity of  $1.0 \text{ \AA/ps}$  is applied at a constant temperature, corresponding to a strain rate of  $\dot{\epsilon} \approx 1.0 \times 10^9 \text{ s}^{-1}$ . This rate aligns with the strain rate employed in previous MD-based tensile tests on NWs [Kang and Cai, 2007, Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024]. The simulations are carried out at three distinct temperatures: specifically, 10 K, 300 K, and 600 K. The Virial theorem [Cormier et al., 2001] is employed for the stress calculations given in Equation 5.19. Utilizing the acquired stress-strain curves, the modulus of elasticity for Si NWs modeled through non-periodic tensile simulations is determined.

Table 5.3: Summary of input parameters used for modeling the tensile and bending behavior of Si NWs with unreconstructed surface state.

| Definition             | Descriptor | Values                                                                                                                                           |
|------------------------|------------|--------------------------------------------------------------------------------------------------------------------------------------------------|
| Critical Dimension     | CD         | Tensile (2, 3, 4, 5, 6, 7, 8, 9, 10 nm)<br>& Bending (2, 3, 4, 5 nm)                                                                             |
| Length to Width Ratio  | AR         | 7, 8, 9, 10, 12, 14, 16, 18, 20                                                                                                                  |
| Interatomic Potentials | POT        | Tersoff (TT3 [Tersoff, 1988] and TM [Munetoh et al., 2007]) & Stillinger-Weber (SW [Stillinger and Weber, 1985] and m-SW [Ganster et al., 2010]) |
| Temperature            | T          | 10, 300, 600 K                                                                                                                                   |
| Boundary Condition     | BC         | Tensile (Non-periodic) & Tensile (Periodic) & Bending                                                                                            |
| Surface State          | SS         | Unreconstructed and Native Oxide (Refs. [Pakzad et al., 2021, Pakzad et al., 2024, Pakzad et al., 2023b] & Section 5.6.8)                        |

*Periodic tensile simulation*

This section covers the MD methodology used to investigate the tensile behavior of Si NWs with unreconstructed surfaces while periodic B.C.s are applied along the NW. Similar to the Si NWs described in Section 5.6.10, atomistic simulations are carried out on Si NWs with  $\langle 110 \rangle$  crystal orientation ( $[110]$ - $x$   $[001]$ - $y$   $[\bar{1}10]$ - $z$ ) utilizing the LAMMPS code [Thompson et al., 2022]. In contrast to the Si NWs discussed earlier, periodic B.C.s are applied along the  $x$ -direction, while the  $y$ - and  $z$ -directions are constrained to model an infinitely long NW segment given in Figure 5.13 (c). The parameters including the CD, AR, interatomic potential, and temperature are repeated for Si NWs studied using this tensile method. The MD simulations start with an energy minimization step using the conjugate gradient method, followed by the assignment of initial velocities based on a Gaussian distribution at the specified temperature. Subsequently, dynamic equilibration at the designated temperature is carried out for 60 ps, utilizing the Nose-Hoover isobaric-isothermal (NPT) ensemble with a time step of 1 fs. Following equilibration, the simulation cell undergoes longitudinal deformation at a strain rate of  $\dot{\epsilon} = 1 \times 10^9 s^{-1}$ , which falls within the suitable range for MD-based tensile testing [Kang and Cai, 2007, Pakzad et al., 2023b], as well as for Si NWs discussed in Section 5.6.10. This ensures consistency in the examination deformation and properties of Si NWs within the scope of this study. The stress-strain curves obtained for Si NWs are utilized to determine the modulus of elasticity, employing the formulation given in Equation 5.19.

*Bending simulation*

Simulations of three-point bending are conducted on double-clamped unreconstructed Si NWs using MD method [Thompson et al., 2022]. Figure 5.13 (c) illustrates the initial atomic configurations of Si NWs, where the width is assigned between 2 nm and 5 nm. The Si NWs have a square cross-section, with the width being denoted as the representative of CD similar to Si NWs discussed in Section 5.6.10 and Section 5.6.10. For bending modeling of Si NWs, the AR, interatomic potential, and temperature assignments are repeated as given in Table 5.3. The length of support

Table 5.4: Surface stress ( $f_{11}$  and  $f_{22}$ ) and surface elastic constants ( $d_{11}$  and  $d_{22}$ ) for unreconstructed Si thin film model with (110) free surface [Zare Pakzad et al., 2023c, Pakzad et al., 2024].

| Structure                | Surface Properties(N/m) |          |          |          |
|--------------------------|-------------------------|----------|----------|----------|
|                          | $f_{11}$                | $f_{22}$ | $d_{11}$ | $d_{22}$ |
| Unreconstructed Si (110) | -1.57                   | -0.95    | +3.40    | -15.10   |

regions denoted as  $L_s$  corresponds to one-eighth of the NW length ( $L$ ) with schematic demonstration of the three-point bending given in Figure 5.13 (d). To simulate the clamped boundary condition, both support regions are constrained in all three dimensions ( $x$ ,  $y$ , and  $z$ ). The non-periodic shrink-wrapped B.C.s are implemented in the  $y$  and  $z$  directions, while periodicity is applied along the  $x$ -direction. The Si NWs undergo a relaxation process using the conjugate gradient method to reach a local minimum configuration. Subsequently, a relaxation process is performed on all NWs at a finite temperature given in Table 5.3 for 60 ps, utilizing a time step of 1 fs. This is accomplished by employing a canonical NVT ensemble with a Nose-Hoover thermostat. The  $F/w$  ratio, which is the ratio of force to deflection, can be determined by analyzing the slope of the initial linear section of the force-deflection response. This ratio is often used to estimate the modulus of elasticity through a linear approach. However, it should be noted that in the case of bending response curves for Si NWs, the displacement of the NW upon loading is expected to be larger than half of the cross-sectional size ( $CD/2$ ). As a result, the response is likely to exhibit a non-linear behavior, as observed in prior experimental and MD studies on the bending of Si NWs [Zare Pakzad et al., 2023c, Pakzad et al., 2021]. In this context, the ExtZP nanomechanical model described in Section 5.6.2 is utilized to estimate the modulus of elasticity of unreconstructed Si NWs. The surface properties for unreconstructed Si with (110) free surface including surface stresses ( $f_{11}$  and  $f_{22}$ ) and surface elastic constants ( $d_{11}$  and  $d_{22}$ ) needed for interpreting the elastic response of Si NWs are extracted from Refs. [Zare Pakzad et al., 2023c, Pakzad et al., 2024] and are given in Table 5.4.



### 5.6.11 Machine Learning

This section provides detailed information on machine learning. Specifically, Section 5.6.11 delves into the intricacies of data mining, while Section 5.6.11 addresses feature selection. Section 5.6.11 elaborates on the details of the machine learning algorithms, and Section 5.6.11 presents the results and evaluates the findings.

#### *Data Mining*

To construct the dataset necessary for training the machine learning algorithms, two primary sources of input are employed. The modeling efforts outlined in Section 5.6.10 generate tensile and bending responses for Si NWs under different parameter sets, with a specific focus on Si NWs featuring the unreconstructed surface state. In light of two distinct interatomic potentials, three designated testing temperatures, and differing Si NW CDs, coupled with nine distinct ARs modeled via different testing methods (B.C.), a comprehensive collection of 1242 Si NWs is established within this study. Additionally, data from previous research conducted by the authors on Si NWs with a native oxide surface state, as documented in relevant literature [Pakzad et al., 2021, Pakzad et al., 2024, Pakzad et al., 2023b] and Section 5.6.8, are assimilated into the overall dataset.

The Si NWs featuring a native oxide surface state exhibit variations in critical dimension, native oxide layer thickness, applied B.C.s (non-periodic tensile, periodic tensile and bending), temperature, and interatomic potentials (Tersoff-Munetoh (TM) [Munetoh et al., 2007] and modified Stillinger-Weber (m-SW) [Ganster et al., 2010]). Notably, two key distinctions arise upon integrating data from Si NWs with these distinct surface conditions. Firstly, the unreconstructed Si NWs maintain their original surface thickness without any native oxide layer, whereas the Si NWs with native oxide exhibit values that account for differing oxide layer thicknesses. Secondly, recognizing the structural deviations resulting from oxygen atom presence in Si NWs with native oxide surfaces, a consolidation is performed concerning the categorization of Tersoff and SW potentials. Consequently, TT3 and TM, as well as SW and m-SW, are grouped within the same potential family, and comparable

values are attributed during dataset preparation. In this context, the Tersoff (TT3 [Tersoff, 1988] and TM [Munetoh et al., 2007]) and Stillinger-Weber (SW [Stillinger and Weber, 1985] and m-SW [Ganster et al., 2010]) represent two distinct families of interatomic potentials within the framework of this article. With the inclusion of the dataset pertaining to Si NWs with native oxide surface states, a total of 72 additional data points are appended to this study's collection. This extension elevates the overall number of data points to 1314, each representing the modulus of elasticity of a unique Si NW.

Certainly, acquisition a substantial number of data points stands as a primary challenge in materials informatics, primarily due to the computational costs associated with acquiring materials and their corresponding target variables. Consequently, datasets frequently comprise a limited quantity of data points. Notably, to the best of our knowledge, the number of data points available for different Si NWs, specifically those investigating elasticity using MD (excluding those presented by the authors [Pakzad et al., 2021, Pakzad et al., 2024, Pakzad et al., 2023b]), is currently less than 300. In this context, every data point within the dataset encompasses six distinct features, as given in Table 5.3, along with a single target variable representing the modulus of elasticity of the Si NW. In the context of ML applications, the intrinsic nature of predictors within the dataset might necessitate preprocessing to enhance the overall performance of the ML process. Particularly, variables within a dataset may display non-normal distributions or have varying scales, both of which can adversely affect the effectiveness of ML algorithms. Therefore, prior to training, a thorough analysis of the dataset will be conducted to understand the data distribution and subsequently apply appropriate data transformation techniques. Through data transformation, the variables are normalized and scaled to ensure fair treatment by ML algorithms. In this study, a z-score normalization (standardization) approach was utilized to achieve standardized scaling and normalization of features, ensuring a mean of zero and a standard deviation of one. Section 5.6.11 will delve into the details associated with descriptors and feature selection for ML algorithms.

### *Feature Selection*

A feature selection process is conducted prior to the analysis of dataset. Within this context, six parameters outlined in Table 5.3 are identified as essential for this task. In this context, features with high correlation are omitted from the scheme, as they would redundantly convey shared information. For example, this is relevant to combinations such as strain rate and time step within the context of MD modeling of Si NWs. Despite selecting six features for this study, evaluating the correlation between these features is crucial, considering both linear and non-linear perspectives. To address potential linear correlations, the Pearson's correlation coefficient (PCC) is computed. To tackle broader correlation issues, the random forest (RF) method, well-known for its efficacy in classification and regression tasks, is also employed for feature correlation analysis. Unlike alternative feature selection methods, the RF method assigns importance scores to variables by ranking them based on their performance during model optimization. This approach allows for a comprehensive assessment of feature correlations, facilitating an enhanced interpretation of findings. Before implementing ML algorithms for data generation, the initial focus is on refining the dimensionality of the dataset by emphasizing the most relevant features. From a modeling perspective, this involves considering factors such as time step, cross-section shape, alternative testing methods like compression, and different types of interatomic potentials like the Modified Embedded Atom Method (MEAM) potential. However, while this approach could enhance the dataset, it carries the risk of introducing an excessive number of input features, potentially leading to overfitting, especially when dealing with a limited number of instances due to the potential high degree of freedom or non-linearity of the problem. Section 5.6.11 will address the specifics pertaining to ML algorithms.

### *Machine Learning Algorithms*

The analysis of the dataset and associated features using ML algorithms follows a two-step process. Initially, the Regression Learner toolbox in MATLAB is utilized to assess various ML models. By training the toolbox's available models, which

encompass Random Forest (RF), K-Nearest Neighbors (KNN), Linear Regression (LR), Decision Trees (DT), Multi-Layer Perceptron (MLP), and Support Vector Machines (SVM), the models exhibiting the most promising performance are identified. This preliminary stage facilitates the selection of appropriate models for a more in-depth exploration of ML algorithms. Within this context, ML models are leveraged, with 70% of the dataset allocated for training and 30% for validation, utilizing 10-fold cross-validation. The evaluation of ML models centers on their predictive accuracy with respect to the test dataset. Transitioning to the second stage of ML modeling, building upon the insights gained from the initial stage, various ML algorithms, namely, RF, KNN, LR, DT, MLP, and SVR, are assessed for their ability to forecast the target variable. Prior to model training, the original dataset is divided into training data, facilitating model optimization, and a test dataset employed to gauge the predictive accuracy of the model on unseen data. The evaluation of ML models is grounded in their predictive errors on the test dataset, measured by root mean squared error (RMSE), mean absolute error (MAE), and coefficient of efficiency ( $R^2$ ), as defined by Equation 5.22, Equation 5.23, and Equation 5.24, respectively. In this respect,  $y_i$  and  $\tilde{y}_i$  are true and predicted values, respectively. Also,  $\bar{y}$  is the average of the predicted values, and  $n$  is the total number of samples. All computations are executed using the scikit-learn library within the Python programming language [Pedregosa et al., 2011]. Upon identifying the most effective models, additional optimization techniques, including hyperparameter tuning, are experimented with to determine optimal configurations. These optimizations are iterated to enhance the training process and mitigate the risk of overfitting given the current training dataset.

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \tilde{y}_i)^2} \quad (5.22)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \tilde{y}_i| \quad (5.23)$$

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \tilde{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (5.24)$$

### *Machine Learning Results*

This section offers a comprehensive analysis of the outcomes obtained from applying ML models. A detailed investigation of the elasticity in Si NWs is conducted using the Python scikit-learn library. In this respect, the analysis of the dataset involves the assessment of different ML algorithms, namely RF, KNN, LR, DT, MLP, and SVR, while varying training data percentages from 30% to 90% with 10% intervals are used in this evaluation. Given the size of the dataset in this study, it is important to split the data thoughtfully, aiming for a balanced distribution in both the training and test datasets to avoid overfitting. To ensure robustness, the random assignment of the dataset for this analysis is repeated across 10 trials. The ML models are evaluated based on their prediction errors on the test dataset. Subsequently, calculations of RMSE, MAE, and  $R^2$  are performed, with their respective standard deviations presented in Figure 5.14 (a), Figure 5.14 (b), and Figure 5.14 (c), respectively. When considering RMSE as the most critical performance evaluation parameter in the context of ML algorithms, a clear distinction emerges in the errors obtained. Specifically, four models – RF, KNN, MLP, and DT – report RMSE values below 10%, while LR and SVR, which both employ linear kernels in this study, exhibit higher RMSE values. This emphasizes the non-linearity of the problem when examining the elasticity of Si NWs. Furthermore, MAE, a common measure of forecast error in time series analysis, confirms the findings from the RMSE analysis, showing a greater dependence on the training data percentage for smaller data subsets. In this context, the calculation of  $R^2$  provides an additional quantitative assessment of the observation of non-linearity. Linear models exhibit a degree of correlation of approximately 80% within the context of prediction and target values, while the remaining four models (RF, KNN, MLP, and DT) demonstrate more than a 95% coefficient of efficiency, underscoring their suitability for this task.

After the discussion on error analysis, a subsequent evaluation and discussion

of algorithms are conducted using a 30% test data percentage, aligning with the optimal error rates observed for the majority of the trained models. As illustrated in Figure 5.14 (d-i), the performance of six algorithms in predicting the modulus of elasticity of Si NWs, relative to the actual modulus of elasticity obtained via MD simulations, is presented. Given the performance discrepancies among various ML models, especially when excluding the linear models (LR and SVR) from consideration within the scope of this study, a more detailed examination of these models becomes essential. To ensure robustness and prevent overfitting, a 10-fold cross-validation approach is employed. Among these algorithms, the RF and DT models emerge as the top performers, followed by KNN and MLP. In contrast, LR and SVR with linear kernels exhibit the least favorable performance. Further analysis of the best-performing models involves hyperparameter tuning, particularly for the RF model. This fine-tuning is implemented to control the maximum depth of individual trees, mitigating the risk of overfitting, while also governing the minimum sample leaf and minimum sample split parameters. Through this process, the following hyperparameter values are determined for the RF model: a maximum depth of 10, a minimum sample leaf of 1, and a minimum sample split of 5. This optimization results in a notable improvement, with a 0.3% reduction in RMSE, a 0.2% reduction in MAE, and a 0.2% increase in R-squared ( $R^2$ ). Similarly, a detailed analysis of hyperparameters for the DT model is carried out, leading to the selection of the following values: a maximum depth of 10, a minimum sample leaf of 3, and a minimum sample split of 5. This hyperparameter tuning results in a 0.6% reduction in RMSE, a 0.1% reduction in MAE, and a significant 0.8% increase in  $R^2$ . These findings underscore the importance of hyperparameter tuning in optimizing the performance of ML models, particularly for decision tree-based algorithms like RF and DT.

Moreover, Figure 5.14 (j) presents a heatmap illustrating the PCCs among the input variables. Notably, the parameters representing dimensionality, specifically CD and AR, exhibit the highest correlation, reaching approximately 0.7. This correlation represents the strongest linear relationship among all the features. However, it is essential to acknowledge the limitations of the PCC method, as it disregards

model performance variations and overlooks non-linear relationships among variables. Consequently, reliance on importance calculations based on the RF method is regarded more reliable, as depicted in Figure 5.14 (k). Furthermore, the effectiveness of the KNN algorithm is closely tied to the hyperparameter  $K$ , which dictates the number of nearest neighbors considered from the training dataset when making predictions for a new data point. To optimize the KNN model, the  $K$  hyperparameter can undergo fine-tuning. Lower values of  $K$ , such as those close to 1, yield predictions closely mirroring patterns in the training data, reducing flexibility but potentially enhancing generalization capabilities. Conversely, higher values of  $K$  introduce more diversity in the neighbor selection process. In this context, Figure 5.14 (l) illustrates the RMSE across a range of  $K$  hyperparameter values, ranging from 1 to 20. The optimal value of  $K$  is determined as 2, corresponding to the minimum error achieved. Furthermore, the article explores the application of the bagging ensemble technique to bolster the stability and accuracy of the KNN model. The reduction in RMSE percentages for various training data percentages is depicted in Figure 5.14 (m) ( $K$ ), highlighting the advantages of this technique in enhancing model performance. Following the optimization process, the predictions for modulus of elasticity in Si NWs, considering different input parameters within the critical dimension range illustrated in Figure 5.3 (b), are carried out using the KNN model. The corresponding ML results are showcased in Fig 5.3b, with standard deviations indicating the tuning of remaining parameters, including other descriptors outlined in Table 5.3.

#### 5.6.12 Error analysis

A multiple-sample uncertainty analysis is conducted to assess the accuracy of measured parameters and their subsequent effects on the prediction of the modulus of elasticity and fracture strength for Si NWs [Moffat, 1988]. Even though individual parameter uncertainties may be insignificant, using several parameters in a calculation can result in uncertainty propagation. To account for this propagation of error, each result is described using three parameters: the overall systematic error,

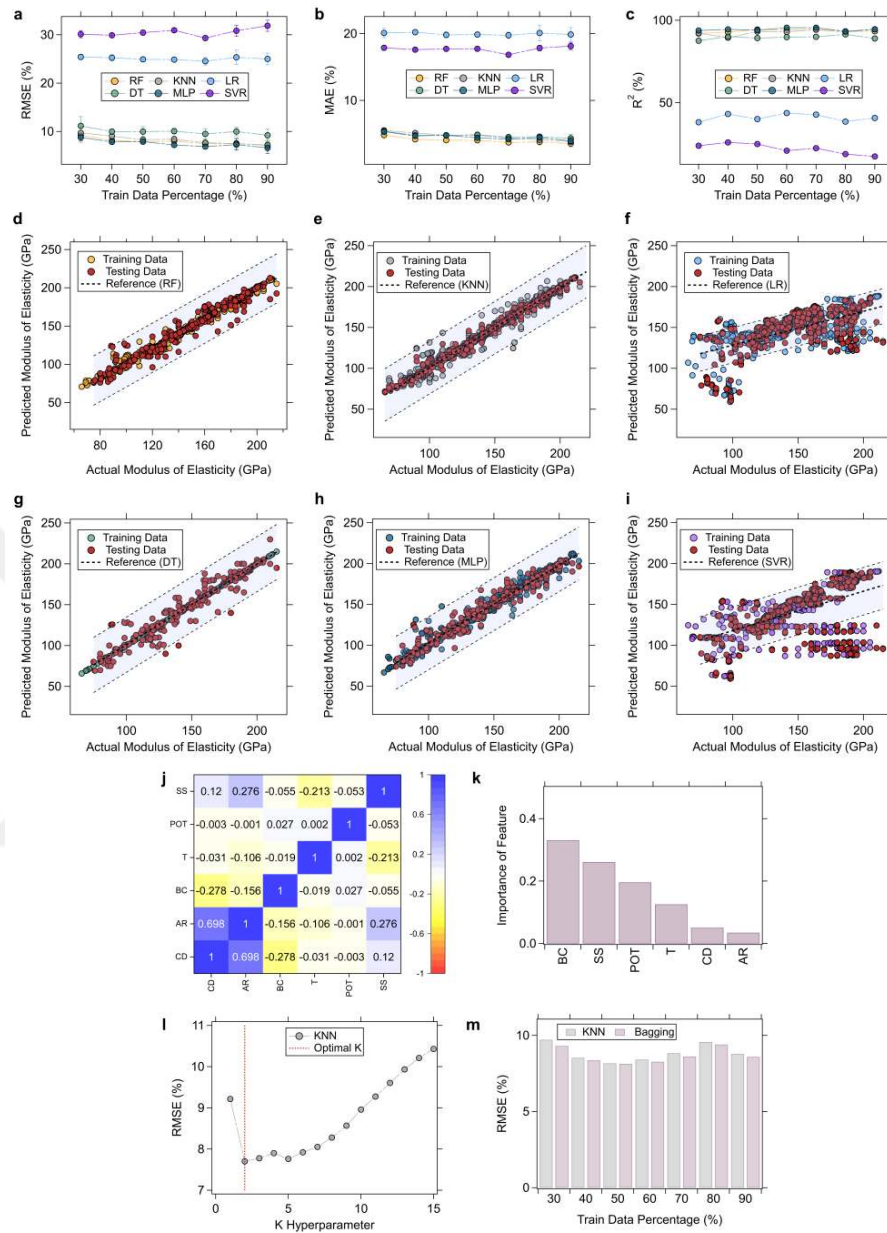


Figure 5.14: The evolution of (a) RMSE, (b) MAE, and (c)  $R^2$  on the test dataset as the proportions of the training dataset change, utilizing RF, KNN, LR, DT, MLP, and SVR algorithms. The predictive performance of (d) RF, (e) KNN, (f) LR, (g) DT, (h) MLP, and (i) SVR algorithms is assessed in relation to the actual modulus of elasticity present in the testing set. The corresponding lines of references, along with their associated standard deviations, are also presented for each model. (j) The heat map illustrates PCCs for the features discussed in Table 5.3. Elevated color intensities signify an increased correlation between the two features, with blue and red indicating negative and positive correlations, respectively. (k) The importance of input variables in terms of their performance, as determined through the RF method. (l) Illustrating the variation in RMSE as the K hyperparameter increases in the KNN algorithm. (m) Evaluating RMSE using the bagging method in comparison to the KNN algorithm.



overall random error, and overall uncertainty. The overall fixed error is determined by taking the root sum square of all residual fixed errors obtained based on analysis conducted upon bending experiment and Raman characterization. The displacement analysis in bending tests via SEM images has yielded errors of up to 6 %. The uncertainty in force calibration of bending experiments is found to be up to 10 %. The systematic errors obtained for the fabrication process is analyzed via cross-sectional HR-TEM images, with a total of 8 samples dedicated for this task. For Raman measurements, the error analysis is conducted through prediction of deviations in intrinsic stress calculations, with a total of 33 samples used. The overall random error is derived from the observed data set of multiple samples and is obtained by performing the nanomechanical estimation for modulus of elasticity and fracture strength on 10 identical Si NWs within each set given from A to G (70 Si NWs in total). The overall uncertainty is calculated as the root sum square of the fixed and random error terms, while considering the number of degrees of freedom in the data set. The calculations for overall systematic and random errors for elastic properties and strength of Si NWs are given in Figure 5.3 (c) and Figure 5.4 (c) of the Article, respectively.

### 5.6.13 References Details

The mapping of the reference work, from which the modulus of elasticity data are obtained, is depicted in Figure 5.1 (a) of the manuscript. The reference articles are provided in the following order: [Li et al., 2003, Zhang et al., 2016, Tsuchiya et al., 2018, Sundararajan et al., 2002, Wollschläger et al., 2016, Sadeghian et al., 2009, Namazu et al., 2000, Zhu et al., 2009]. The specific color coding corresponding to each reference is indicated in Figure 5.15.

The mapping of the reference work, from which the fracture strength data are obtained, is depicted in Figure 5.1 (b) of the manuscript. The reference articles are provided in the following order: [Namazu et al., 2000, Sundararajan et al., 2002, Bernal et al., 2014, Alan et al., 2006a, Alan et al., 2006b, Fujii et al., 2013, Wilson et al., 1996, Passi et al., 2012, Johansson et al., 1988, Jarzabek et al., 2014, Arkan

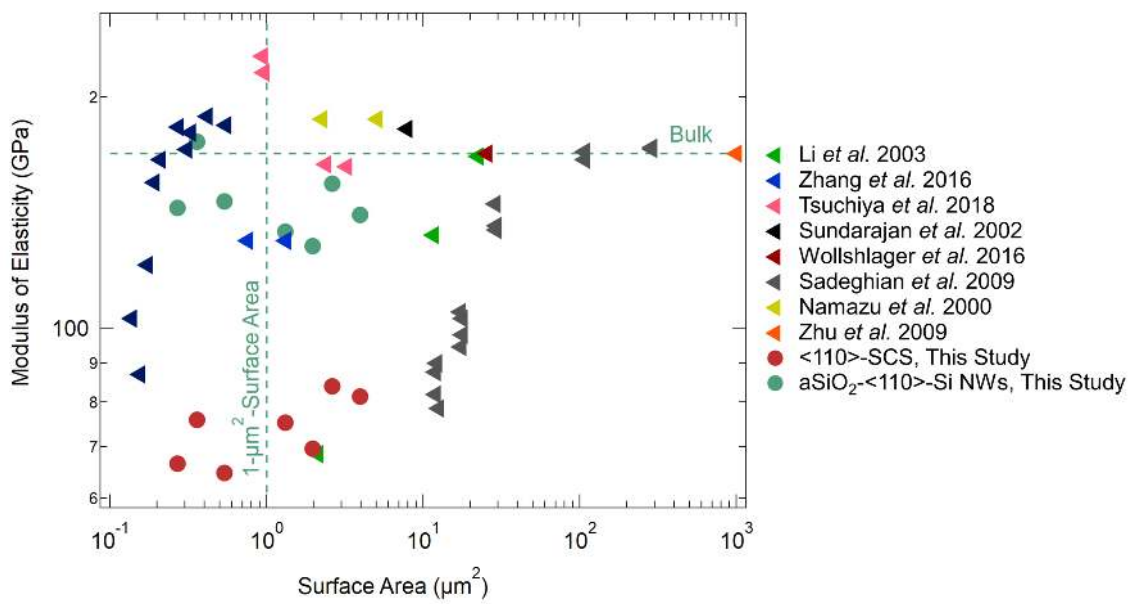


Figure 5.15: The mapping of the reference work, from which the modulus of elasticity data are obtained, is illustrated in Figure 5.1 (a) of the manuscript. The associated reference articles are listed in the following order: [Li *et al.*, 2003, Zhang *et al.*, 2016, Tsuchiya *et al.*, 2018, Sundararajan *et al.*, 2002, Wollschläger *et al.*, 2016, Sadeghian *et al.*, 2009, Namazu *et al.*, 2000, Zhu *et al.*, 2009]. The corresponding color coding for each reference is indicated in Figure 5.15.

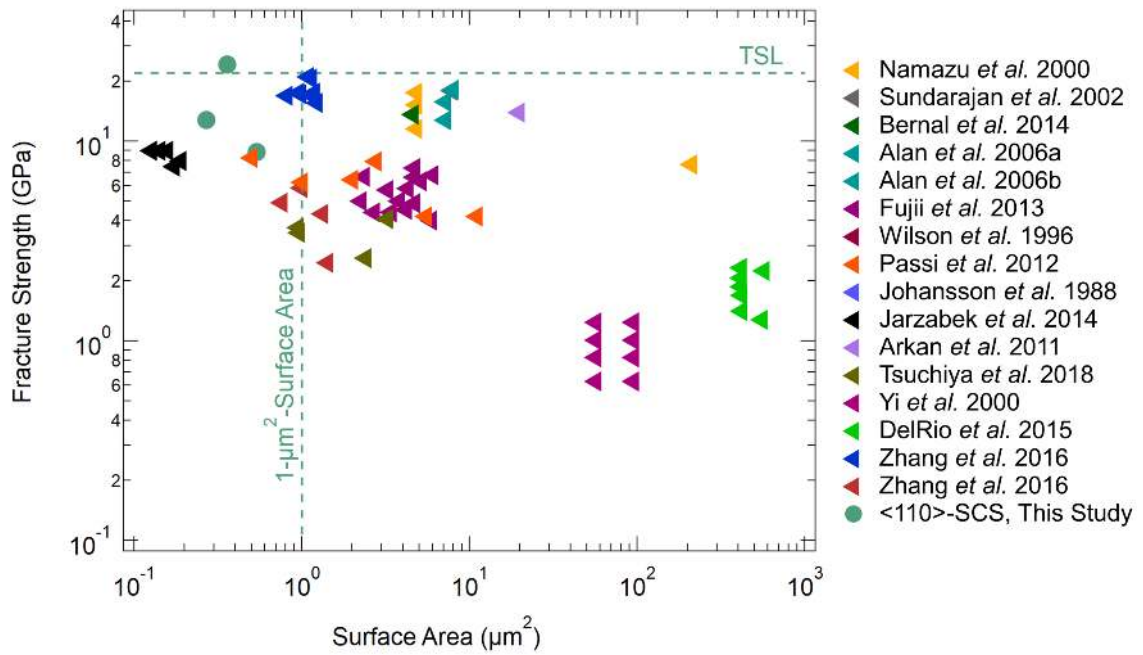


Figure 5.16: The mapping of reference works, from which the fracture strength data are derived, is illustrated in Figure 5.1 (b) of the manuscript. The reference articles are provided in the following order: [Namazu et al., 2000, Sundararajan et al., 2002, Bernal et al., 2014, Alan et al., 2006a, Alan et al., 2006b, Fujii et al., 2013, Wilson et al., 1996, Passi et al., 2012, Johansson et al., 1988, Jarzabek et al., 2014, Arkan et al., 2011, Tsuchiya et al., 2018, Yi et al., 2000, DelRio et al., 2015, Zhang et al., 2016]. The specific color coding for each reference is indicated in Figure 5.16.

et al., 2011, Tsuchiya et al., 2018, Yi et al., 2000, DelRio et al., 2015, Zhang et al., 2016]. The specific color coding corresponding to each reference is indicated in Figure 5.16.

The mapping of the reference work, from which the modulus of elasticity data via MD method are obtained, is depicted in Figure 5.3 of the manuscript. The reference articles are provided in the following order: [Kang and Cai, 2007, Kang and Cai, 2010, Jing et al., 2009a, Jing et al., 2009b, Jing and Meng, 2010a, Xu and Kim, 2019, Xu and Kim, 2020, Park et al., 2005, Liu and Shen, 2012, Liu et al., 2015]. The specific color coding corresponding to each reference is indicated in Figure 5.17. The literature domain for experimental references are covered previously in Figure 5.15.

The mapping of the reference work, from which the fracture strength data are

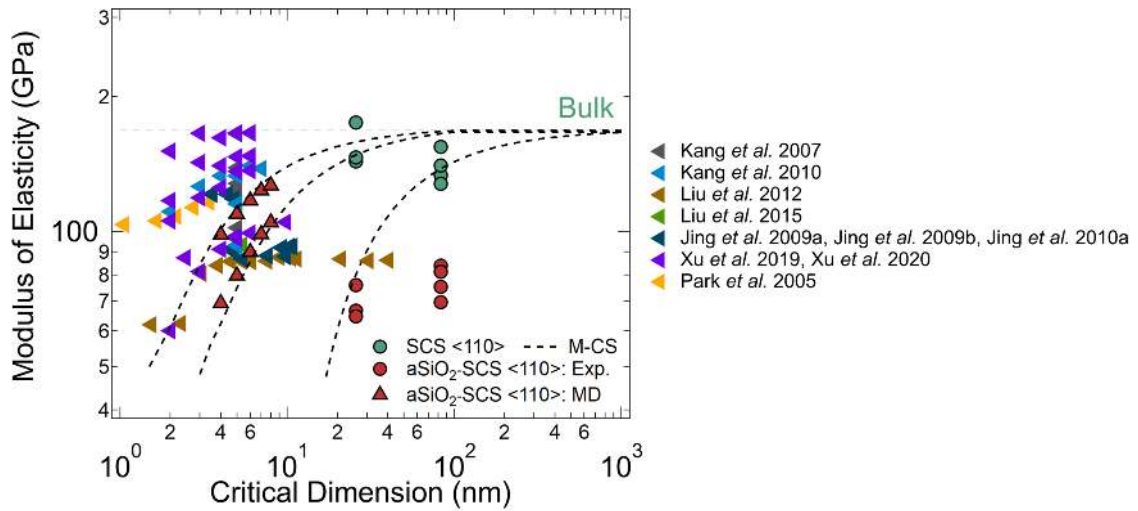


Figure 5.17: Figure 5.17 illustrates the mapping of reference works contributing to the modulus of elasticity data obtained via the MD method. The provided reference articles are listed in the following order: [Kang and Cai, 2007, Kang and Cai, 2010, Jing et al., 2009a, Jing et al., 2009b, Jing and Meng, 2010a, Xu and Kim, 2019, Xu and Kim, 2020, Park et al., 2005, Liu and Shen, 2012, Liu et al., 2015].

obtained, is depicted in Figure 5.4 (a) of the manuscript. The reference articles are provided in the following order as i) grown: [DelRio et al., 2015, Zhu et al., 2009, Gordon et al., 2009, Zhang et al., 2010a, Zhang et al., 2016, Kim et al., 2011, Hoffmann et al., 2006, Tang et al., 2012, Stan et al., 2012b, Stan et al., 2012a, Steighner et al., 2011, Wagesreither et al., 2014, Kushima et al., 2012, Passi et al., 2012, Tabib-Azar et al., 2005], ii) wet etch: [DelRio et al., 2015, Yi et al., 2000, Sato et al., 1998] given in Figure 5.17 (a) and iii) dry etch: [DelRio et al., 2015, Zhang et al., 2016, Tsuchiya et al., 2018, Arkan et al., 2011, Jarzabek et al., 2014, Sundararajan et al., 2002, Namazu et al., 2000, Wilson et al., 1996, Bernal et al., 2014, Alan et al., 2006a, Alan et al., 2006b, Fujii et al., 2013, Johansson et al., 1988], and iv) mechanical: [DelRio et al., 2015, Tsuchiya et al., 2001] given in Figure 5.18 (b). The specific color coding corresponding to each fabrication technology is indicated in Figure 5.17 (a) and Figure 5.18 (b). For more comprehensive insights into the fracture strength of SCS, readers are advised to consult additional sources or pertinent literature on the subject [Cook, 2006, DelRio et al., 2022, Namazu, 2023].

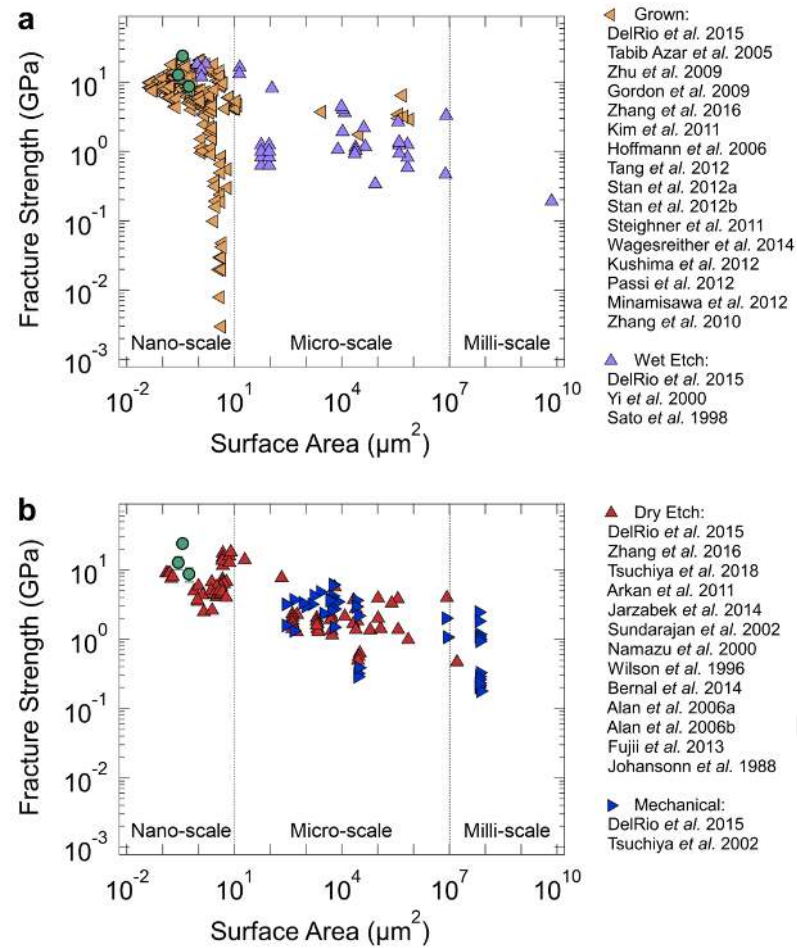


Figure 5.18: Mapping of reference works contributing to fracture strength data is presented in Figure 5.4. (a) The provided references are categorized based on fabrication methods: (i) grown: [DelRio *et al.*, 2015, Zhu *et al.*, 2009, Gordon *et al.*, 2009, Zhang *et al.*, 2010a, Zhang *et al.*, 2016, Kim *et al.*, 2011, Hoffmann *et al.*, 2006, Tang *et al.*, 2012, Stan *et al.*, 2012b, Stan *et al.*, 2012a, Steighner *et al.*, 2011, Wagesreither *et al.*, 2014, Kushima *et al.*, 2012, Passi *et al.*, 2012, Tabib-Azar *et al.*, 2005], and (ii) wet etch: [DelRio *et al.*, 2015, Yi *et al.*, 2000, Sato *et al.*, 1998]. (b) The provided references are categorized based on fabrication methods: (iii) dry etch: [DelRio *et al.*, 2015, Zhang *et al.*, 2016, Tsuchiya *et al.*, 2018, Arkan *et al.*, 2011, Jarzabek *et al.*, 2014, Sundararajan *et al.*, 2002, Namazu *et al.*, 2000, Wilson *et al.*, 1996, Bernal *et al.*, 2014, Alan *et al.*, 2006a, Alan *et al.*, 2006b, Fujii *et al.*, 2013, Johansson *et al.*, 1988], and (iv) mechanical: [DelRio *et al.*, 2015, Tsuchiya *et al.*, 2001].

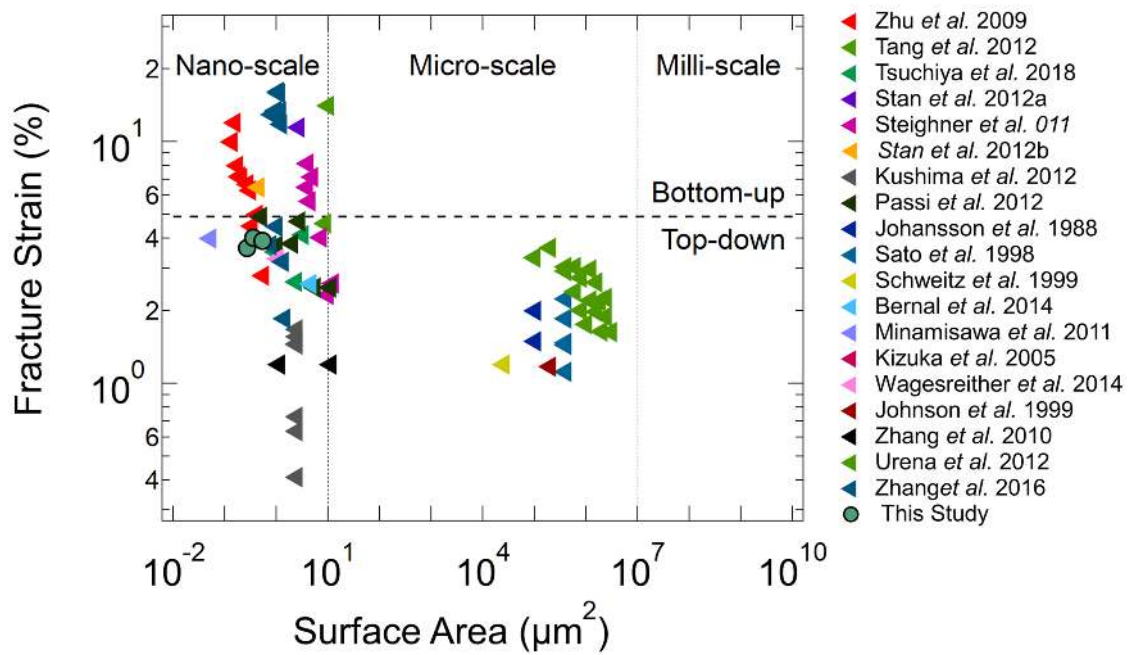


Figure 5.19: The mapping of reference works contributing to the fracture strain data is illustrated in Figure 5.4 (b) of the Article. The provided references are arranged in the following order: [Zhu et al., 2009, Tang et al., 2012, Tsuchiya et al., 2018, Stan et al., 2012a, Stan et al., 2012b, Steighner et al., 2011, Kushima et al., 2012, Passi et al., 2012, Johansson et al., 1988, Sato et al., 1998, Bernal et al., 2014, Minamisawa et al., 2012, Kizuka et al., 2005, Zhang et al., 2016, Zhang et al., 2010a, Johnson et al., 1999, Urena et al., 2012, Schweitz and Ericson, 1999, Wagesreither et al., 2014]. The specific color coding corresponding to each reference is indicated here.

The mapping of the reference work, from which the fracture strain data are obtained, is depicted in Figure 5.4 (b) of the Article. The reference articles are provided in the following order: [Zhu et al., 2009, Tang et al., 2012, Tsuchiya et al., 2018, Stan et al., 2012a, Stan et al., 2012b, Steighner et al., 2011, Kushima et al., 2012, Passi et al., 2012, Johansson et al., 1988, Sato et al., 1998, Bernal et al., 2014, Minamisawa et al., 2012, Kizuka et al., 2005, Zhang et al., 2016, Zhang et al., 2010a, Johnson et al., 1999, Urena et al., 2012, Schweitz and Ericson, 1999, Wagesreither et al., 2014]. The specific color coding corresponding to each reference is indicated in Figure 5.19.

The mapping of the reference work, from which the modulus of elasticity data are obtained for different orientations of Si, is depicted in Figure 5.20. The reference



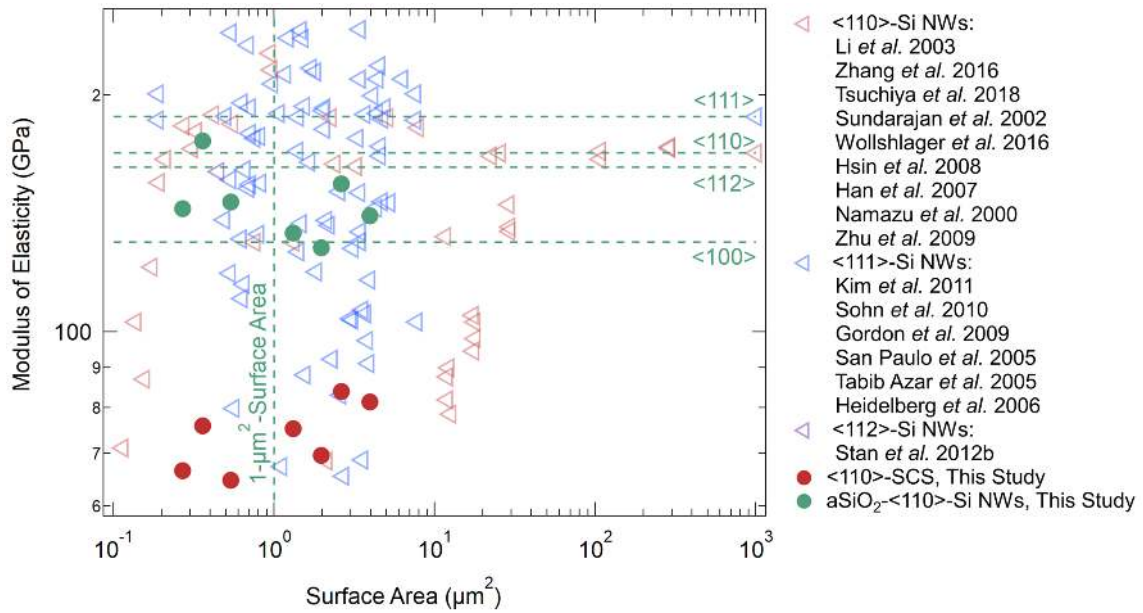


Figure 5.20: The mapping of reference works, from which modulus of elasticity data are obtained for different orientations of Si, is depicted. The reference articles are provided in the following order: < 110>-Si NWs [Li et al., 2003, Zhang et al., 2016, Tsuchiya et al., 2018, Sundararajan et al., 2002, Wollschläger et al., 2016, Hsin et al., 2008, Han et al., 2007, Namazu et al., 2000, Zhu et al., 2009], < 111>-Si NWs [Kim et al., 2011, Sohn et al., 2010, Gordon et al., 2009, Tabib-Azar et al., 2005, San Paulo et al., 2005, Heidelberg et al., 2006], and < 112>-Si NWs [Stan et al., 2012b].

articles are provided in the following order: < 110>-Si NWs: [Li et al., 2003, Zhang et al., 2016, Tsuchiya et al., 2018, Sundararajan et al., 2002, Wollschläger et al., 2016, Hsin et al., 2008, Han et al., 2007, Namazu et al., 2000, Zhu et al., 2009], < 111>-Si NWs: [Kim et al., 2011, Sohn et al., 2010, Gordon et al., 2009, Tabib-Azar et al., 2005, San Paulo et al., 2005, Heidelberg et al., 2006], and < 112>-Si NWs: [Stan et al., 2012b]. For further information regarding the modulus of elasticity of SCS and Si NWs, we would recommend referring to other sources or literature available on this topic [Yang et al., 2022, Wang et al., 2017, Nasr Esfahani and Alaca, 2019, Park et al., 2009, Furmanchuk et al., 2012].

The mapping of the reference work, from which the fracture strength data are obtained for different orientations of Si, is depicted in Figure 5.21 with an extended range of surface area compared to Figure 5.1 (b). The reference articles are provided

in the following order: [Namazu et al., 2000, Sundararajan et al., 2002, Bernal et al., 2014, Alan et al., 2006a, Alan et al., 2006b, Fujii et al., 2013, Wilson et al., 1996, Passi et al., 2012, Johansson et al., 1988, Jarzabek et al., 2014, Arkan et al., 2011, Tsuchiya et al., 2018, Yi et al., 2000, Kim et al., 2011, Zhu et al., 2009, Hoffmann et al., 2006, Tang et al., 2012, Gordon et al., 2009, Stan et al., 2012b, Stan et al., 2012a, Kizuka et al., 2005, Steighner et al., 2011, Tabib-Azar et al., 2005, Wilson et al., 1996, Schweitz and Ericson, 1999, Minamisawa et al., 2012, Sato et al., 1998, Kushima et al., 2012, Johnson et al., 1999, Zhang et al., 2010a, Tsuchiya et al., 2001, Wagesreither et al., 2014, Urena et al., 2012, DelRio et al., 2015, Zhang et al., 2016, DelRio et al., 2016, Li et al., 2005].



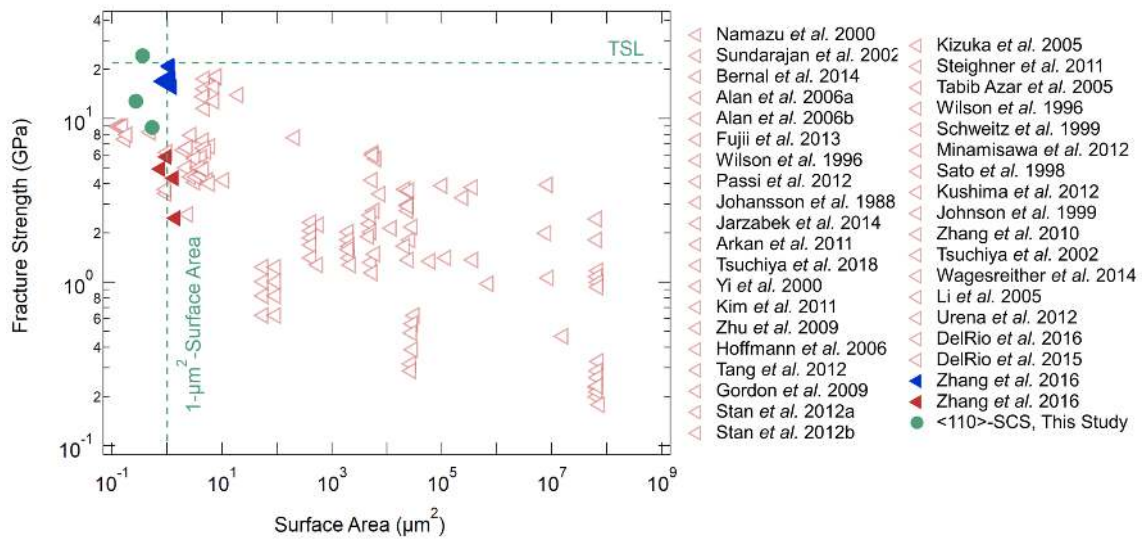


Figure 5.21: The mapping of reference works, from which fracture strength data are obtained for different orientations of Si, is presented with an extended range of surface area compared to Figure 5.1 (b). The reference articles are provided in the following order: [Namazu et al., 2000, Sundararajan et al., 2002, Bernal et al., 2014, Alan et al., 2006a, Alan et al., 2006b, Fujii et al., 2013, Wilson et al., 1996, Passi et al., 2012, Johansson et al., 1988, Jarzabek et al., 2014, Arkan et al., 2011, Tsuchiya et al., 2018, Yi et al., 2000, Kim et al., 2011, Zhu et al., 2009, Hoffmann et al., 2006, Tang et al., 2012, Gordon et al., 2009, Stan et al., 2012b, Stan et al., 2012a, Kizuka et al., 2005, Steighner et al., 2011, Tabib-Azar et al., 2005, Wilson et al., 1996, Schweitz and Ericson, 1999, Minamisawa et al., 2012, Sato et al., 1998, Kushima et al., 2012, Johnson et al., 1999, Zhang et al., 2010a, Tsuchiya et al., 2001, Wagesreither et al., 2014, Urena et al., 2012, DelRio et al., 2015, Zhang et al., 2016, DelRio et al., 2016, Li et al., 2005].

## Chapter 6

# INVESTIGATION OF THE BENDING BEHAVIOR IN SILICON NANOWIRES: A NANOMECHANICAL MODELING PERSPECTIVE

### **6.1 Overview**

Nanowires play a pivotal role across a spectrum of disciplines such as nanoelectromechanical systems, nanoelectronics, and energy applications. As nanowires continue to diminish in dimensions, their mechanical characteristics are increasingly influenced by surface attributes. This research delves into the elastic properties of silicon nanowires, which vary in dimensions and crystal orientations, employing diverse nanomechanical models. Through molecular dynamics simulations and the application of five models namely, Heidelberg, Hudson, Zhan, SimpZP, and ExtZP, the analysis of force-deflection responses reveals the intricate interplay among elastic properties, crystal orientation, and the chosen model. To accurately account for unreconstructed states, surface properties are examined for different silicon surface orientations. Each crystal orientation exhibits distinct trends, with surface properties showing a substantial influence on estimated elasticity. A thorough grasp of surface effects and anisotropic properties is crucial for unraveling nanowire mechanics. This study drives both the understanding of size-dependent behaviors and the enhancement of insights into nanoscale surface characteristics of silicon nanowires.

### **6.2 Introduction**

Nanowires (NWs) hold great promise as fundamental components for advancing future nanoelectromechanical systems [Bachtold et al., 2022], nanoelectronics [Li et al., 2023, Zhang et al., 2021], with notable applications in highly sensitive sen-

sors [Karimzadehkhoei et al., 2023, Akbari-Saatlu et al., 2020, Maita et al., 2023] and cutting-edge energy technologies [Panda et al., 2022]. The remarkable advancements in fabrication methods [Wang et al., 2016a, Liang et al., 2023], technological applicability [Alaca and Karimzadehkhoei, 2023], and multi-scale modeling techniques [Momeni et al., 2020, Zare Pakzad et al., 2023c] have sparked great interest in the extensive characterization of NWs. The miniaturization of NWs leads to a significant increase in the ratio of surface area to volume giving rise to remarkable physical properties distinguishing them from bulk structures [Nasr Esfahani and Alaca, 2019, Wang et al., 2017, Huang et al., 2023]. In this context, the surface properties of NWs assume a notably significant role and are regarded as pivotal factors that influence their mechanical attributes [Müller and Saúl, 2004, Zare Pakzad et al., 2023c, Pakzad et al., 2023b]. Furthermore, intrinsic effects such as the stresses generated in NWs during fabrication, assembly, and surface interactions are recognized as dominant parameters that have significant effects on the performance and properties of NWs [Zare Pakzad et al., 2023c, Nasr Esfahani et al., 2022, Fedorov et al., 2019, Li et al., 2021, Ureña et al., 2013, Yokogawa et al., 2017, Lorenzoni et al., 2016, Dolabella et al., 2020, Spejo et al., 2020]. Nanomechanical modeling techniques are developed as a means to interpret the behavior of NWs at the nanoscale. The classical surface elasticity theory proposed by Gurtin and Murdoch [Gurtin and Ian Murdoch, 1975] has found extensive application in studying the size-dependent mechanical properties of NWs. As dimensions are further scaled down, various surface models are incorporated into nanomechanical modeling approaches in an attempt to elucidate the deformation behavior at the nanoscale regime [He and Lilley, 2008, Song et al., 2011, Chen et al., 2006b]. In this regard, different formulations of the Young-Laplace model (YL) have been utilized in numerous studies to interpret the properties of NWs. These include the original formulation of YL [Chen et al., 2006b], the modified YL [He and Lilley, 2008, Zare Pakzad et al., 2021], and the extended YL [Song et al., 2011, Zare Pakzad et al., 2023c]. Furthermore, various core-shell models have been developed as structural frameworks that comprise a core with the modulus of the bulk material and a surface shell [Yao et al.,

2012, Xu et al., 2016, Xiao et al., 2022]. These models are utilized to interpret and analyze the impact of surface properties on the overall behavior of the NWs [Li et al., 2022, Miller and Shenoy, 2000, Pakzad et al., 2023b].

Silicon (Si) NWs have been extensively investigated as fundamental components in semiconductor manufacturing due to their unique properties [Nasr Esfahani and Alaca, 2019, Wang et al., 2017, Ye et al., 2019]. Despite numerous studies on the size-dependent mechanical properties of Si NWs, conflicting reports have led to the need for a more detailed examination of the scale effect [Zare Pakzad et al., 2023c, Pakzad et al., 2023b, Yang et al., 2022]. Specifically, the size-dependent modulus of elasticity of Si NWs has been addressed using various computational and experimental methods, resulting in discrepancies regarding the scale effect [Nasr Esfahani and Alaca, 2019, Yang et al., 2022, Nasr Esfahani and Alaca, 2019]. The importance of nanomechanical model selection is highlighted in a recent study, where deviations of up to 85 GPa are attributed to the specific choice of the model [Zare Pakzad et al., 2023c]. Considering the challenges in fabrication, testing, and characterization, modeling remains a critical step in the successful interpretation of results [Zare Pakzad et al., 2021, Zare Pakzad et al., 2023c]. The use of bending experiments, aided by advancements in testing methods and *in-situ* approaches, has gained significant importance in revealing the properties of Si NWs [Espinosa et al., 2013]. Within this framework, the development of nanomechanical models that account for large deflections observed in Si NWs has been ongoing [Heidelberg et al., 2006, Ngo et al., 2006, Zare Pakzad et al., 2023c, Zare Pakzad et al., 2021]. Previous nanomechanical models, such as those proposed by Heidelberg *et al.* [Heidelberg et al., 2006] for large deflection due to axial extension, extended with initial tension effects by Hudson *et al.* [Hudson et al., 2013], incorporating surface effects based on modified YL model by Zhan *et al.* [Zhan and Gu, 2012], and combined effects by Zare Pakzad *et al.* [Zare Pakzad et al., 2021], make this research area particularly intriguing for further exploration. Introducing the ExtZP model [Zare Pakzad et al., 2023c], the recent multi-scale approach presents a comprehensive formulation that accounts for large deflections, incorporates anisotropic surface properties using the extended YL

model, and considers intrinsic terms encompassing effects arising from surface and initial tension conditions. Moreover, the modeling of the surface properties goes beyond mathematical formulation and also requires an examination of surface state and orientation-dependent properties, such as surface stress and surface elasticity constants. Moreover, recent studies by Zare Pakzad *et al.* [Zare Pakzad et al., 2023c, Pakzad et al., 2021] propose a reliable approach to compare unreconstructed and native oxide surface states for (100)- and (110)-Si surfaces. As surface effects continue to gain significance, molecular dynamics (MD) and density functional theory (DFT) simulations are playing vital roles in revealing the size-dependent trends in the elastic properties of Si NWs [Pakzad et al., 2023b, Pakzad et al., 2021, Lee and Rudd, 2007, Pakzad et al., 2024]. In line with this, MD simulations are used to subject Si NWs to tensile [Xu and Kim, 2019, Kang and Cai, 2007, Pakzad et al., 2023b, Pakzad et al., 2024], vibrational [Kim et al., 2006, Park et al., 2005], and bending tests [Zhuo and Beom, 2018, Ilinov and Kuronen, 2014], providing valuable insights into their mechanical properties.

The objective of this study is to explore the elastic properties of Si NWs through the application of nanomechanical modeling, considering different critical dimensions and crystallographic orientations [Heidelberg et al., 2006, Hudson et al., 2013, Zhan and Gu, 2012, Zare Pakzad et al., 2021, Zare Pakzad et al., 2023c]. The models are utilized to interpret the large deflection bending deformations observed in three-point bending tests, allowing for the acquisition and comparison of the modulus of elasticity of Si NWs. The surface properties of Si thin films with different crystal orientations at their free surface are calculated. Furthermore, the calculated intrinsic stresses generated in Si NWs are determined. These results are utilized to comprehensively examine and compare the effectiveness of various nanomechanical models. The study establishes a multi-scale framework for developing a strategy to investigate the size-dependency of Si NW properties, particularly considering unreconstructed surface states. Through this work, valuable insights into the surface characteristics of Si NWs are provided, contributing to an improved understanding of their mechanical properties at the nanoscale.

### 6.3 Methods and Materials

This section encompasses four segments, which focus on the methods used to interpret the selection of nanomechanical models and their effects on the calculated elastic responses of Si NWs. These include the analytical constitution of the models, formulations for effective bending rigidity, three-point bending simulations of Si NWs using MD, and atomistic simulations of surface properties. The methods are utilized to interpret the elastic response of Si NWs with varying sizes and crystal orientations through different nanomechanical models. The order in which these methods are described is as follows: Section 6.3.1 provides details about the existing nanomechanical models employed to interpret the bending response in NWs. Section 6.3.2 discusses the integration of effective modulus of elasticity definitions into the models, along with their respective formulations that incorporate surface analogy, elucidating the bending rigidity details. Section 6.3.3 delves into the bending simulations performed on Si NWs via MD method. Finally, Section 6.3.4 presents the atomistic method employed to calculate surface properties (surface stress and surface elasticity constants) for different orientations of unreconstructed Si film.

#### 6.3.1 Nanomechanical Models

The section begins by introducing the Heidelberg model, which represents the most general version of large deflection models utilized in the interpretation of bending deformations in NWs [Heidelberg et al., 2006]. Following that, Section 6.3.1 introduces an extended version of the Heidelberg model called the Hudson model [Hudson et al., 2013], which incorporates intrinsic stress induced by initial tension/compression. In Section 6.3.1, Zhan *et al.*'s modification of the Heidelberg model [Zhan and Gu, 2012] is discussed, including the modified YL surface model to incorporate surface properties. Section 6.3.1 explains the large deflection model proposed by Zare Pakzad *et al.* [Zare Pakzad et al., 2021], referred to as SimpZP. This model incorporates both intrinsic stress induced by initial tension/compression and the modified YL surface model. Finally, in Section 6.3.1, a recently developed nanomechanical model, known

as the ExtZP model [Zare Pakzad et al., 2023c], is presented. It integrates the extended YL model and intrinsic stresses induced by both surface effects and initial tension/compression. These nanomechanical models enable the prediction of the modulus of elasticity ( $E$ ) for Si NWs by employing different sets of parameters as inputs. Figure 6.1 (a) provides an overview, schematically illustrating the effective parameters associated with each model, including large deflection, intrinsic stress, and surface properties.

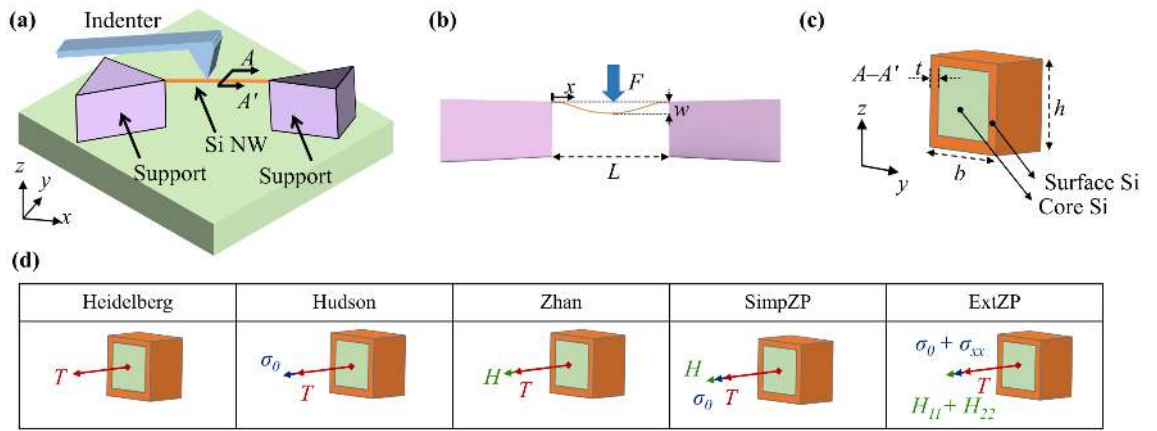


Figure 6.1: (a) Schematic representation of Si NW, clamped by support regions and subjected to the force applied by an indenter. (b) Schematic of a NW of length  $L$  under bending test with applied load  $F$ , and subsequent deformation  $w$  at its center. (c) Cross-sectional representation of the NW with associated height ( $h$ ), width ( $b$ ), and surface layer thickness ( $t$ ). (d) Effective terms of different nanomechanical models are given here.

### Heidelberg Model

The Heidelberg model presents the most general method for interpreting the bending behavior of Si NWs when subjected to large deformation during a three-point bending test. The governing equation for a NW of length  $L$  and of rectangular cross section loaded at its midsection by a point load  $F$  (Figure 6.1 (a)) is given in Equation 6.1.

$$EI \frac{\partial^4 w}{\partial x^4} - T \frac{\partial^2 w}{\partial x^2} = \frac{F}{2} \left( -\delta(x) + 2\delta\left(x - \frac{L}{2}\right) - \delta(x - L) \right) \quad (6.1)$$

In Equation 6.1,  $w$  represents the transversal displacement in the  $z$ -direction,  $x$  denotes the longitudinal axis of the beam,  $I$  represents the moment of inertia,  $T$  signifies the overall tension along the NW, and  $\delta$  is the Dirac delta function, as depicted in Figure 6.1 (b). The first term in Equation 6.1 arises from the bending of the beam, while the second term is associated with the stretching along the axial direction of the beam, often referred to as large deflection in nanomechanics. The axial tension term can be expressed as Equation 6.2.

$$T = \frac{EA}{2L} \int_0^L \left( \frac{\partial w}{\partial x} \right)^2 dx \quad (6.2)$$

By integrating Equation 6.1 and Equation 6.2 with respect to  $x$ , and taking into account the usual clamped boundary conditions (B.C.s) at both ends of the NW, as well as the cross-sectional area denoted as  $A$ , Equation 6.3 is obtained.

$$F = \frac{192EI}{L^3} w\left(\frac{L}{2}\right) f(\alpha) \quad (6.3)$$

Equation 6.3 is commonly known as the linear beam deflection approximation, with the relationship  $f(\alpha) = 1$ . However, when a precise solution method is employed, the function  $f(\alpha)$  yields Equation 6.4.

$$f(\alpha) = \frac{\alpha}{48 - \frac{192 \tanh(\sqrt{\alpha}/4)}{\sqrt{\alpha}}} \quad (6.4)$$

The value of  $\alpha$ , which is connected to the maximum deflection through Equation 6.5 is utilized to calculate  $f(\alpha)$  in order to predict the modulus of elasticity of Si NWs using Heidelberg model.

$$\begin{aligned} & \left( \frac{\alpha \cosh^2(\frac{\sqrt{\alpha}}{4})}{2 + \cosh(\frac{\sqrt{\alpha}}{2}) - 6 \frac{\sinh(\frac{\sqrt{\alpha}}{2})}{\sqrt{\alpha}}} \right) \left( 1 - 4 \frac{\tanh(\sqrt{\alpha}/4)}{\sqrt{\alpha}} \right)^2 \\ & = \Delta Z_{center}^2 \left( \frac{E}{I} \right) \end{aligned} \quad (6.5)$$



### Hudson Model

According to the Hudson model [Hudson et al., 2013], in order to analytically include residual stresses resulting from initial tension/compression into the Heidelberg model, it is essential to incorporate the term  $T_0$ , which represents the initial axial force along the NW. This term is added to Equation 6.2 with an updated formulation provided in Equation 6.6. The Hudson model utilizes a governing equation that is similar to the Heidelberg model, thereby allowing it to account for the effects of embedded initial stresses.

$$T = T_0 + \frac{EA}{2L} \int_0^L \left( \frac{\partial w}{\partial x} \right)^2 dx \quad (6.6)$$

The presence of the term  $T_0$  in the formulation signifies the residual term that is embedded within the NW, arising from fabrication or assembly-induced stresses. By solving Equation 6.1 and Equation 6.6 according to the Hudson model, the exact analytical solution provided in Equation 6.7 is derived.

$$\begin{aligned} \left(1 - \frac{L^2 T_0}{\alpha EI}\right) \left(\frac{EA}{T_0 + EA}\right) \left(\frac{\alpha \cosh^2\left(\frac{\sqrt{\alpha}}{4}\right)}{2 + \cosh\left(\frac{\sqrt{\alpha}}{2}\right) - 6 \frac{\sinh\left(\frac{\sqrt{\alpha}}{2}\right)}{\sqrt{\alpha}}}\right) \\ \left(1 - 4 \frac{\tanh(\sqrt{\alpha}/4)}{\sqrt{\alpha}}\right)^2 = \Delta Z_{center}^2 \left(\frac{E}{I}\right) \end{aligned} \quad (6.7)$$

It is worth mentioning that an approximate version of Hudson's model is proposed by Yaish *et al.* [Yaish et al., 2015], where the function  $f(\alpha)$  is approximated as Equation 6.8.

$$f(\alpha) = 1 + 2.412 \times 10^{-2} \alpha - 1.407 \times 10^{-6} \alpha^2 \quad (6.8)$$

### Zhan Model

The Zhan model [Zhan and Gu, 2012], which incorporates a surface model based on the modified YL equation, introduces updates to the formulation of the Heidelberg model. These updates are reflected as surface stress and surface elasticity

constant given in Equation 6.9. As the analytical bending formulation incorporates the surface model, the concept of the effective modulus of elasticity, represented as  $E^*$ , becomes necessary. Consequently, all formulations utilizing surface embedded models consider both the effective modulus of elasticity and the effective moment of inertia ( $I^*$ ). Subsequently, this article will delve into the specifics of the bending rigidity formulation for determining the modulus of elasticity of Si NWs Section 6.3.2. Equation 6.9 shows the governing equation provided by Zhan model.

$$(EI)^* \frac{\partial^4 w}{\partial x^4} - T \frac{\partial^2 w}{\partial x^2} - H \frac{\partial^2 w}{\partial x^2} = \frac{F}{2} \left( -\delta(x) + 2\delta\left(x - \frac{L}{2}\right) - \delta(x - L) \right) \quad (6.9)$$

In Equation 6.9,  $H$  represents the surface parameter that incorporates the surface stress,  $f_{11}$ , and the surface elasticity constant,  $d_{11}$  with detailed form given in Equation 6.10.

$$H = 2hd_{11}\epsilon_x + 2f_{11}h \quad (6.10)$$

In Equation 6.10,  $h$  represents the thickness of the NW, and  $\epsilon_x$  denotes the axial strain. By solving Equation 6.9, following a similar approach as the previous models, the solution given in Equation 6.11 is obtained.

$$\left(1 - \frac{2f_{11}hL^2}{\alpha(EI)^*}\right) \left( \frac{\alpha \cosh^2\left(\frac{\sqrt{\alpha}}{4}\right)}{2 + \cosh\left(\frac{\sqrt{\alpha}}{2}\right) - 6\frac{\sinh\left(\frac{\sqrt{\alpha}}{2}\right)}{\sqrt{\alpha}}} \right) \left(1 - 4\frac{\tanh(\sqrt{\alpha}/4)}{\sqrt{\alpha}}\right)^2 = \Delta Z_{center}^2 \left( \frac{(EA)^* + 2d_{11}h}{(EI)^*} \right) \quad (6.11)$$

In this regard,  $E^*$  for the Si NW is derived by numerically solving Equation 6.11. The bending rigidity associated with the modified YL model is utilized to predict the modulus of elasticity of the Si NW. Section 6.3.2 will elaborate on the precise formulation concerning the bending rigidity aligned with Zhan model.

### SimpZP Model

The SimpZP model [Zare Pakzad et al., 2021] incorporates both fabrication induced residual stress,  $\sigma_0$ , and surface effects,  $H$ , via modified YL formulation. In this context, this model leverages the governing terms outlined in Equation 6.12, wherein Equation 6.6 replaces Equation 6.2 to represent the axial extension term, considering the embedded initial tension/compression component. Essentially, this approach integrates the formulations provided by the Heidelberg, Hudson, and Zhan models, encompassing all the previously discussed terms associated with these models. The solution provided by SimpZP model is given in Equation 6.12.

$$\begin{aligned} & \left(1 - \frac{L^2 T_0}{\alpha(EI)^*}\right) \left(\frac{(EA)^*}{T_0 + (EA)^*}\right) \left(1 - \frac{2f_{11}hL^2}{\alpha(EI)^*}\right) \\ & \left(\frac{\alpha \cosh^2(\frac{\sqrt{\alpha}}{4})}{2 + \cosh(\frac{\sqrt{\alpha}}{2}) - 6\frac{\sinh(\frac{\sqrt{\alpha}}{2})}{\sqrt{\alpha}}}\right) \left(1 - 4\frac{\tanh(\sqrt{\alpha}/4)}{\sqrt{\alpha}}\right)^2 \\ & = \Delta Z_{center}^2 \left(\frac{(EA)^* + 2d_{11}h}{(EI)^*}\right) \end{aligned} \quad (6.12)$$

In accordance with the SimpZP formulation, the bending rigidity formulation derived from the modified YL model is integrated with this model to provide the relation between  $E$  and  $E^*$ . Similar to Zhan model, in Section 6.3.2, the specific formulation regarding the bending rigidity, in alignment with the SimpZP model, will be elaborated upon.

### ExtZP Model

The model proposed by Zare Pakzad *et al.* [Zare Pakzad et al., 2023c], ExtZP model, represents a multiscale extension of prior models, where the treatment of the surface is enhanced by incorporating two new sets of effective parameters: i) anisotropic surface parameters,  $H_{11}$  and  $H_{22}$ , and ii) surface-induced residual stresses,  $\sigma_{xx}$ . Consequently, the ExtZP approach represents the most comprehensive method for interpreting the bending response of Si NWs. In this approach, Equation 6.13 incorporates the surface terms derived from the extended YL surface model, which

are combined with the governing equation presented in Equation 6.9 and the initial extension term expressed in Equation 6.6. In this formulation,  $b$  represents the NW width.

$$H = H_{11} + H_{22} + bh\sigma_{xx} = 2bf_{11} + 2hf_{22} + 2bd_{11} + 2hd_{22} + bh\sigma_{xx} \quad (6.13)$$

With terms  $H_{11}$  and  $H_{22}$  defined as effective surface terms embedding the surface constants and geometrical representation of involved side surfaces [Song et al., 2011] the complete form of ExtZP model can be rewritten as Equation 6.14 where  $(EI)^*$  represents the effective flexural rigidity. The indices 11 and 22 denote the corresponding directions for the involved planar surfaces.

$$\begin{aligned} (EI)^* \frac{\partial^4 w}{\partial x^4} - T \frac{\partial^2 w}{\partial x^2} - 2bf_{11} \frac{\partial^2 w}{\partial x^2} - 2hf_{22} \frac{\partial^2 w}{\partial x^2} \\ - 2bd_{11} \frac{\partial^2 w}{\partial x^2} - 2hd_{22} \frac{\partial^2 w}{\partial x^2} - bh\sigma_{xx} \frac{\partial^2 w}{\partial x^2} = \\ \frac{F}{2} \left( -\delta(x) + 2\delta\left(x - \frac{L}{2}\right) - \delta(x - L) \right) \end{aligned} \quad (6.14)$$

Expanding upon the terms present in Equation 6.14, there are five terms that account for surface effects. These terms consist of the surface stress components ( $f_{11}$  and  $f_{22}$ ), surface elasticity constants ( $d_{11}$  and  $d_{22}$ ), and the residual stress induced by the surface ( $\sigma_{xx}$ ). The exact solution for the nanomechanical model is given in Equation 6.15. Section 6.3.2 will provide the bending rigidity formulation for the ExtZP model, which is based on the extended YL approach.

$$\begin{aligned} \left(1 - \frac{L^2 T_0}{\alpha(EI)^*}\right) \left(\frac{(EA)^*}{T_0 + (EA)^*}\right) \left(1 - \frac{L^2 H_{11}}{\alpha(EI)^*}\right) \left(1 - \frac{L^2 H_{22}}{\alpha(EI)^*}\right) \\ \left(\frac{\alpha \cosh^2(\frac{\sqrt{\alpha}}{4})}{2 + \cosh(\frac{\sqrt{\alpha}}{2}) - 6\frac{\sinh(\frac{\sqrt{\alpha}}{2})}{\sqrt{\alpha}}}\right) \left(1 - 4\frac{\tanh(\sqrt{\alpha}/4)}{\sqrt{\alpha}}\right)^2 = \\ \Delta Z_{center}^2 \left(\frac{(EA)^* + 2d_{11}b + 2d_{22}h + bhE^*}{(EI)^*}\right) \end{aligned} \quad (6.15)$$

### 6.3.2 Bending Rigidity Calculation

To estimate the value of  $E$ , the connection between classical bending rigidity and effective bending rigidity is employed, which relies on surface properties and geometric definitions. The formulation for the effective bending rigidity, as given by Equation 6.16, utilizes a modified YL method [He and Lilley, 2008, Wang and Feng, 2007] that aligns with the Zhan and SimpZP models.

$$(EI)^* = EI + (E_s)\left(\frac{bh^2}{2} + \frac{h^3}{6}\right) \quad (6.16)$$

In this context, the ExtZP model requires the calculation of the modulus of elasticity, which relies on the effective bending rigidity formulated using the extended YL model [Song et al., 2011, Zare Pakzad et al., 2023c], as expressed in Equation 6.17.

$$(EI)^* = EI + (E_s + \tau_0)\left(\frac{bh^2}{2} + \frac{h^3}{6}\right) \quad (6.17)$$

These formulations designate the average values of surface stresses ( $f_{11}$  and  $f_{22}$ ) and surface elasticity constants ( $d_{11}$  and  $d_{22}$ ) as  $\tau_0$  and  $E_s$ , respectively. In the field of nanomechanical models, these terms are commonly known as the surface modulus and initial surface stress, as discussed in the literature [He and Lilley, 2008]. More detailed information regarding the formulation of previous models [Heidelberg et al., 2006, Zhan and Gu, 2012, Hudson et al., 2013, Zare Pakzad et al., 2021, Zare Pakzad et al., 2023c] and related expressions for bending rigidity [Song et al., 2011, He and Lilley, 2008, Wang and Feng, 2007] can be found in other sources.

### 6.3.3 Bending Modeling

Simulations of three-point bending are conducted on double-clamped Si NWs using MD method [Plimpton, 1995]. Figure 6.2 illustrates the initial atomic configurations of Si NWs, where the width ( $h$ ) and height ( $b$ ) are varied between 2 nm and 5 nm. The Si NWs have a cubic cross-section, with the width being equal to the height. In this regard, the length ( $L$ ) of the Si NW remains constant at 600 nm for different

critical dimensions. Furthermore, it should be noted that support regions exist on each side of the Si NW and have a length ( $L_s$ ) of 60 nm. It is crucial to mention that both the length of the NW and the length of the support regions are kept constant across all critical dimensions of the Si NWs. This ensures a length-to-width aspect ratio (AR) greater than 10 for all NW critical dimensions, effectively excluding any potential length-related effects [Pakzad et al., 2023b]. A constant surface layer thickness ( $t$ ) of 0.5 nm is assumed for all Si NWs studied here. To maintain consistency in cross-section designs and accurate examination of surface constants, it is common to observe rectangular or square geometries in top-down fabricated Si NWs with  $\langle 100 \rangle$  and  $\langle 110 \rangle$  orientations [Nasr Esfahani and Alaca, 2019]. On the other hand, circular cross-sections are frequently encountered in bottom-up fabricated Si NWs with  $\langle 111 \rangle$  and  $\langle 112 \rangle$  orientations [Nasr Esfahani and Alaca, 2019]. In order to maintain consistency in defining the height and thickness of the Si NWs and to accurately analyze surface constants, square cross-sections have been chosen for all four orientations investigated in this study. This decision ensures that the cross-section designs are uniform across the orientations ( $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$  and  $\langle 112 \rangle$ ), enabling precise comparisons and comprehensive analysis of the Si NWs. To simulate the clamped B.C., the boundary regions at both ends are fixed in all three dimensions ( $x$ ,  $y$ , and  $z$ ). The non-periodic shrink-wrapped B.C.s are applied in all directions. The Si NWs undergo a quasi-static relaxation process using the conjugate gradient method to reach a local minimum configuration. Subsequently, a relaxation process is performed on all NWs at a temperature of 1.0 K for 40 ps, utilizing a time step of 1 fs. This is accomplished by employing a canonical NVT ensemble with a Nose-Hoover thermostat. The Tersoff-T3 potential [Tersoff, 1988] as an empirical function composed of two-body terms depending on the local environment is used for the modeling of Si NWs in this work. The associated Si NW stress state,  $\pi_{ij}$ , is calculated using the virial theorem [Zimmerman et al., 2004], given in Equation 6.18.

$$\pi_{ij} = \frac{1}{2\Omega_0} \left[ \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \frac{1}{r^{\alpha\beta}} \frac{\partial V(r^{\alpha\beta})}{\partial r} (v_i^{\alpha\beta} v_j^{\alpha\beta}) \right] \quad (6.18)$$

In Equation 6.18,  $\Omega_0$  stands for the atomic volume in an undeformed system with  $N$  as the total number of atoms where associated atomic volume for Si is calculated via relaxation of related structure with further details given in Ref. [Pakzad et al., 2021]. Atomic distances between atoms  $\alpha$  and  $\beta$  are represented as  $r_{\alpha\beta}$ .  $v_j^\alpha$  stands for the position of atom  $\alpha$  along  $j$  direction, i.e.,  $v_j^{\alpha\beta} = v_j^\alpha - v_j^\beta$  and  $V$  represents the interatomic potential. The  $F/w$  ratio, which is the ratio of force to deflection, can be determined by analyzing the slope of the initial linear section of the force-deflection response. This ratio is often used to estimate the modulus of elasticity through a linear approach. However, it should be noted that in the case of bending response curves for Si NWs, the displacement of the NW upon loading is expected to be larger than half of the cross-sectional size ( $h/2$ ). As a result, the response is likely to exhibit a non-linear behavior, as observed in prior experimental and MD studies on the bending of NWs [Zare Pakzad et al., 2023c, Pakzad et al., 2021]. In this context, the nanomechanical models described in Section 6.3.1 will be utilized to estimate the modulus of elasticity for Si NWs with various crystallographic orientations and critical dimensions.

#### 6.3.4 Surface Properties Modeling

To quantify the surface stress components ( $f_{11}$  and  $f_{22}$ ) and surface elastic constants ( $d_{11}$  and  $d_{22}$ ) for four orientations of Si NWs, Martin's method can be applied to the thin film structures given in Figure 6.3. By employing periodic boundary conditions in the  $x$ - and  $y$ -directions, an infinite film model with a finite thickness ( $L_z$ ) in the  $z$ -direction is obtained. The evaluation area ( $A_{film}$ ) consists of two free surfaces facing each other, and the film must be sufficiently thick to prevent interaction between these two surfaces. The dimensions, crystallographic orientations, numbers of atoms, and evaluation areas are listed in Table 6.1. The atomic structures are designed to be 8 times the lattice constants of Si along each crystallographic direction. This

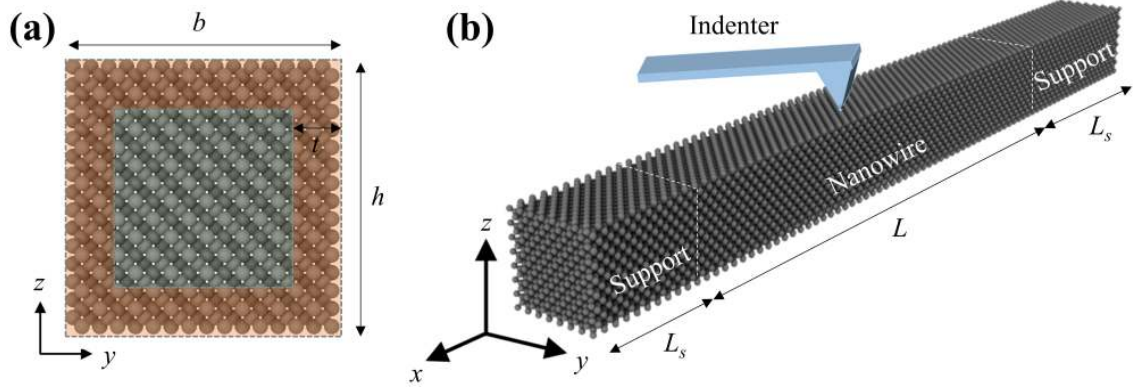


Figure 6.2: (a) The initial configuration of Si NW of width,  $b$ , height,  $h$ , and surface layer thickness,  $t$ . (b) The perspective view of a double-clamped NW showing the atomic configuration of a Si NW under 3-point bending simulation using a spherical indenter with associated support regions. The NW length ( $L$ ) and support region length ( $L_s$ ) are shown here.

Table 6.1: Dimensions, number of atoms and evaluation areas of unreconstructed Si thin film structures with associated crystallographic orientations.

| Structure | Si Orientation      |               |       | Dimensions [nm] |      |      | No. of atoms | $A_{film}$ [nm <sup>2</sup> ] |
|-----------|---------------------|---------------|-------|-----------------|------|------|--------------|-------------------------------|
|           | $x$                 | $y$           | $z$   | $x$             | $y$  | $z$  |              |                               |
| Si (100)  | [100]               | [010]         | [001] | 4.35            | 4.35 | 4.35 | 4224         | 37.8                          |
| Si (110)  | $[\bar{1}10]$       | [001]         | [110] | 6.15            | 4.35 | 6.15 | 8448         | 53.5                          |
| Si (111)  | $[\bar{1}\bar{1}2]$ | $[1\bar{1}0]$ | [111] | 7.10            | 6.15 | 7.52 | 16378        | 87.3                          |
| Si (112)  | $[1\bar{1}0]$       | $[11\bar{1}]$ | [112] | 6.15            | 7.52 | 7.10 | 16356        | 106.8                         |

ensures an appropriate thickness for the film, allowing for accurate calculations of surface stresses and surface elastic constants.

To determine the surface stress components, the structures are initially equilibrated at a temperature of 0.01 K using NPT dynamics. Afterward, the total energy is minimized using the steepest descent and conjugate gradient techniques. The surface stress components are then calculated by assuming a film thickness of  $L_z$ , and are formulated according to Equation 6.19. In this equation, the parameter  $\eta$  represents the average strain resulting from the relaxation process [Izumi et al.,



2004, Pakzad et al., 2021, Zare Pakzad et al., 2023c]. The Tersoff-T3 potential [Tersoff, 1988] is used for the modeling of Si thin films.

$$f_{ij}(\eta) = f_{ij}^{film}(\eta) - f_{ij}^{bulk}(\eta) \quad (6.19)$$

The estimation of bulk surface stress requires a separate analysis using the bulk model. The surface stress for the film model can be determined by utilizing the stress tensor definition, denoted as  $\sigma_{ij}^{film}$ , as described in Equation 6.20. For more comprehensive information regarding the stress tensor of thin films, additional details can be found elsewhere [Izumi et al., 2004, Pakzad et al., 2021, Zare Pakzad et al., 2023c].

$$f_{ij}^{film}(\eta) = \sigma_{ij}^{film}(\eta) \frac{L_z}{2} \quad (6.20)$$

The surface elastic constants ( $d_{ijkl}$ ) are defined as the second-order derivatives of surface energy with respect to strain under plane-stress conditions. To calculate the elastic constants for both the bulk ( $C_{ijkl}^{bulk}$ ) and film ( $C_{ijkl}^{film}$ ) models, specific considerations are made. For the bulk model, the elastic constants are defined under plane-stress conditions ( $C_{ijkl}^{bulk,plane}$ ), which can be determined using the relationships provided in Equation 6.21, Equation 6.22, and Equation 6.23 [Izumi et al., 2004, Pakzad et al., 2021, Zare Pakzad et al., 2023c].

$$C_{11}^{bulk,plane} = C_{11} - \frac{C_{13}^2}{C_{33}} \quad (6.21)$$

$$C_{22}^{bulk,plane} = C_{22} - \frac{C_{12}^2}{C_{33}} \quad (6.22)$$

$$C_{12}^{bulk,plane} = C_{12} - \frac{C_{12}C_{13}}{C_{33}} \quad (6.23)$$

The relationship between the plane-stress elastic constants of the bulk and film models and the surface elastic constants is expressed by Equation 6.24 [Izumi et al., 2004, Pakzad et al., 2021, Zare Pakzad et al., 2023c]. To obtain elastic constants, infinitesimal strains are applied to the simulation box in different directions and the resulting variation of the energy is measured.

$$C_{ijkl}^{film,plane} = C_{ijkl}^{bulk,plane} - \frac{2}{L_z} d_{ijkl} \quad (6.24)$$

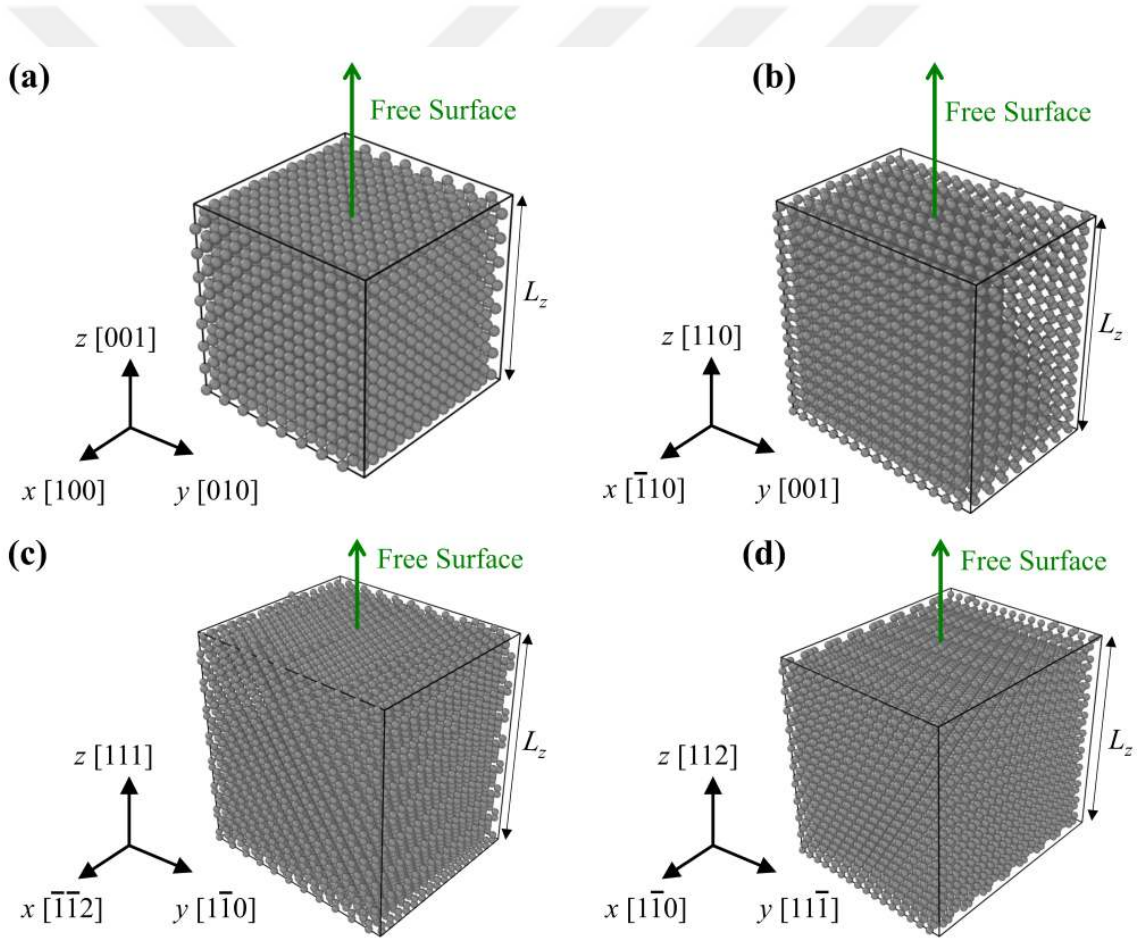


Figure 6.3: The atomic structures used for calculating surface properties of unreconstructed Si thin films with different crystallographic orientations and associated free surfaces in the  $z$ -direction. The depicted structures correspond to Si orientations of (a) Si (100), (b) Si (110), (c) Si (111), and (d) Si (112).

## 6.4 Results

The section begins by establishing surface parameters, such as surface stresses and surface elastic constants, for different orientations of unreconstructed Si thin films (Section 6.4.1). Next, the bending simulation results for Si NWs modeled using MD with varying critical dimension and crystallographic orientations are presented in Section 6.4.2. Subsequently, the force-deflection relationships resulting from the simulations are examined to extract the modulus of elasticity of the Si NWs. The modulus of elasticity results are interpreted using different models from the existing literature (Section 6.4.3).

### 6.4.1 Surface Properties of Si

Despite numerous studies employing atomistic [Pakzad et al., 2021, Pishkenari and Rezaei, 2017, Izumi et al., 2004, Xu and Kim, 2019, Park, 2008], DFT [Melis et al., 2015, Melis et al., 2016, Lee and Rudd, 2007, Jung and Shin, 2017], finite element [Quagliotti et al., 2013, Delph, 2008, Payne et al., 1989, Miyamoto, 1994, Alerhand et al., 1988], and experimental [Pennelli et al., 2012] approaches to investigate the surface constants of Si, a consensus regarding surface stress profiles and the subsequent calculation of constants for different crystalline orientations and surface conditions is lacking. A recent study has provided insights into the surface constants of unreconstructed and oxidized Si thin films offering valuable analysis regarding the surface properties of crystalline Si with different surface states [Zare Pakzad et al., 2023c]. In line with that investigation, the unreconstructed Si thin films with (100), (110), (111), and (112) free surface orientations shown in Figure 6.3 are examined for the calculation of surface properties including surface stresses,  $f_{11}$  and  $f_{22}$ , and surface elasticity constants,  $d_{11}$  and  $d_{22}$ . The methodology described in Section 6.3.4 is employed to analyze nanoscale Si thin films. The validity of this approach has been previously verified on various Si surfaces, including amorphous and unreconstructed structures, using different interatomic potentials. These previous studies, conducted through MD and DFT, have demonstrated good agreement with the results obtained

Table 6.2: Surface stress and surface elastic constants calculated for unreconstructed Si structures with associated crystallographic orientations.

| Structure | Si Orientation      |               |       | Surface Stress [N/m] |          |           | Surface Elasticity [N/m] |          |           |
|-----------|---------------------|---------------|-------|----------------------|----------|-----------|--------------------------|----------|-----------|
|           | $x$                 | $y$           | $z$   | $f_{11}$             | $f_{22}$ | $f_{avg}$ | $d_{11}$                 | $d_{22}$ | $d_{avg}$ |
| Si (100)  | [100]               | [010]         | [001] | -0.88                | -0.88    | -0.88     | -8.77                    | -8.77    | -8.77     |
| Si (110)  | $[\bar{1}10]$       | [001]         | [110] | -1.57                | -0.95    | -1.26     | +3.40                    | -15.10   | -5.85     |
| Si (111)  | $[\bar{1}\bar{1}2]$ | $[1\bar{1}0]$ | [111] | -0.88                | -1.23    | -1.06     | -18.67                   | +8.42    | -5.12     |
| Si (112)  | $[1\bar{1}0]$       | $[11\bar{1}]$ | [112] | -4.42                | -2.11    | -3.27     | -25.10                   | +22.38   | -1.36     |

from the current method [Shchipalov, 2000, Miller and Shenoy, 2000]. To calculate surface stress, Equation 6.19 is utilized, taking into account the film thickness ( $L_z$ ), and the resulting planar surface stresses are presented in Table 6.2. Additionally, the surface elasticity constants are computed using Equations 6.21, 6.22, and 6.23, with the values also provided in Table 6.2. The local stresses along the thin film structures are calculated using Equation 6.18, considering the estimated atomic volume. The surface elastic constants are obtained for the film structures using limited thicknesses, while the bulk models are separately examined. Equation 6.24, with the associated film thickness of  $L_z$ , is employed for this purpose. Table 6.2 further illustrates the average surface stress and surface elasticity constants for each orientation of the free surface. Remarkably, the obtained surface stress and surface elasticity constants for Si (100) and Si (110) crystal orientations align precisely with prior reports [Zare Pakzad et al., 2023c, Pishkenari and Rezaei, 2017, Izumi et al., 2004, Pakzad et al., 2021, Shchipalov, 2000]. To the best of our knowledge, there is currently no existing study that provides surface constants for (111) and (112) Si thin films. The surface properties obtained here will be utilized in Section 6.4.2 to interpret the bending response of Si NWs using different surface formulations integrated into nanomechanical models.

#### 6.4.2 Bending Response of Si NWs

In Figure 6.4 (a), the graph demonstrates the correlation between force and deflection ( $F - w$ ) during a three-point bending test of a Si NW simulated using the MD method. Five significant deformation points ( $p_1$  to  $p_5$ ) are identified for detailed examination of the  $F - w$  behavior, and accompanying snapshots of the bending deformation of the Si NW profile are presented in Figure 6.4 (b). The gray shaded region (between points  $p_1$  and  $p_2$ ) depicted in Figure 6.4 (a) represents the range of deformation occurring in the middle of the Si NW, reaching approximately  $h/2$ , before transitioning into non-linearity, indicating large deflection during Si NW deformation. Likewise, Figure 6.4 (b) illustrates the deflection level attained at  $p_2$  as the bending continues in the mid-section, eventually reaching the ultimate force level. The point  $p_3$  exhibits the deviation observed between nanomechanical modeling and  $F - w$  response given here. The ultimate force is also shown as point  $p_4$ . Finally, the fracture snapshot corresponding to Si NW failure is denoted as  $p_5$ . The response of the Si NW demonstrates a nonlinear relationship between force and displacement, covering a force range of up to 180 nN and a corresponding deflection range of up to 10 nm at the center of the NW. Examination of Si NWs with different crystal orientations and critical dimensions shows that incorporating surface properties like surface stresses and surface elastic constants (given in Table 6.2), along with intrinsic stresses, into the relevant models becomes essential to effectively apply various nanomechanical models for fitting the obtained  $F - w$  responses. In this respect, MD simulations are utilized to determine the intrinsic stresses induced in Si NWs of different sizes and orientations. Once the relaxation process reaches a steady state, the atomic stresses along the longitudinal direction ( $x$ -axis) are computed for each Si NW using Equation 6.18. Table 6.3 presents the calculated surface-induced residual stresses for Si NWs with varying critical dimensions and orientations. In this study, it is assumed that the surface-induced residual stress represents the total intrinsic stress which will also be regarded as an initial tensile/compressive stress within the associated models. Intrinsic stresses in Si NWs have been reported in previous studies, including both computational [Zhan and Gu,

2012] and experimental [Zare Pakzad et al., 2023c, Calahorra et al., 2015, Nasr Esfahani et al., 2022, Dolabella et al., 2020, Spejo et al., 2020] investigations. These studies have observed intrinsic stress values in Si NWs within a range of 100 MPa to 1.2 GPa. The nanomechanical model fitting shown in Figure 6.4 (a) corresponds to the ExtZP model, which is obtained by incorporating the relevant surface and intrinsic parameters. The detailed estimation of the modulus of elasticity for Si NWs with various dimensions and crystallographic orientations using nanomechanical models, as described in Section 6.3.1, is provided in Section 6.4.3.

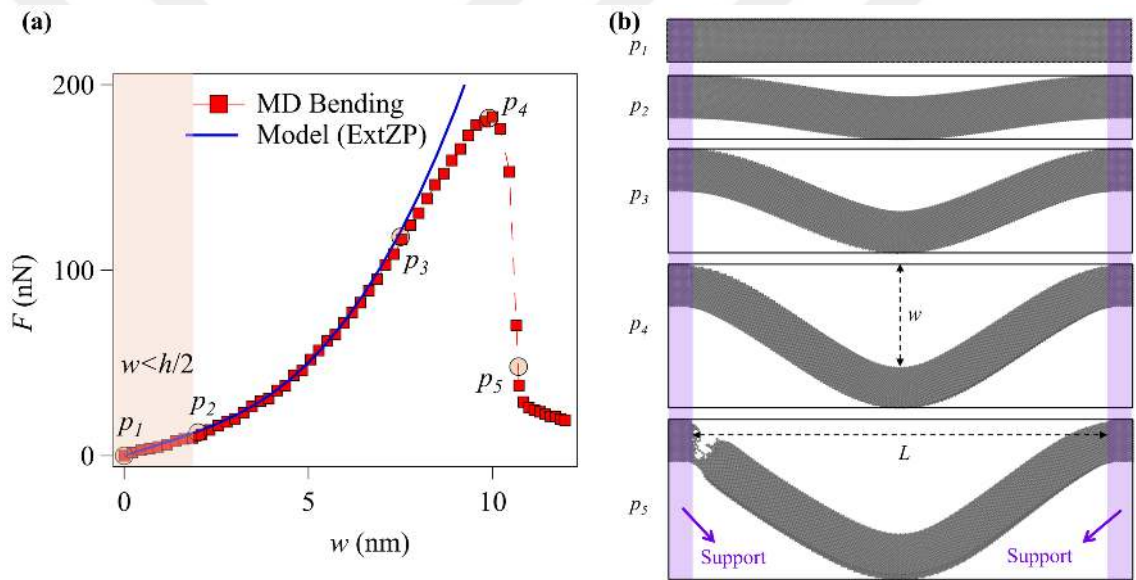


Figure 6.4: (a) Force vs. deflection data obtained through 3-point bending simulation of a Si NW of  $h = 4$  nm and fitted curve using the ExtZP model. (b) Atomic configurations of a Si NW and snapshots upon deformation of the Si NW during bending experiment.

### 6.4.3 Interpretation of Results

This section provides a detailed explanation of the interpretation of force-deflection responses for Si NWs with different dimensions and crystal orientations. Previous studies [Heidelberg et al., 2006, Zhan and Gu, 2012, Zare Pakzad et al., 2023c] have used a fitting procedure that begins with small deflections and extends to include progressively larger displacements. It is important to note that each nanomechanical

Table 6.3: Intrinsic stresses of Si NWs with different critical dimensions and crystallographic orientations obtained via MD simulations.

| Structure                | Si Orientation |               |                     | Intrinsic Stress [GPa] |           |           |           |
|--------------------------|----------------|---------------|---------------------|------------------------|-----------|-----------|-----------|
|                          | $x$            | $y$           | $z$                 | $h = 2nm$              | $h = 3nm$ | $h = 4nm$ | $h = 5nm$ |
| Si $\langle 100 \rangle$ | [100]          | [010]         | [001]               | 0.69                   | 0.51      | 0.53      | 0.38      |
| Si $\langle 110 \rangle$ | [110]          | [001]         | $[\bar{1}10]$       | 1.87                   | 1.46      | 1.23      | 0.77      |
| Si $\langle 111 \rangle$ | [111]          | $[1\bar{1}0]$ | $[\bar{1}\bar{1}2]$ | 1.73                   | 0.98      | 1.26      | 0.80      |
| Si $\langle 112 \rangle$ | [112]          | $[11\bar{1}]$ | $[\bar{1}\bar{1}0]$ | 1.48                   | 0.81      | 1.05      | 0.65      |

model attributes the nonlinearity of the  $F - w$  curve to different sets of parameters, including axial extension, intrinsic stress, and surface effects. Thus, each obtained  $F - w$  curve is analyzed using five nanomechanical models, utilizing the appropriate input parameters, to obtain the modulus of elasticity of the Si NW. Among the models used, the ExtZP model is the comprehensive method that incorporates the surface stress ( $f_{11}$  and  $f_{22}$ ) and surface elastic constants ( $d_{11}$  and  $d_{22}$ ) provided in Table 6.2, as well as the intrinsic stresses given in Table 6.3, along with geometric details for interpreting the bending response. The SimpZP model considers the intrinsic stresses provided here as the initial tension ( $\sigma_0$ ) and incorporates the surface properties  $f_{11}$  and  $d_{11}$  during the fitting procedure. The Zhan model relies on the previously given surface constants ( $f_{11}$  and  $d_{11}$ ) without including any intrinsic terms. In contrast, the Hudson model includes the intrinsic term based on the initial tension adopted from Table 6.3, without incorporating any surface properties. Finally, the Heidelberg model performs the fitting procedure without including any surface or intrinsic terms. The bending rigidity formulations provided in Section 6.3.2 are utilized with the previously mentioned details specific to each nanomechanical model, taking advantage of the relevant surface properties. The procedure outlined for estimating the modulus of elasticity using the provided models and the fitting curve shown in Figure 6.4 (a) has been applied to Si NWs. The results are presented in Figure 6.5 for different crystal orientations. Specifically, the modulus of elasticity estimation

for  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ , and  $\langle 112 \rangle$ -oriented Si NWs, with  $h$  ranging from 2.0 to 5.0 nm, is shown in Figure 6.5 (a), Figure 6.5 (b), Figure 6.5 (c), and Figure 6.5 (d), respectively. The bulk modulus of elasticity for each corresponding orientation is also given as dashed lines [Nasr Esfahani and Alaca, 2019].

The trend observed for Si NWs with varying crystal orientations is a decrease in the modulus of elasticity as the critical dimension  $h$  increases, though the rate of decrease varies depending on the orientation and the specific nanomechanical model employed. Specifically, for  $\langle 100 \rangle$ -oriented Si NWs given in Figure 6.5 (a), the modulus of elasticity estimation remains relatively constant for different critical dimensions, while incorporating the Heidelberg and Hudson models. When incorporating the surface and/or intrinsic terms in the Zhan, SimpZP, and ExtZP models, there is a consistent decreasing trend of  $E$  as the critical dimension  $h$  increases. The differences observed among these three models can be attributed to the utilization of distinct combinations of inputs, despite sharing a similar overall decreasing trend. For  $\langle 110 \rangle$ -oriented Si NWs given in Figure 6.5 (b), different decreasing trends are observable using the nanomechanical models. With the Heidelberg and Hudson model having higher estimation at 2.0 nm critical dimension, a similar constant trend is obtained with increase in  $h$ . However, the Zhan, SimpZP, and ExtZP models depict a decreasing  $E$  for Si NWs with increasing  $h$ .

Expanding the discussion to  $\langle 111 \rangle$ -Si NWs, as shown in Figure 6.5 (c), a clear decreasing trend of the modulus of elasticity can be observed for all the nanomechanical models used in this study. The estimations consistently demonstrate a similar trend when considering the effect of critical dimensions on the Si NWs. However, similar to the previous orientations, the Zhan, SimpZP, and ExtZP models yield higher estimations of  $E$  compared to the Heidelberg and Hudson models. For  $\langle 112 \rangle$ -Si NWs, as shown in Figure 6.5 (d), the trend of the modulus of elasticity also exhibits a similar decrease, but with differences between the models at each critical dimension. Once again, the Heidelberg and Hudson models provide lower estimations compared to the other three models. It is worth noting that the combination of parameters included in the nanomechanical models for the four crystal



orientations studied here can result in differences of up to 100 GPa in the estimation of  $E$ , which is a significant variation. In particular, in the case of the smallest critical dimension ( $h$  of 2.0 nm), where surface effects are anticipated to exhibit a more significant influence due to the size effect, models that encompass surface properties yield higher estimations, displaying more substantial deviations when contrasted with the Heidelberg and Hudson models. Notably, both the Heidelberg and Hudson models lack formulations that include surface-related terms, leading to inadequate estimations of the modulus of elasticity for Si NWs with critical dimensions below 10 nm. As the size increases, the surface contribution becomes less pronounced, leading to closer estimations among different models.

In the investigation of size-dependent elastic properties of Si NWs, especially in cases of smaller dimensions, it becomes crucial to meticulously account for the inclusion of terms, particularly those relating to surface properties. When comparing the outcomes of the three models incorporating surface terms, it becomes apparent that both the Zhan and SimpZP models employ a common surface model known as the modified YL model. Depending on whether intrinsic terms are taken into account or not, divergences emerge between these two models. The Zhan model consistently yields higher estimates of the modulus of elasticity for all four orientations and critical dimensions. Conversely, the SimpZP model, which incorporates a tensile intrinsic stress during the fitting procedure, is anticipated to offer lower estimates of  $E$  depending on the critical dimension and the magnitude of the intrinsic stress. Furthermore, it is important to emphasize that among the four orientations studied in this work ( $\langle 110 \rangle$ ,  $\langle 111 \rangle$ ,  $\langle 112 \rangle$ ), only the ExtZP model benefits from the inclusion of anisotropic surface constants modeled via extended YL model given in Table 6.2. The remaining four models dismiss some or all of these surface terms, depending on their respective formulations. Previous findings emphasizing the significance of the native oxide surface state [Zare Pakzad et al., 2023c, Pakzad et al., 2021, Pakzad et al., 2023b, Pakzad et al., 2024] can be extended via present study on unreconstructed Si NWs. This highlights not only the importance of the surface state itself but also the anisotropic effects of surface properties. The se-

lection of an appropriate model is crucial to avoid potential misinterpretations, as improper model selections may lead to misleading conclusions regarding the nature of unreconstructed Si surfaces and their impact on Si NW behavior. Given the discrepancies observed in the literature regarding experimental and computational estimations of the modulus of elasticity in Si NWs, the values obtained in this study are in line with the prior reports [Zare Pakzad et al., 2023c, Nasr Esfahani and Alaca, 2019, Wang et al., 2017, Yang et al., 2022].

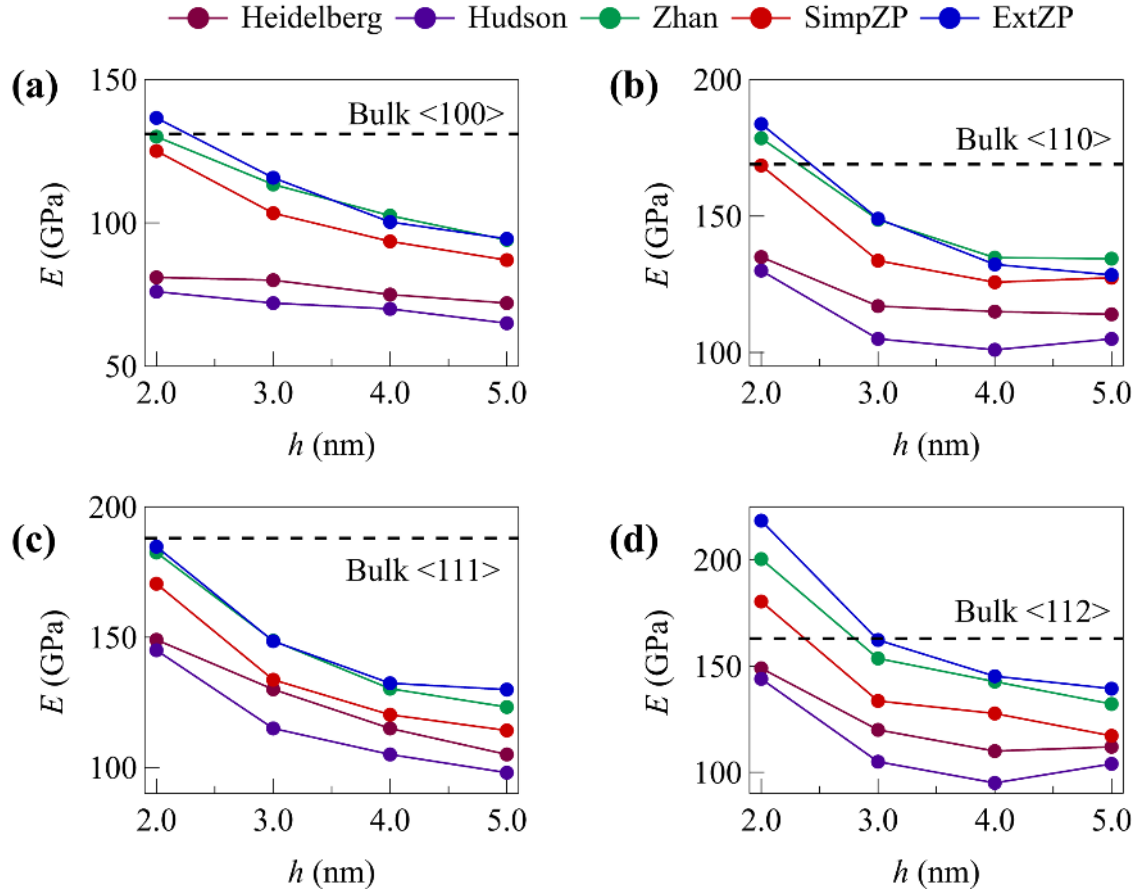


Figure 6.5: The modulus of elasticity estimations for Si NWs with (a)  $\langle 100 \rangle$ , (b)  $\langle 110 \rangle$ , (c)  $\langle 111 \rangle$ , and (d)  $\langle 112 \rangle$  crystal orientations. The Si NWs have different size in  $h$  ranging between 2 to 5 nm. The bulk modulus of elasticity for each orientation of Si is shown.

## **6.5 Conclusion**

This study exhibits the pivotal role that surface properties play in the mechanical behavior of Si NWs. By delving into the elastic properties of Si NWs with varying dimensions and crystal orientations through a diverse range of nanomechanical models, the intricate relationship between elastic properties, crystal orientation, and the chosen nanomechanical model has been unveiled. The analysis of force-deflection responses via MD simulations yields invaluable insights into the behavior of Si NWs at the nanoscale. These findings underscore the significance of meticulously modeling surface effects and incorporating anisotropic surface properties to attain a comprehensive grasp of Si NW mechanics. Additionally, the distinct trends observed in Si NWs with different crystal orientations emphasize the necessity of accounting for crystal orientation effects when scrutinizing their mechanical properties. This knowledge contributes to the ongoing exploration of size-dependent behaviors in Si NWs and enhances our comprehension of their surface attributes. A thorough comprehension of the effects originating from surface and crystal orientation aspects will undoubtedly expedite the development of more efficient and reliable NW-based technologies in the future.

## Chapter 7

# THE ROLE OF NATIVE OXIDE ON THE MECHANICAL BEHAVIOR OF SILICON NANOWIRES

### 7.1 Overview

Molecular dynamics simulations are employed to study the effect of native oxide on the size-dependent mechanical properties of silicon nanowires. Despite their immense potential as essential building blocks in nanoelectromechanical systems, mechanical behavior of silicon nanowires still needs further attention for a full understanding. The leading source of ambiguity can be traced back to the fact that the presence of native oxide on silicon nanowire surfaces is ignored when interpreting nanomechanical test data, when it comes, for example, to converting force and deflection measurements to stress and strain. This problem needs immediate attention, because, first, nanowires have a significant surface area, and second, native oxide is the dominant surface state. With prior work reporting conflicting dimensional and computational viewpoints regarding the effect of native oxide on silicon nanowires properties, size dependence of nanowire mechanical properties is investigated here with great attention placed on critical size and atomistic simulation perspectives. For this purpose, Tersoff-Munetoh and modified Stillinger-Weber potentials are employed in this intensive computational study to address the influence of size and crystal orientation on nanowire elastic behavior and tensile strength. As a result, a striking set of differences is obtained. First, the presence of native oxide layer is observed to decrease both the modulus of elasticity and the ultimate strength. The reduction in the modulus of elasticity is observed to be as much as 30% and 40% for  $\langle 100 \rangle$  and  $\langle 110 \rangle$ -oriented nanowires, respectively. Similarly, the reduction in the ultimate strength is estimated to be as much as 20% using the modified

Stillinger-Weber potential, which proved to be more suitable for strength analysis compared to Tersoff-Munetoh potential. Finally, the failure behavior is studied through the ductile failure probability calculations, where a higher size-dependent failure probability is observed for decreasing nanowire width upon oxidation. These results shed light on the background of existing inconsistencies between experimental and numerical findings in the literature, as opposing trends for silicon nanowire stiffness and strength were reported with decreasing size. The study provides a guideline to quantify the scale effect in silicon nanowire mechanical behavior as a combined outcome of oxide thickness, nanowire size and crystal orientation and thus to reduce the extent of uncertainties originating from inadequate interpretation of nanomechanical test data.

## **7.2 Introduction**

Among the low-dimensional nanoscale materials that increasingly find applications in high-performance devices of diverse nature, nanowires (NWs) and nanotubes are of particular interest due to their utilization in the fields of electronics, energy harvesting and storage, sensing and communications [Alaca and Karimzadehkhoei, 2023, Wang et al., 2017, Rojo et al., 2013, Nasr Esfahani and Alaca, 2019, Zhu, 2017, Dasgupta et al., 2014]. In the specific case of silicon (Si) NWs, this trend is fueled by a multitude of applications ranging from gate-all-around transistors [Guerfi and Larrieu, 2016, Sacchetto et al., 2009] to next-generation mass spectrometers [Sannicolo et al., 2016, Sage et al., 2018] with the latter representing a nanoelectromechanical system (NEMS) [Ekinici and Roukes, 2005]. Such NEMS devices entail the potential of extreme miniaturization of today's sensors. Demonstrated by a series of exploratory studies [Zhu et al., 2020, Kilinc et al., 2020, Miani et al., 2021], this miniaturization brings about the benefits of improved sensitivity and power consumption in sensor applications. Due to its ease of integration with electronics, maturity of fabrication technologies, and well-understood transduction via piezoresistivity, Si remains in the forefront of the miniaturization effort [Wang et al., 2017, Nasr Esfahani and Alaca, 2019]. As Si NWs serve as the core mechan-

ical building block in NEMS applications, a solid understanding of the scale effect on the mechanical properties is an inherent part in NEMS design and implementation. However, it is also the very scale that poses significant challenges for NW characterization [Nasr Esfahani and Alaca, 2019, DelRio et al., 2015].

These challenges take different forms in experimental and modeling studies. In mechanical characterization experiments, physical requirements for reliable testing, such as alignment of the Si NW sample with respect to loading axis and imposing suitable boundary conditions are very stringent [Elhebeary and Saif, 2017b]. Various testing techniques including bending, uniaxial loading, indentation, and resonance address certain aspects of these requirements with varying levels of success [Nasr Esfahani and Alaca, 2019, Zhu, 2017, Zare Pakzad et al., 2021]. In addition to the issues related to the mechanical nature of testing, challenges due to processing and metrology — sample preparation, device calibration and setup resolution in addition to the extraordinary challenges of *in-situ* characterization — contribute to the fact that the resulting spread in measurements remains significant. As a result, Si NW strength below the critical dimension of 400 nm is currently reported to cover several orders of magnitude ranging from 100 MPa up to 21 GPa, the theoretical strength of the crystal [Nasr Esfahani and Alaca, 2019, Zhu, 2017, DelRio et al., 2015]. On the other hand, theoretical approaches including molecular dynamics (MD) simulations, *ab initio* and first-principal methods [Nasr Esfahani and Alaca, 2019, Wang et al., 2017] are very powerful techniques to study the mechanical properties using the force fields. In a similar fashion, such efforts also result in a wide range of estimations of Si NW mechanical properties [Nasr Esfahani and Alaca, 2019]. This can be predominantly attributed to an inconsistent use of constitutive models for the study of surface bond reconstruction and nonlinearity in elasticity [Nasr Esfahani and Alaca, 2019, Zhu, 2017, Wang et al., 2017], and thus deserves a closer scrutiny.

Size-dependent mechanical properties of Si NWs have been modeled by MD simulations considering primarily parameters such as the NW diameter [Jing et al., 2009a, Jing et al., 2009b, Kang and Cai, 2010, Liu and Shen, 2012, Xu and Kim, 2019, Xu, 2020] and its geometrical shape [Justo et al., 2007, Liu et al., 2015, Yang

et al., 2009]. Surface-related properties of NWs were also addressed [Liu and Shen, 2012, Justo et al., 2007] taking surface stress [Esfahani and Alaca, 2018] and side surface crystalline orientations [Zhuo and Beom, 2019] into account. In addition to atomic simulations, continuum formulation was employed as well to address size dependence [Nasr Esfahani and Alaca, 2019, Esfahani and Alaca, 2018]. However, most studies – both MD and continuum – considered the unreconstructed and passivated Si NW surfaces [Kang and Cai, 2007, Xu and Kim, 2019, Jing and Meng, 2010b, Godet et al., 2015, Guénolé et al., 2011] while studying surface stress [Esfahani and Alaca, 2018] and surface elasticity [Yao et al., 2012], thereby ignoring the presence of the native oxide as the primary surface structure [Chen et al., 2018, Steinruck et al., 2014, Watanabe et al., 2004, Al-Bayati et al., 1991]. This native oxide layer, known to be amorphous silicon dioxide ( $\text{aSiO}_2$ ) [Morita et al., 1990, Steinruck et al., 2014], affects the local structure through creating interfaces and introducing defects [Poindexter et al., 1981, McDowell et al., 2011, Baumer et al., 2004]. This becomes especially significant at the nanoscale, where minuscule variations in the oxide thickness and shape can lead to major changes in Si NW properties [Chen et al., 2018, Sadeghian et al., 2009, Sadeghian et al., 2010, Xu, 2020, He and Galli, 2012, Zhou et al., 2003, Ilinov and Kuronen, 2014]. Despite the degree to which the native oxide is expected to affect Si NW mechanical behavior, to our knowledge, very limited work has been reported so far. For example, the existence of a compressive stress near the  $\text{aSiO}_2/\text{Si}$  interface was demonstrated in Si NWs [Ohta et al., 2007] which can alter the surface stress state due to surface reconstruction. Another study on bending properties of oxidized Si NWs reported the reduction in NW stiffness due to the oxide layer when compared with pure Si NWs [Ilinov and Kuronen, 2014]. More recently, the effect of the native oxide was investigated via MD tensile modeling, where the effective modulus of elasticity and fracture strength were reported to decrease with increasing oxide thickness [Pakzad et al., 2021, Xu, 2020]. Furthermore, predicting a negligible size effect in the case of Si nanocantilevers, findings of such theoretical studies remain in stark contrast with those of experimental investigations [Sadeghian et al., 2009, Park, 2008]. In addition

to the surface state, such disagreement between theory and experiment can also be linked to the specific interatomic potential used in MD simulations [Liu et al., 2015]. There are numerous interatomic potentials developed for Si and oxygen (O) including the Tersoff-Munetoh [Munetoh et al., 2007], Stillinger-Weber (SW) [Watanabe and Ohdomari, 1999, Watanabe et al., 1999], modified SW [Ganster et al., 2010], and Vashishta [Vashishta et al., 1990] potentials. Similar to the elastic behavior, size-dependent brittle-to-ductile transition and orientation-dependent failure of Si NWs were previously studied using various interatomic models [Kang and Cai, 2007, Kang and Cai, 2010, Zhuo and Beom, 2018, Östlund et al., 2009, Liu and Shen, 2012]. In this regard, there are studies putting forward both the slip mechanism [Yang et al., 2009, Godet et al., 2009] and the crystal-to-amorphous phase transition [Han et al., 2007, Huang et al., 2009] as the source of ductility.

It is against this background that the present work is concerned with the mechanical behavior of Si NWs with a native oxide surface layer. MD simulations are used to model Si NW tensile behavior with an unreconstructed surface and native oxide using the Tersoff- Munetoh [Munetoh et al., 2007] and modified SW [Ganster et al., 2010] potentials. The impact of the native oxide on the modulus of elasticity, yield and ultimate strength is studied in  $\langle 100 \rangle$  and  $\langle 110 \rangle$ , the two most relevant crystallographic orientations found in top-down fabrication of Si NWs [Nasr Esfahani and Alaca, 2019]. Furthermore, due to expected rectangular/square geometry of NWs upon top-down fabrication, the selection of the cross-sections are decided to be square opposite to circular cross-sections commonly encountered in  $\langle 111 \rangle$  oriented Si NWs as outcome of bottom-up fabrication attempts [Nasr Esfahani and Alaca, 2019, Tang et al., 2012]. In the remainder of this paper, details of the interatomic potentials and simulation methods are discussed first. This is followed by a case study on the native oxide effect on two different orientations with varying interatomic potential, oxide thickness and NW length-to-width ratio. Furthermore, the analytical approach based on the core-shell model is employed for the comparison with MD results. The paper is concluded with a study on the orientation and interatomic-potential-dependent failure behavior in the presence of native oxide.



### 7.3 Materials and Methods

In this section, first the description of methods used to perform atomistic study on tensile behavior of Si NWs with and without native oxide is given. This includes geometrical definition and interatomic potentials used in this study. This is followed by the details of the analytic model, utilized for the estimation of the effective modulus of elasticity of NWs.

MD simulations are employed to study the impact of native oxide on the tensile behavior of Si NWs. NWs with native oxide are denoted as aSiO<sub>2</sub>-Si NWs throughout the rest of this work. Si NWs with unreconstructed surfaces are simply denoted as Si NWs. MD simulations are carried out on Si NWs along  $\langle 100 \rangle$  and  $\langle 110 \rangle$  crystal orientations using LAMMPS [Plimpton, 1995]. The initial configurations of Si NWs and aSiO<sub>2</sub>-Si NWs are schematically shown in Figure 7.1. Periodic boundary conditions (B.C.s) were applied along  $x$ -direction, while applying fixed boundary condition along  $y$ - and  $z$ -directions to model a part of an infinite NW. The interaction between atoms in Si NWs and aSiO<sub>2</sub>-Si NWs are modeled by the Tersoff-Munetoh [Munetoh et al., 2007] (TM), and modified SW [Ganster et al., 2010] (m-SW) potentials. The details of the corresponding expressions and coefficients of the formulations for the TM and m-SW potentials can be found in the associated references [Munetoh et al., 2007, Ganster et al., 2010]. Figure 7.1 shows the geometrical definitions of the NW including width ( $W$ ), oxide thickness ( $t$ ), and length ( $L$ ) while the length-to-width ( $L/W$ ) ratio is denoted as the aspect ratio (AR).

MD simulations are performed at a temperature of 10  $K$  to obtain a quasi-static system. An initial velocity with a Gaussian distribution was assigned at a temperature of 10  $K$ . This was followed by the energy minimization using the conjugate gradient method as a static relaxation. This energy minimization removes any excessive stress in the atomic structure for the dynamic equilibrium step. Then the structure was dynamically equilibrated at 10  $K$  for 60 ps using the Nose-Hoover isobaric-isothermal (NPT) ensemble with a time step of 1 fs. After the equilibration,

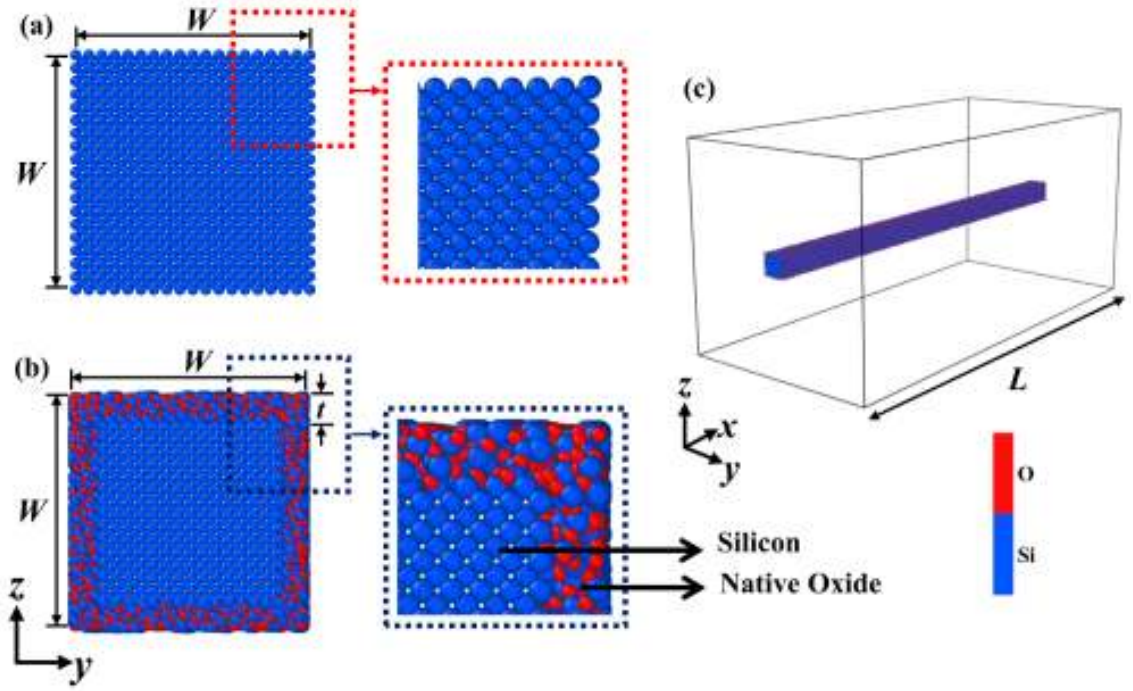


Figure 7.1: Cross-sections of models for (a) Si NWs and (b) aSiO<sub>2</sub>-Si NWs studied here where surface condition of NWs are represented with close-ups. Si and O atoms are shown with blue and red spheres respectively. (c) The simulation box with a representative aSiO<sub>2</sub>-Si NW with periodic B.C. applied along the NW direction ( $x$ ) and non-periodic B.C.s applied along two other directions ( $y$ -direction and  $z$ -direction). Dimensional parameters defining NW sizes as width ( $W$ ), length ( $L$ ) and native oxide thickness ( $t$ ) are shown here.

the simulation cell was deformed along the NW longitudinal direction with a strain rate of  $\dot{\epsilon} = 5 \times 10^9 \text{ s}^{-1}$ , which is in the range of strain rates suitable for tensile tests in MD simulations [Kang and Cai, 2007]. For a quasistatic system with negligible thermal oscillations, atomic stress based on the virial theorem [Cormier et al., 2001] can be written as:

$$\pi_{ij} = \frac{1}{2\Omega_0} \left[ \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \frac{1}{r^{\alpha\beta}} \frac{\partial V(r^{\alpha\beta})}{\partial r} (v_i^{\alpha\beta} v_j^{\alpha\beta}) \right] \quad (7.1)$$

where  $\Omega_0$  stands for the atomic volume in an undeformed system with  $N$  as the total number of atoms. Atomic distances between atoms  $\alpha$  and  $\beta$  are represented as  $r^{\alpha\beta}$ .  $v_j^\alpha$  stands for the position of atom  $\alpha$  along  $j$  direction, *i.e.*  $v_j^{\alpha\beta} = v_j^\alpha - v_j^\beta$

and  $V$  represents the interatomic potential. The virial stress can be computed as a sum over all atoms (and atom pairs) in the simulation cell and then divided by the cell volume, *i.e.* the volume of the NW in this work.

The structure of aSiO<sub>2</sub>-Si NWs can be considered as an aSiO<sub>2</sub> layer encapsulating a crystalline Si core. Hence, the core-shell model can be utilized as the basic approach to implement the surface effect on the elastic response. The core-shell model describes the NW as a combination of a core and a surface region with a distinct set of elastic properties. Considering a finite thickness of  $t$  for the surface layer, the modulus of elasticity of the NW,  $E$ , under tensile load is given in Equation 7.2 where the moduli of elasticity of bulk Si and aSiO<sub>2</sub> are denoted by  $E_{Si}$  and  $E_{aSiO_2}$ , respectively [Xu et al., 2010, Chen et al., 2006a].

$$E = E_{Si} \left[ 1 + 4 \left( \frac{E_{aSiO_2}}{E_{Si}} - 1 \right) \left( \frac{t}{W} - \frac{t^2}{W^2} \right) \right] \quad (7.2)$$

Although the core-shell models are capable of considering the surface effect, a close estimation of  $E_{aSiO_2}$  and  $t$  are required. In this work,  $E_{Si}$  and  $E_{aSiO_2}$  are computed via tensile MD simulations, while Equation 7.2 is used for the estimation of the accuracy and trends of NW tensile simulation results. To estimate  $E_{Si}$  and  $E_{aSiO_2}$ , tensile tests are performed with the TM and m-SW potentials using periodic boundary conditions in all directions. Thus, the effect of native oxide on the mechanical behavior of Si NWs is studied using both MD and analytical models.

## 7.4 Results and Discussion

The influence of native oxide on the mechanical properties of Si NWs will be presented in this section through studying i) modulus of elasticity, ii) ultimate strength, and iii) fracture behavior. Results will be presented in the following sequence:

- In the first step, the reliability of interatomic potentials is studied for Si NWs and aSiO<sub>2</sub>-Si NWs of the same size.
- Then, the effect of oxide thickness and AR is investigated using TM and m-SW interatomic potentials.

- Next, a comparison with the core-shell model is carried out to evaluate limits associated with using analytical methods to estimate the modulus of elasticity.
- Then the impact of the native oxide on the ultimate strength of Si NWs is studied based on both potentials.
- This is followed by a benchmark study on the role of crystal orientation on the performance of interatomic potentials.
- At the end of this section, the failure behavior of aSiO<sub>2</sub>-Si NWs is compared to that of Si NWs.

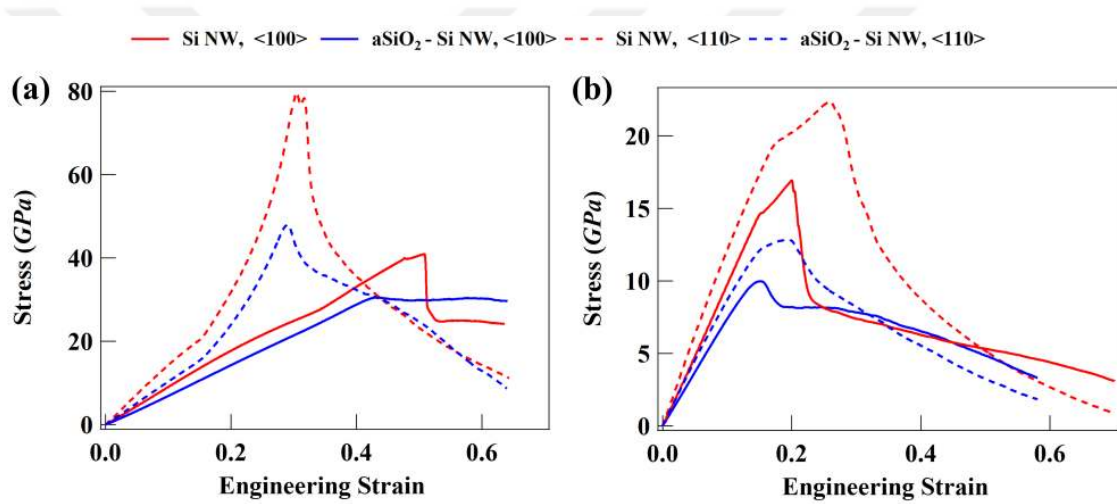


Figure 7.2: Stress-strain curves of Si NWs and aSiO<sub>2</sub>-Si NWs modeled using the (a) TM, and (b) m-SW potentials. The associated orientations of Si crystal in NWs as  $\langle 100 \rangle$ -Si and  $\langle 110 \rangle$ -Si are depicted with solid and dashed lines, respectively. The corresponding change in stress-strain curves of Si NWs with native oxide (blue curves) compared to Si NWs with unreconstructed surface (red curves) exhibit the change in modulus of elasticity (slope of stress strain curve at strains  $< 4\%$ ) and ultimate strength (maximum stress) of NWs due to presence of native oxide.

For a comparison of the TM and m-SW interatomic models, the mechanical properties of NWs are studied with  $L = 100$  nm,  $W = 5$  nm, and  $t = 0.5$  nm. Figure 7.2 depicts the stress-strain curves for Si NWs and aSiO<sub>2</sub>-Si NWs modeled with both potentials. For small strains, the stress-strain relation is linear representing the elastic regime for all NWs, where the modulus of elasticity can be directly estimated. The stress then changes non-linearly reaching the ultimate strength. Beyond this

Table 7.1: Modulus of elasticity and ultimate strength values calculated using different interatomic potentials for Si NWs and aSiO<sub>2</sub>-Si NWs.

| NW                            | Potential | Modulus of Elasticity<br>(GPa) | Ultimate Strength<br>(GPa) |
|-------------------------------|-----------|--------------------------------|----------------------------|
| Si < 100 >                    | TM        | 85.6                           | 41.0                       |
| aSiO <sub>2</sub> -Si < 100 > |           | 63.4                           | 30.6                       |
| Si < 110 >                    |           | 145.8                          | 79.4                       |
| aSiO <sub>2</sub> -Si < 110 > |           | 101.6                          | 47.8                       |
| Si < 100 >                    | m-SW      | 97.1                           | 16.9                       |
| aSiO <sub>2</sub> -Si < 100 > |           | 73.0                           | 15.3                       |
| Si < 110 >                    |           | 128.4                          | 22.3                       |
| aSiO <sub>2</sub> -Si < 110 > |           | 91.7                           | 14.8                       |

point, and accompanied by necking, it decreases until fracture. The modulus of elasticity and ultimate strength measured from the stress-strain curves for Si NWs and aSiO<sub>2</sub>-Si NWs are summarized in Table 7.1. Results show a reduction in the modulus of elasticity of aSiO<sub>2</sub>-Si NWs compared to that of Si NWs. This change is about 25% and 30% for NWs along < 100 > and < 110 > crystal orientations, respectively.

The yield stress and strain analysis are performed by defining the starting point of deviation of the stress-strain curves from the linear curve with the slope of the predicted modulus of elasticity below 4% strain. The linear regime associated with stress-strain curves used for the modulus of elasticity estimations is given in Supplementary 7.6.1. The stress-strain curves for NWs modeled with the TM potential in Figure 7.2 (a) show a linear increase up to a yield strain of 7.5% for Si NWs, whereas such deformation is limited to 4% for aSiO<sub>2</sub>-Si NWs. Such yield analysis shows a decrease in the yield strength from 5.6 GPa and 11.6 GPa for Si NWs to 2.5 GPa and 5.8 GPa for aSiO<sub>2</sub>-Si NWs in < 100 > and < 110 >, respectively. A similar inspection with the m-SW potential demonstrated in Figure 7.2 b) shows a

yield strain and a yield strength of 10% and 9.7 GPa decrease to 5.5% and 5.0 GPa upon oxidation, respectively. Exploration of yield strain and strength for  $\langle 110 \rangle$ -oriented Si NW and aSiO<sub>2</sub>-Si NWs using the m-SW potential indicates a similar reduction from 8% and 10.3 GPa to 5% and 4.9 GPa, respectively.

In the non-linear region of the stress-strain plots in Figure 7.2, a reduction in Si NW ultimate strength is observed for both crystal orientations. A decrease of 33% and 21% is obtained with the TM and m-SW potentials, respectively. Regardless of the surface state, there is a significant difference between the TM and m-SW potentials in predicting the ultimate strength. The reliability of these two potentials can be studied through comparing Figure 7.2 with experimental studies [Nasr Esfahani and Alaca, 2019, Zare Pakzad et al., 2021, DelRio et al., 2015, Wang et al., 2017]. The ultimate strength reported in experimental observations ranges between 10 GPa up to 23 GPa [Nasr Esfahani and Alaca, 2019], where the ultimate strength predicted for aSiO<sub>2</sub>-Si NWs modeled by the m-SW potential is in a similar range. In contrast, the TM potential overestimates the ultimate strength which can be linked to the soft cut-off scheme in the Tersoff potential [Le and Nguyen, 2014, Esfahani, 2022, Bartók et al., 2018]. Despite similarities of stress-strain curves obtained via both interatomic potentials for strains  $< 0.1$ , the overestimation of strength using the TM potential is reflected in results shown in Supplementary 7.6.2. This overestimation in the TM potential can be linked to the cut-off distance considered in the empirical model [Le and Nguyen, 2014, Belytschko et al., 2002, Le and Nguyen, 2015]. With prior examples of failure strength overprediction observed at nanoscale modelling efforts, it should be noted that recent MD simulations with Tersoff and Tersoff-like potentials would estimate the fracture strength and strain due to the problem of the cut-off function [Le and Nguyen, 2014]. Further discussion and details on the discrepancies between the TM and m-SW potentials to predict the mechanical properties is provided in Supplementary 7.6.2. Despite this challenge, the TM potential will be still used to study the native oxide effect on the mechanical behavior of NWs, considering that the TM potential is capable to accurately model the modulus of elasticity reduction due to the native oxide effect. Previously

reported modulus of elasticity for Si NWs by experimental efforts [Nasr Esfahani and Alaca, 2019, Zare Pakzad et al., 2021] is in the range of 65 GPa up to 230 GPa, comparable with the estimated modulus of elasticity for aSiO<sub>2</sub>-Si NWs using the TM and mod-SW potentials as summarized in Table 7.1. Considering the deficiency of the TM potential to model the ultimate strength values, comparison of the fracture behavior with experimental work [Nasr Esfahani and Alaca, 2019] will be carried out via m-SW potential only. A similar reduction in the mechanical properties of Si NWs with amorphous silica layer was reported previously [Xu, 2020]. As discussed earlier, the strain rate considered here is in the same range as those of previous MD studies of NW tensile tests [Kang and Cai, 2007]. The impact of the strain rate on the modeling of Si and aSiO<sub>2</sub>-Si NWs NW tensile properties by the TM and m-SW potentials is presented in Supplementary 7.6.1. The findings exhibit an almost negligible change of the modulus of elasticity and ultimate strength.

Having studied the performance of interatomic potentials, the impact of  $t$  on the mechanical properties of Si NWs is studied next. The native oxide thickness depends on parameters such as the crystallographic orientation and surface preparation [Shir et al., 2006]. Previous theoretical studies report a native oxide thickness ranging between 0.2 nm to 1.0 nm [Xu, 2020]. However, the oxide can be as thick as 2.0 nm using thermal oxidation processes [Ohta et al., 2007]. To understand the influence of native oxide on the elastic behavior, at first, the effect of  $t$  is investigated for various AR. Tensile tests are carried out on NWs with  $W = 5$  nm to 9 nm and  $t = 0.5$  nm and 1.0 nm.

Figure 7.3 shows the modulus of elasticity according to the TM and m-SW potentials. Results generally exhibit a negligible dependence of the modulus of elasticity on AR for both surface states. The only considerable increase in the modulus of elasticity is observed for aSiO<sub>2</sub>-Si NWs with  $W = 6$  nm, if  $AR < 15$ . Further examination of the results in Figure 7.3 reveals a significant reduction of modulus of elasticity with increasing  $t$ , a direct result of the native oxide. However, the size effect on the modulus of elasticity for Si NWs remains insignificant in both crystal orientations. In addition, there is a size-dependent elastic response in aSiO<sub>2</sub>-

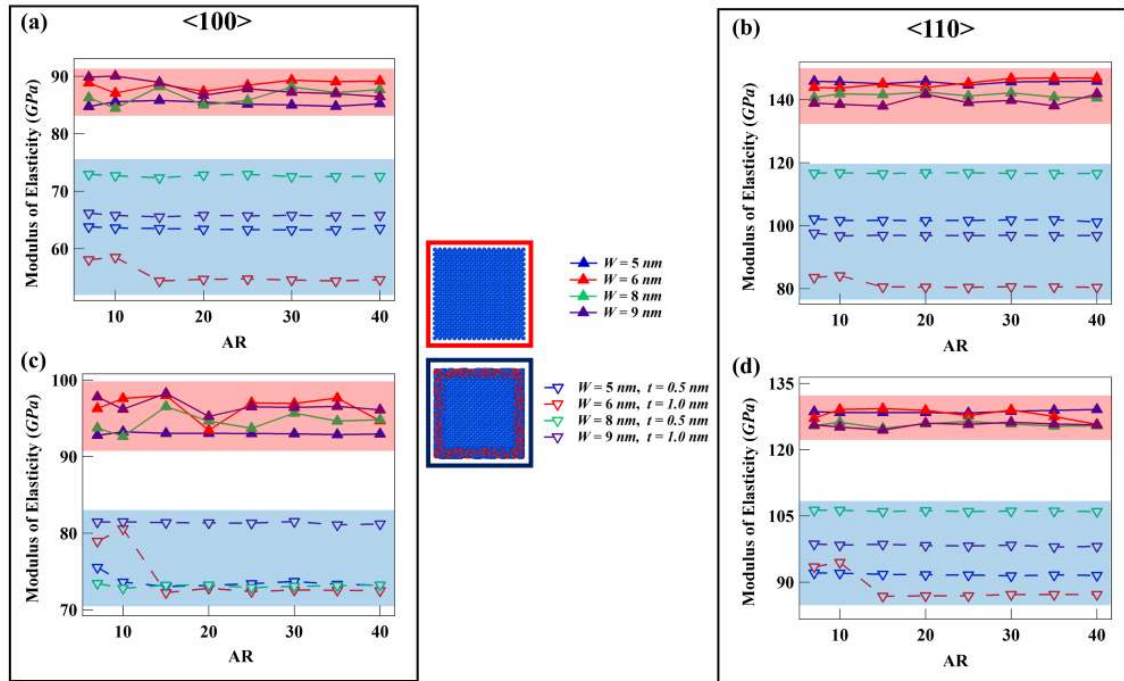


Figure 7.3: The modulus of elasticity as a function of AR for Si NWs and aSiO<sub>2</sub>-Si NWs along (a)  $\langle 100 \rangle$  and (b)  $\langle 110 \rangle$  crystal orientations modeled by the TM potential and along (c)  $\langle 100 \rangle$  and (d)  $\langle 110 \rangle$  crystal orientations modeled by the m-SW potential. Different widths (and different native oxide thicknesses for aSiO<sub>2</sub>-Si NWs) of NWs are examined where Si NWs and aSiO<sub>2</sub>-Si NWs are color-coded with red and blue color codes on modulus of elasticity vs. AR graphs with different levels of reduction due to combined effects of size, native oxide thickness, crystalline orientation, and interatomic potential effects.

Si NWs, where increasing  $W$  at a constant  $t$ , increases the modulus of elasticity. This size effect becomes negligible in aSiO<sub>2</sub>-Si NWs of  $\langle 100 \rangle$  modeled by the m-SW potentials, which can be traced back to the combined effect of  $W$ , crystal orientation and interatomic potential.

In addition to the interatomic potential, crystal orientation has a drastic impact on the modulus of elasticity. As discussed earlier in the context of native oxide effect on modulus of elasticity of Si NWs, the results in Figure 7.3 b) and Figure 7.3 (d) also confirm that native oxide reduces the modulus of elasticity for  $\langle 110 \rangle$ -oriented aSiO<sub>2</sub>-Si NWs in a range of 15% to 42%, depending on  $W$  and  $t$ . This change on the modulus of elasticity as a result of native oxide is in a range of 12% to 32%



Table 7.2: Modulus of elasticity of the bulk,  $E_{Si}$  and  $E_{aSiO_2}$ .

| Material                 | Potential | Modulus of Elasticity of the Bulk (GPa) |
|--------------------------|-----------|-----------------------------------------|
| Si $\langle 100 \rangle$ | TM        | 87.4                                    |
| Si $\langle 110 \rangle$ |           | 133.1                                   |
| aSiO <sub>2</sub>        |           | 59.4                                    |
| Si $\langle 100 \rangle$ | m-SW      | 94.1                                    |
| Si $\langle 110 \rangle$ |           | 120.3                                   |
| aSiO <sub>2</sub>        |           | 111.7                                   |

for  $\langle 100 \rangle$  NWs as shown in Figure 7.3 (a) and Figure 7.3 (c). This observation indicates that the native oxide effect on the elastic behavior in  $\langle 110 \rangle$  is stronger compared to  $\langle 100 \rangle$ . This can be linked to a larger difference between the elastic moduli of aSiO<sub>2</sub> and Si  $\langle 110 \rangle$  compared to Si along  $\langle 100 \rangle$ . The comparison of the modulus of elasticity for Si NWs and aSiO<sub>2</sub>-Si NWs exhibits a drastic effect of the native oxide on NWs with smaller  $W$ . For instance, the reduction in modulus of elasticity observed for aSiO<sub>2</sub>-Si NWs of  $W$  of 5 nm and 6 nm is more significant compared to  $W$  of 8 nm and 9 nm.

In the next step, an analytical model, *i.e.* the core-shell model, is used to verify the impact of the native oxide on the size-dependent elastic behavior of Si NWs. For this purpose,  $E_{Si}$  and  $E_{aSiO_2}$  of Equation 7.2 are predicted using MD simulations and are listed in Table 7.2. These results are in good agreement with previous theoretical and MD studies [Ilinov and Kuronen, 2014, Park et al., 2005] as well as experimental measurements [Wortman and Evans, 1965]. A modulus of elasticity around 70-75 GPa was reported previously [Ni et al., 2006, Scholze, 1991, Silva et al., 2006, Dávila et al., 2009, Yuan and Huang, 2012, Yuan and Huang, 2013] for aSiO<sub>2</sub>, while in this study the TM potential predicts a lower  $E_{aSiO_2}$  compared to the m-SW potential as shown in Table 7.2. To examine the native oxide effect on the modulus of elasticity by the core-shell model, different oxide thicknesses are considered for aSiO<sub>2</sub>-Si NWs as shown in Figure 7.4. Starting from the TM potential,

the modulus of elasticity of NWs of  $\langle 100 \rangle$  modeled by MD changes from 70 GPa to 55 GPa with  $t$  increasing from 0.25 nm to 1.0 nm, while the core-shell model predicts a reduction from 80 GPa to 70 GPa. Similarly, the modulus of elasticity of  $\langle 110 \rangle$  NWs decreases with increasing  $t$  using both MD and core-shell methods, while some deviation between the predictions is observed. This discrepancy between MD simulations and the core-shell model increases in the case of the m-SW potential, where MD simulations predict a change from 80 GPa to 70 GPa in contrast to the core-shell model estimating an almost constant  $E$  of 100 GPa. A similar difference between MD simulations and core-shell model is observed in  $\langle 110 \rangle$  NWs as well. MD results show a reduction in  $E$  from 105 GPa to 85 GPa by changing  $t$  from 0.25 nm to 1.0 nm, while the core-shell model estimates an almost constant  $E$  of 120 GPa. Stress-strain curves associated with each modulus of elasticity estimation depicted in Figure 7.4 are presented in Supplementary 7.6.2. A previous MD study on the oxide effect in Si NWs reported a similar reduction in  $E$  with increasing  $t$  [Xu, 2020]. Despite such differences between modulus of elasticity predictions using MD and core-shell model, both methods clearly confirm the reduction due to the native oxide effect in aSiO<sub>2</sub>-Si NWs. The difference between the predictions of the modulus of elasticity by the core-shell model and MD can be traced back to the non-continuous elasticity definition in core-shell model at the interface of bulk core Si and surface shell oxide regions. Such general assumption in core-shell model violates the continuity condition at the interface of the two layers and leads to unphysical interpretations of NW elastic response. To address this shortcoming, alternative approaches such as the modified core-shell models were proposed [Xu et al., 2016, Yao et al., 2012]. Similarly, core-shell model also falls short of considering intrinsic effects such as stresses generated due to the formation of native oxide on NW surfaces with recent studies revealing stresses up to 2 GPa induced in Si NWs as a direct outcome of native oxide formation [Nasr Esfahani et al., 2022].

As the next stage, the TM and m-SW potentials are used to study the effect of native oxide on the ultimate strength of Si NWs and aSiO<sub>2</sub>-Si NWs. The case of AR = 20 was already discussed in connection with Table 7.1. Figure 7.5 now

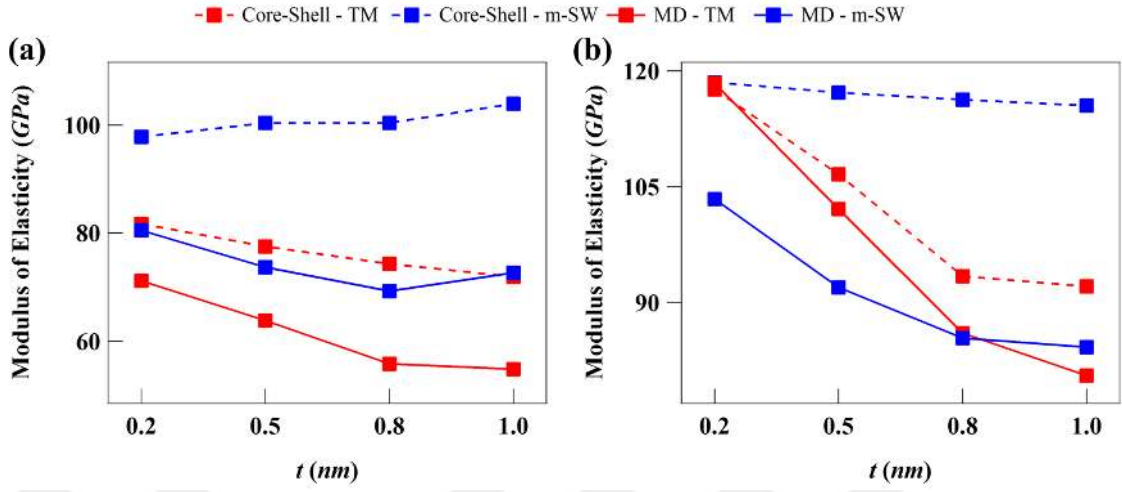


Figure 7.4: The modulus of elasticity predicted based on the core-shell model and MD simulations for aSiO<sub>2</sub>-Si NWs of core Si thickness of 4 nm and AR = 20 along (a)  $\langle 100 \rangle$  and (b)  $\langle 110 \rangle$  as a function of the native oxide thickness,  $t$ . Results demonstrate and compare the level of success in modulus of elasticity estimation for aSiO<sub>2</sub>-Si via analytical and MD methods with combined effects native oxide thickness, interatomic potential, and crystalline orientation of Si.

depicts the ultimate strength as a function of AR. First of all, results regularly exhibit reduction of strength with oxidation. This reduction is in the range of 5% to 40% in the case of  $\langle 100 \rangle$ -oriented aSiO<sub>2</sub>-Si NWs, depending on  $W$ ,  $t$  and interatomic potential, as shown in Figure 7.5 (a) and Figure 7.5 (c). For  $\langle 110 \rangle$ , the reduction in strength is between 29% to 42% as depicted in Figure 7.5 (b) and Figure 7.5 (d). The amount of reduction in the ultimate strength for aSiO<sub>2</sub>-Si NWs of  $\langle 110 \rangle$  is higher compared to NWs of  $\langle 100 \rangle$ . This could be traced back to the differences between the ultimate strengths of core crystals compared to the native oxide. Analyzing the impact of  $t$  on the ultimate strength of aSiO<sub>2</sub>-Si NWs as a function of AR reveals a decreasing ultimate strength of aSiO<sub>2</sub>-Si NWs with increasing  $t$ . The SW potential predicts a raise in the ultimate strength with increasing AR of Si NWs, while the size effect on the ultimate strength is negligible for aSiO<sub>2</sub>-Si NWs. This is in agreement with previous studies, where the impact of oxide layer on the ultimate strength of Si NWs covered with amorphous silica was demonstrated as a reduction from 25 GPa to 8 GPa [Xu, 2020]. Results obtained

here for Si NWs can be compared with previous MD simulations. For instance, elastic properties in Table 7.1 are comparable with previous studies on  $\langle 100 \rangle$  Si NWs with estimations ranging from 40 GPa up to 125 GPa depending on the NW size, interatomic potential and thermodynamic state such as temperature [Liu and Shen, 2012, Liu et al., 2015, Jing et al., 2009a, Zhuo and Beom, 2019]. Similarly, modulus of elasticity values reported for  $\langle 110 \rangle$  Si NWs [Kang and Cai, 2007, Kang and Cai, 2010, Liu et al., 2015, Jing et al., 2009a, Jing et al., 2009b, Xu, 2020, Xu and Kim, 2019] are comparable with results presented in Table 7.1 ranging between 60 GPa to 170 GPa. Parameters such as cross-section, AR, temperature, and the interatomic potential cause such a wide range of prediction for modulus of elasticity of Si NWs of different orientations.

After studying the elastic and strength properties, the native oxide effect on the fracture behavior is examined next. Previous studies report different fracture properties in Si NWs, where a range of ductile, brittle or a mixture of both were observed among MD models using different potentials such as the Tersoff-T3, SW and modified Embedded Atom Method (MEAM) potentials [Kang and Cai, 2007, Xu and Kim, 2019, Liu and Shen, 2012, Kang and Cai, 2010, Xu and Kim, 2020, Xu, 2020]. To distinguish the brittle fracture from the ductile behavior, various parameters are recommended as ductility measures by various studies focusing on fracture of NWs [Kang and Cai, 2007, Xu and Kim, 2019]. The ductility parameter suggested by Kang and Cai [Kang and Cai, 2007] combines the effect of ideal tensile strength and ideal shear strength with Schmid factor predicting a ductile fracture behavior for the Tersoff and SW potentials and reporting brittle fracture modes mostly for the MEAM potentials. In contrast, Xu and Kim [Xu and Kim, 2019] introduced a definition to quantify the slip deformation due to the development of cleavage surfaces on  $(110)$  plane and  $\{111\}$  plane family, while the brittle fracture in Si NWs were reported similar to the findings of the ductility parameter model [Kang and Cai, 2007], confirming a consistent brittle behavior.

To quantify the ductile/brittle failure, a parameter denoted as the ductile failure probability ( $p$ ) was introduced considering complete brittle and complete ductile

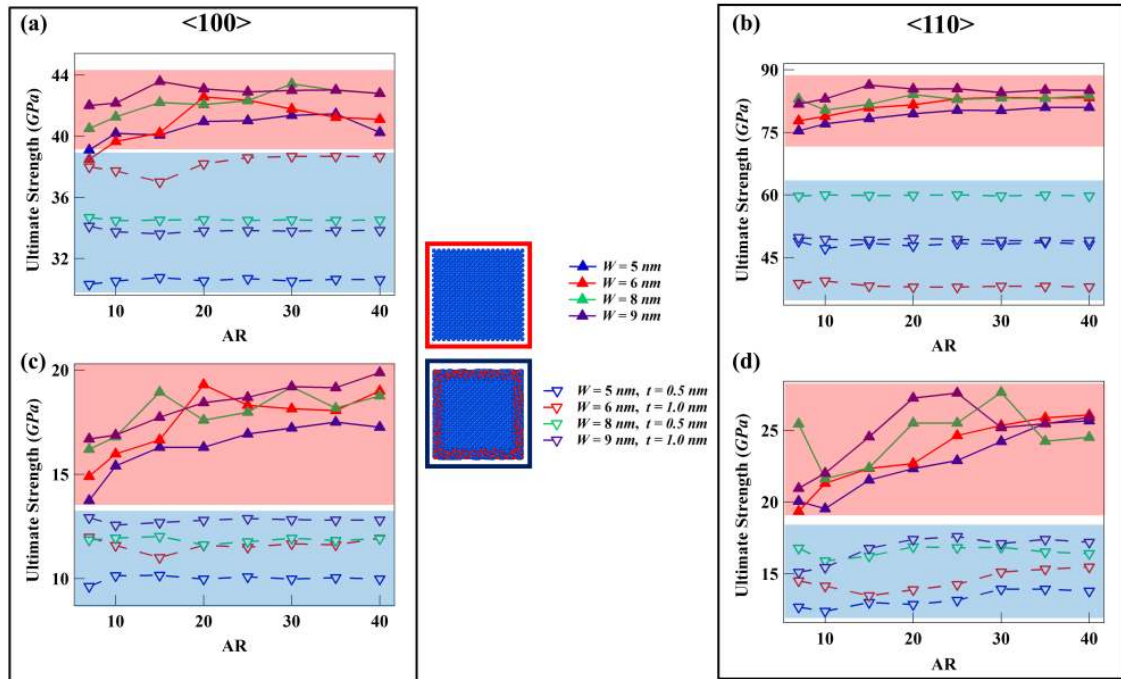


Figure 7.5: The ultimate strength as a function of AR for Si NWs and aSiO<sub>2</sub>-Si NWs along (a) < 100 > and (b) < 110 > crystal orientations modeled by the TM potential and along (c) < 100 > and (d) < 110 > crystal orientations modeled by the m-SW potential. Different widths (and different native oxide thicknesses for aSiO<sub>2</sub>-Si NWs) of NWs are examined where Si NWs and aSiO<sub>2</sub>-Si NWs are color-coded with red and blue color codes on ultimate strength vs. AR graphs with different levels of reduction due to combined effects of size, native oxide thickness, crystalline orientation, and interatomic potential effects.

failure for  $p = 0$  and  $p = 1$ , respectively [Xu and Kim, 2019]. The definition of this parameter is based on the type of fracture categorized as full and partial failures due to necking and slip or cleavage in above mentioned planar directions. The ductile failure parameter is defined as  $p = (W_0 - W_{fail})/W_0$ , where  $W_0$  is the nominal width and  $W_{fail}$  is the width at the failure as shown in Figure 7.6 (a). The criterion for the full necking case is taken as  $p > p_{cr} = 0.5$  as suggested previously [Xu and Kim, 2019], where the NW remains connected even after the width reduces to less than a half of the nominal value. For all NWs studied in this work, ductile fracture was consistently observed as expected from the TM and m-SW potentials, an observation in parallel with previous findings [Kang and Cai, 2007, Kang and Cai, 2010, Godet et al., 2015]. Similar ductile fracture was observed for aSiO<sub>2</sub>-Si NWs as shown in Figure 7.6 (b) demonstrating full necking during failure. Initiation of the partial reduction in  $W$  is represented in left snapshots of Figure 7.6 (a) and Figure 7.6 (b).  $W$  is reduced to less than a half of its nominal value due to the full necking while both parts remain connected as shown in the right snapshots of respective figures.

Some partial necking behavior was also observed in aSiO<sub>2</sub>-Si NWs while most of NWs failed due to a full necking. Ductile failure probability calculations were performed on NWs represented in Figure 7.5 and  $AR = 20$ . Results in Figure 7.6 (c) show a reduction in the ductile probability with increasing  $W$ , indicating an increased probability of ductile fracture with reduced  $W$  in both crystal orientations modeled by TM and m-SW potentials. The reduction in ductile failure probability with increasing  $W$  as depicted in Figure 7.6 (c) agrees well with previous reports on ductility of Si NWs using Tersoff or MEAM-based interatomic potentials [Kang and Cai, 2007, Xu and Kim, 2019]. Moreover, Figure 7.6 (c) also exhibits ductile failure estimation for aSiO<sub>2</sub>-Si NWs via both interatomic potentials. The deviations obtained for failure predictions of aSiO<sub>2</sub>-Si NWs are associated with crystallographic orientation, critical dimension, and oxide layer thickness effects. Hence, ductile failure mechanisms can be captured in Si NWs with a native oxide surface using two common interatomic potentials for Si-O interactions, namely Tersoff and SW. A similar change in the fracture behavior was reported previously for Si NWs

[Kang and Cai, 2010, Xu and Kim, 2019]. Failure analysis also shows an insignificant dependence of ductile failure probability on NW orientation. Two leading parameters in such a probability analysis are strain rate and temperature, while previous studies demonstrated slightly less ductile behavior at lower strain rates and lower temperatures [Kang and Cai, 2007, Xu and Kim, 2019, Xu, 2020]. This work utilized a moderate strain rate which is more suitable for tensile simulation of NWs at low temperatures below 10 K for the minimization of the kinetic effects. As a result, a higher size-dependent failure probability for aSiO<sub>2</sub>-Si NWs is obtained with a  $W$  of 5 nm and 6 nm compared to  $W$  of 8 nm and 9 nm as depicted in Figure 7.6 (c). Similarly, previous works on the failure behavior of Si NWs with amorphous silica layer show that NWs with thinner oxide layers fail by necking, while increasing the oxide thickness leads to brittle fracture of Si NWs [Xu, 2020]. Calculating  $p$  for aSiO<sub>2</sub>-Si NWs at different temperatures can be helpful for the examination of the brittle-to-ductile transition temperature in Si NWs [Xu and Kim, 2019, Kang and Cai, 2007].

## 7.5 Conclusion

This work investigates the effect of native oxide on the size-dependent mechanical behavior of Si NWs. For this purpose, mechanical properties of pure Si NWs and aSiO<sub>2</sub>-Si NWs are compared using MD simulations with TM and m-SW interatomic potentials. The uniaxial tensile deformation is imposed with a strain rate of  $\dot{\epsilon} = 5 \times 10^9 s^{-1}$  at temperatures below 10 K while using periodic B.C.s along the NW length and applying fixed B.C.s along the other two axes. The effect of critical factors such as crystal orientation, oxide thickness, interatomic potential, and AR are examined. The following set of conclusions can be made:

- Both interatomic potentials are found to be reliable for modeling the modulus of elasticity of Si NWs and aSiO<sub>2</sub>-Si NWs. On the other hand, the m-SW potential is found to estimate the ultimate strength comparable to previous theoretical and experimental findings. In contrast, the TM potential overestimates the ultimate strength, which can be linked to the soft cut-off scheme in the Tersoff potential.

- Furthermore, the core-shell model is used to verify the impact of native oxide on the size-dependent elastic behavior of Si NWs.

- Results demonstrate an insignificant size effect on the elastic behavior of Si NWs for both crystal orientations, while the native oxide layer reduces the modulus of elasticity considerably with increasing oxide thickness. Similarly, the ultimate strength of aSiO<sub>2</sub>-Si NWs is found to be drastically lower than that of Si NWs due to the presence of native oxide. Moreover, the ultimate strength estimations exhibit a negligible AR effect for Si NWs and aSiO<sub>2</sub>-Si NWs.

- The reduction in the modulus of elasticity can be as significant as 42%, while strength is observed to diminish by 21%. Such significant reductions in mechanical properties of Si NWs are clear indications of the size effect particularly elaborated as core Si size and native oxide thickness for aSiO<sub>2</sub>-Si NWs in this study.

- To quantify the failure behavior of aSiO<sub>2</sub>-Si NWs, ductile failure probability is calculated with mixed behavior observed with full necking failure as the most dominant fracture condition. With decreasing NW width, a higher probability of ductile fracture is observed in Si NWs compared to aSiO<sub>2</sub>-Si NWs.

- The significant variations in properties and failure mode of Si NWs compared to those exhibited by aSiO<sub>2</sub>-Si NWs verifies the extremely important and useful outcome of including the native oxide in the interpretation of size dependence of Si NW properties.

- Finally, the contribution of native oxide should be assessed further via combining computational and experimental efforts to examine the physical mechanisms behind size-dependent mechanical behavior of Si NWs.

In fact, various studies considered Si NW surface as a significant factor contributing to mechanical properties including failure mechanisms. However, the present study clearly reveals the important role played by the native oxide layer on the size-dependent mechanical behavior of Si NWs. By doing so, it also sheds further light on the background of various conflicting reports in the literature such as opposing trends of modulus of elasticity estimations with reduced size scale. The findings can serve as a powerful tool for interpretation of size-dependency in properties of Si



NWs, as – to the best of our knowledge – no previous MD study exists for inspection of size-dependent properties in Si NWs with native oxide surface condition. The reductions observed in Si NW modulus of elasticity and strength due to the presence of native oxide heavily depend on the thickness of oxide layer. With the probability of ductile failure fracture reduced for Si NWs and aSiO<sub>2</sub>-Si NWs with increasing  $W$ , further study on the prediction of the critical dimension for the initiation of brittle fracture is suggested. Methods such as ideal shear strength calculation of Ref. [Kang and Cai, 2007] can be used for this purpose. This is a very valuable insight for the interpretation of experimental observations and extraction of properties from measured data. Elimination of assumptions such as pure Si surface instead of native oxide will further help reduce both the discrepancies between computational and experimental findings and the resulting scatter in estimated modulus of elasticity and fracture strength of Si NWs. Overall, the present study highlights the importance of native oxide layer on the size-dependent mechanical behavior of Si NWs shedding further light on the background of various conflicting reports in the literature. This work can be extended by incorporating a detailed analysis of the interface between the crystalline Si core and native oxide as well as an examination of further – such as thermal – properties of Si NWs.

## 7.6 Supporting Information

### 7.6.1 Strain Rate Effect

The effect of strain rate on the mechanical behavior of Si NWs is studied using LAMMPS code. Tensile response of Si and aSiO<sub>2</sub>-Si NWs are examined via using two different strain rates here. The simulations are repeated using the TM and m-SW interatomic potentials. Figure 7.7 shows the tensile properties of Si NWs and aSiO<sub>2</sub>-Si NWs with  $\langle 100 \rangle$  and  $\langle 110 \rangle$  crystal orientations tested with strain rates,  $\dot{\epsilon} = 1 \times 10^8 \text{ s}^{-1}$ . Figures 7.7 (a) and (b) exhibit the stress-strain graphs for NWs tested using the TM and m-SW interatomic potentials, respectively.

The modulus of elasticity and ultimate strength of NWs modeled by the TM and

Table 7.3: Modulus of elasticity and ultimate strength values calculated using different interatomic potentials for Si NWs and aSiO<sub>2</sub>-Si NWs tested via two different strain rates.

| Material                      | Potential | $\dot{\epsilon} = 1 \times 10^8 s^{-1}$ |           | $\dot{\epsilon} = 5 \times 10^9 s^{-1}$ |           |
|-------------------------------|-----------|-----------------------------------------|-----------|-----------------------------------------|-----------|
|                               |           | $E$ (GPa)                               | $S$ (GPa) | $E$ (GPa)                               | $S$ (GPa) |
| Si < 100 >                    | TM        | 85.9                                    | 29.8      | 85.6                                    | 40.2      |
| aSiO <sub>2</sub> -Si < 100 > |           | 71.4                                    | 28.9      | 63.6                                    | 30.5      |
| Si < 110 >                    |           | 145.5                                   | 43.3      | 145.7                                   | 77.0      |
| aSiO <sub>2</sub> -Si < 110 > |           | 112.3                                   | 40.3      | 101.7                                   | 47.1      |
| Si < 100 >                    | m-SW      | 93.6                                    | 13.5      | 93.2                                    | 15.4      |
| aSiO <sub>2</sub> -Si < 100 > |           | 78.7                                    | 9.3       | 73.6                                    | 10.1      |
| Si < 110 >                    |           | 128.8                                   | 16.9      | 128.4                                   | 19.5      |
| aSiO <sub>2</sub> -Si < 110 > |           | 97.9                                    | 10.4      | 92.0                                    | 10.4      |

m-SW potentials are listed in Table 7.3. For the modulus of elasticity estimations using two different strain rates, the deviations are below 10% for all NWs tested here via the TM and m-SW potentials. For ultimate strength estimations via m-SW potential, the predictions could deviate up to 15%. However, for NWs modeled using the TM potential, the overprediction due to cut-off function of this potential can be clearly observed and the results deviate up to 70%. As discussed earlier, the ultimate strength estimations via TM potential are not reliable. The interested reader is encouraged to follow the literature cited in the References [Bartók et al., 2018, Le and Nguyen, 2014, Belytschko et al., 2002] for further elaboration on the origin of cut-off functions and the subsequent effects on overestimation of strength via Tersoff-like potentials. Observation of differences up to 10% for modulus of elasticity and up to 15% for ultimate strength (via m-SW potential) estimations with respect to strain rate selection shows the negligible impact of strain rate on the results presented in this work. Moreover, the deviations observed in this study are in an acceptable range of relative errors reported for different interatomic potentials of Si where the predictions are compared with results from a DFT reference model

[Nasr Esfahani et al., 2022].

### 7.6.2 Effect of native oxide thickness

The effect of native oxide thickness on the mechanical behavior of Si NWs is studied using LAMMPS. Tensile response of Si and aSiO<sub>2</sub>-Si NWs is examined by considering four different oxide thicknesses. The simulations are repeated using the TM and m-SW interatomic potentials. Figure 7.8 (a) and (b) demonstrate the stress-strain relation for aSiO<sub>2</sub>-Si NWs with  $\langle 100 \rangle$  and  $\langle 110 \rangle$  orientation, respectively. The NWs have different oxide layer thicknesses ranging between 0.25 nm to 1.00 nm given in Figure 7.4. Results demonstrate the stress-strain curves associated with the modulus of elasticity estimations given before.

A comparison between stress-strain curves obtained via the TM and m-SW potentials on identical NWs reveals similar linear responses for strains up to 0.1, while it also shows a clear overestimation of strength in the case of TM potential. The overestimation of the maximum force needed to break an interatomic bond is controlled by the cut-off function of the potential. It is also proven that the original cut-off function by the Tersoff potential leads to overestimations in strength estimations for different materials as evident from previous studies [Bartók et al., 2018, Le and Nguyen, 2014, Belytschko et al., 2002]. A solution is proposed by setting the small and the large cut-off distances as equal [Le and Nguyen, 2014]. Since, to our knowledge, there is no prior study examining the original versions of the TM and m-SW on Si and aSiO<sub>2</sub>-Si NWs, interatomic potentials are used in their original form with no further modifications. The interested reader is encouraged to follow the cited literature to gain further understanding of the origin of cut-off functions and subsequent effects on overestimation of strength via Tersoff-based potentials.

### 7.6.3 Linear regime for modulus of elasticity estimation

Figures 7.9 (a) and (b) demonstrate the stress-strain relations for Si and aSiO<sub>2</sub>-Si NWs with  $\langle 100 \rangle$  and  $\langle 110 \rangle$  orientations modeled using the TM and m-SW potentials, respectively, respectively. Results demonstrate the stress-strain curves

up to a strain of 0.04 associated with the region used for modulus of elasticity estimations given before.

Figures 7.10 (a) and (b) demonstrate the stress-strain relation for aSiO<sub>2</sub>-Si NWs with  $\langle 100 \rangle$  and  $\langle 110 \rangle$  orientations, respectively. Results demonstrate the stress-strain curves up to a strain of 0.04 associated with the region used for modulus of elasticity estimations given before.



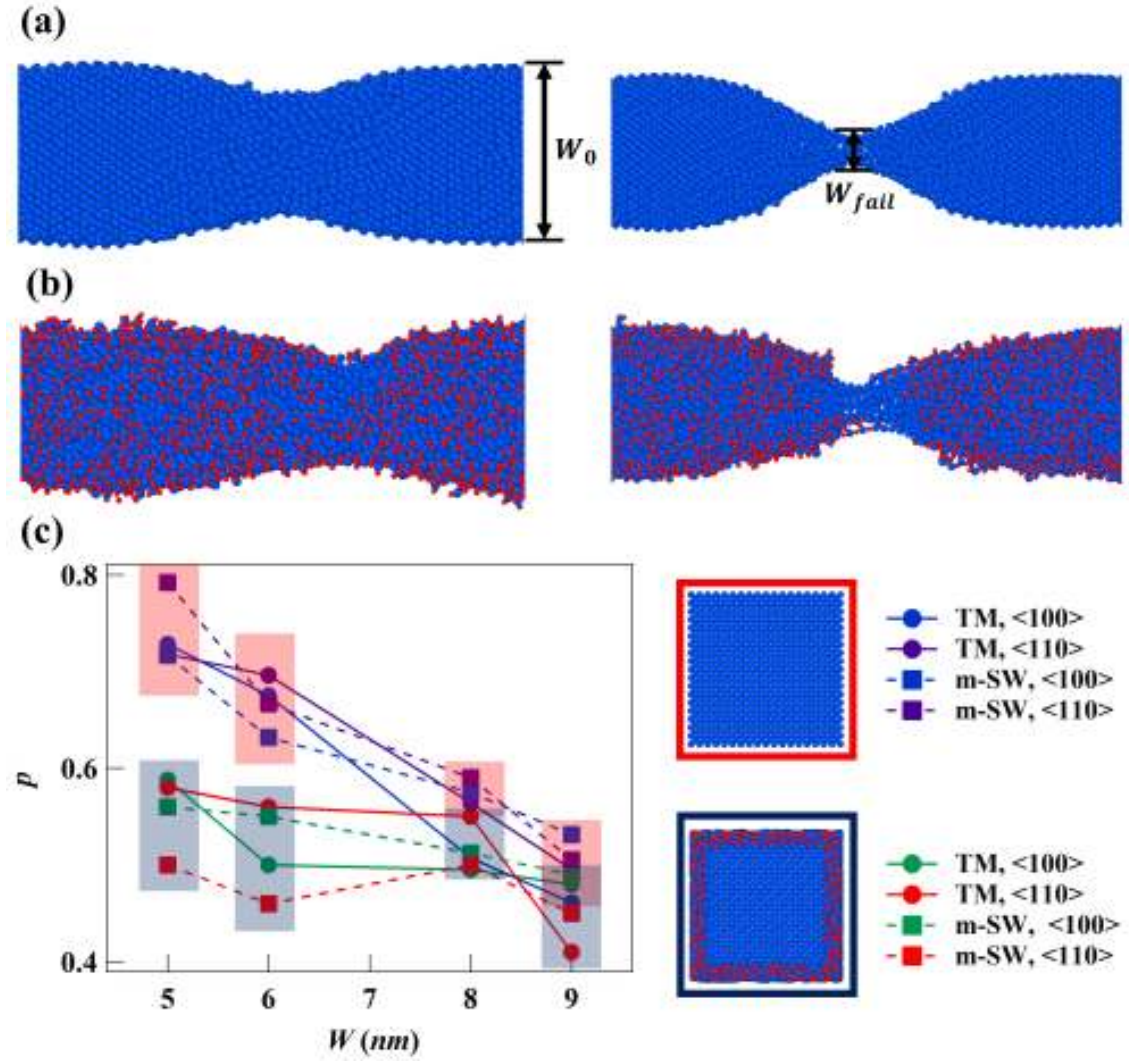


Figure 7.6: Full necking failure of NWs in (a) Si NW, and (b) aSiO<sub>2</sub>-Si NW (Blue spheres represent Si and red spheres denote O atoms) where the nominal width ( $W_0$ ) shown in left images and width at failure ( $W_{fail}$ ) of the NWs are used for ductile failure probability calculations. (c) Ductile failure probability of Si NWs and aSiO<sub>2</sub>-Si NWs with associated failure probability estimations color-coded for Si NWs with and without native oxide in red and blue, respectively. The ductile failure probability calculations are conducted for different width of NWs while examining both crystalline orientations ( $\langle 100 \rangle$ -Si and  $\langle 110 \rangle$ -Si) and both interatomic potentials (TM and m-SW) studied in this work.

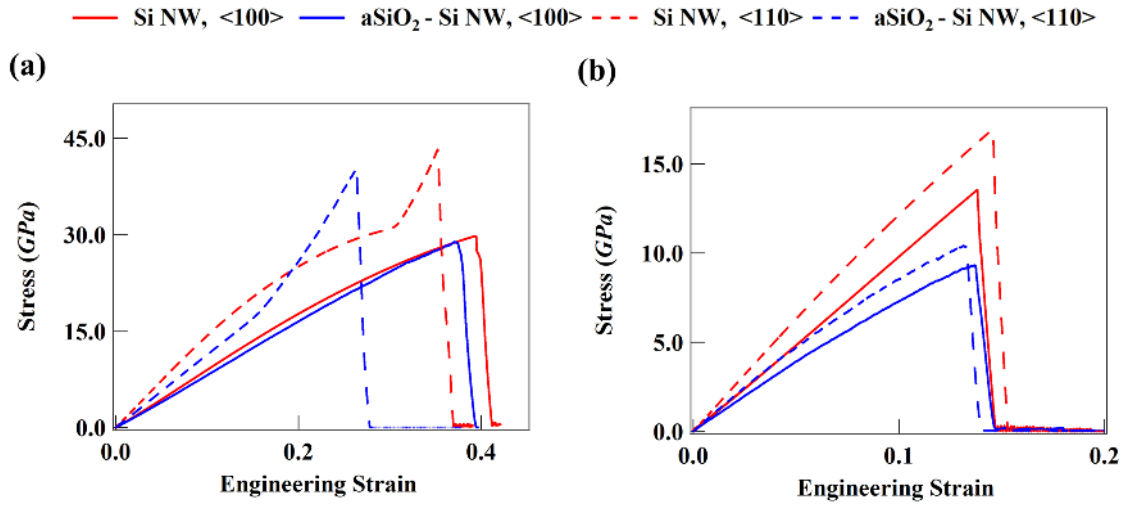


Figure 7.7: Stress-strain curves of Si NWs and aSiO<sub>2</sub>-Si NWs modeled using (a) the TM and (b) m-SW potentials and AR of 10 tested using  $\dot{\epsilon} = 1 \times 10^8 s^{-1}$ .

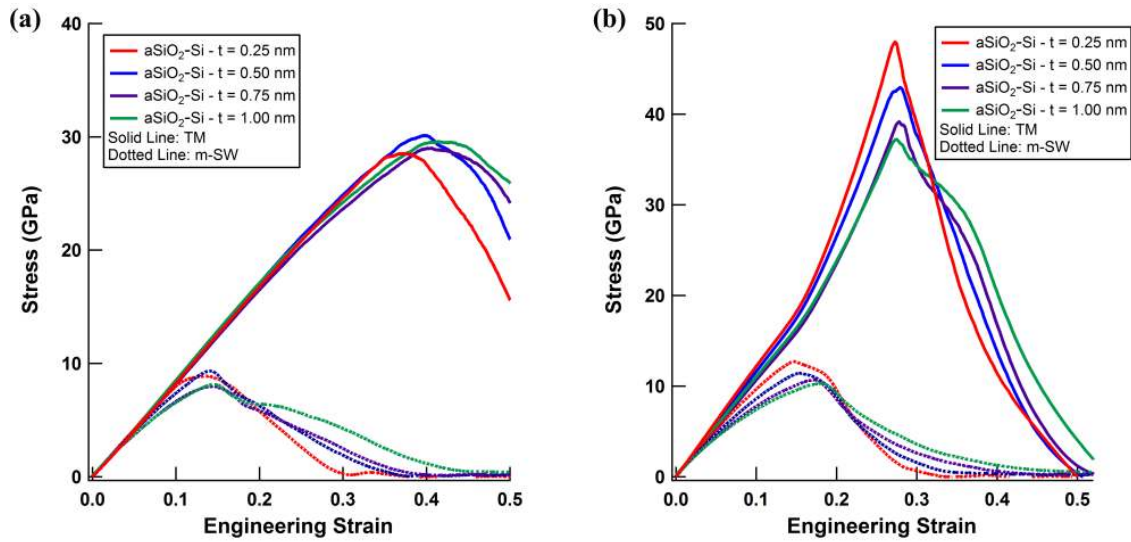


Figure 7.8: Stress-strain curves of aSiO<sub>2</sub>-Si NWs modeled with associated orientations for Si crystal in NWs as (a) <100>, and (b) <110>. The results for TM and m-SW interatomic potentials are depicted with solid and dotted lines, respectively.

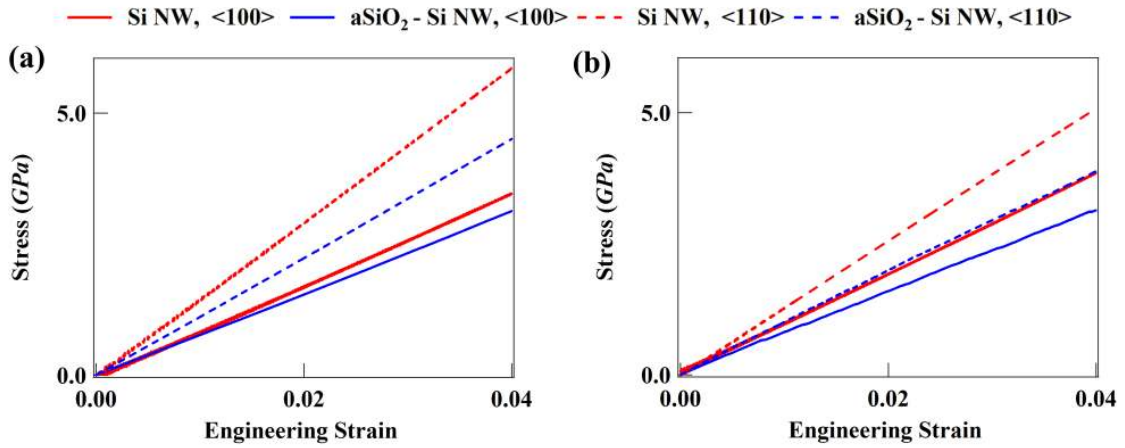


Figure 7.9: Stress-strain curves of Si NWs and aSiO<sub>2</sub>-Si NWs modeled using (a) the TM potential and (b) m-SW potentials plotted up to 0.04 strain used for estimation of modulus of elasticity.

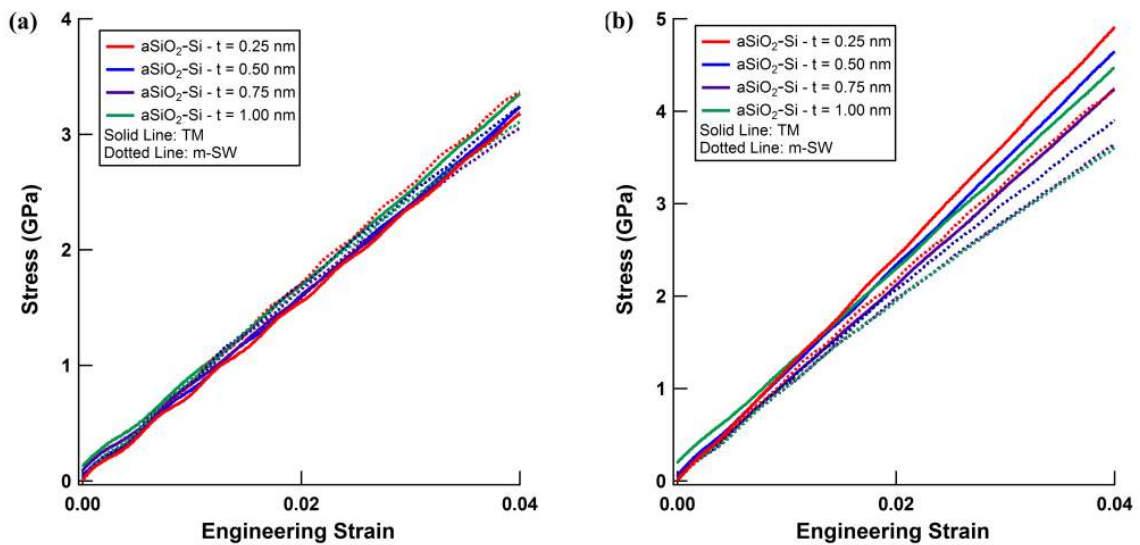


Figure 7.10: Stress-strain curves of aSiO<sub>2</sub>-Si NWs modeled with associated orientations for Si crystal in NWs as (a) < 100 >, and (b) < 110 >. The resulted for TM and m-SW interatomic potentials are depicted with solid and dotted lines, respectively. The stress-strain curves correspond to the linear regime of curves shown in Figure 7.8 plotted up to 0.04 of strain, used for estimation of modulus of elasticity.

## Chapter 8

# AN ANALYTICAL-ATOMISTIC MODEL FOR ELASTIC BEHAVIOR OF SILICON NANOWIRES

### 8.1 Overview

Silicon nanowires entail significant potential as sensors in nanoelectromechanical systems. Despite its crucial impact in such applications, inconsistent trends in mechanical behavior reported in computational and experimental studies remain unexplained. Hence, scale effect in even the most fundamental elastic properties requires clarification. This work introduces a multiscale model to bridge the existing gap between atomistic simulations and experimental observations encountered around a critical dimension of 10 nm. The combined approach of this work is based on molecular dynamics and modified core-shell model and captures the scale effect over a substantial size range. The evolution of the modulus of elasticity is thus studied and linked to nanowire critical dimension through the parameterization of surface inhomogeneity. The developed method is also validated through an analysis of native oxide revealing an average modulus of elasticity of 75 GPa. The method's applicability can be extended to similar one-dimensional structures with unique surface states.

### 8.2 Introduction

Silicon nanowires (Si NWs) exhibit a distinctive set of properties enabling their use in applications such as sensing, energy conversion and communication [Karimzadehkhoei et al., 2023, Nehra et al., 2020, Yang et al., 2021]. Compared to other one-dimensional nanostructures, the ease of their integration and miniaturization due to their compatibility with semiconductor manufacturing puts Si NWs in a unique position



to serve as the main transducer building block in nanoelectromechanical systems (NEMS) and nanoelectronic devices [Sessi et al., 2020, Zafar et al., 2018, Sage et al., 2018, Tintelott et al., 2021, Sreejith et al., 2023, Tran et al., 2023]. There is extensive literature studying the effect of miniaturization on the physical properties of Si NWs as a prerequisite for the development of innovative applications [Nasr Esfahani and Alaca, 2019, Wang et al., 2017, Yang et al., 2022, Zare Pakzad et al., 2023c, Nasr Esfahani et al., 2022, Zare Pakzad et al., 2021, Namazu, 2023, Zare Pakzad et al., 2023b, Zare Pakzad et al., 2023a]. In this regard, Si NW mechanical properties have drawn considerable attention, where several discrepancies exist among reported trends regarding the dependence of mechanical behavior on scale [Nasr Esfahani and Alaca, 2019, Yang et al., 2022]. Furthermore, most nanomechanical tests on Si NWs were reported for a critical dimension (CD) in excess of 10 nm, while computational studies were mainly restricted to CDs below 10 nm. This dimensional limitation from both experimental and computational perspectives has led to the loss of a common ground between the two approaches, thereby delaying the development of an understanding regarding the size dependence in Si NW mechanical properties [Nasr Esfahani and Alaca, 2019, Wang et al., 2017, Yang et al., 2022].

Surface effects, the leading outcome of miniaturization, are found to be an important factor influencing NWs properties [Nasr Esfahani and Alaca, 2019, Pakzad et al., 2023b]. The surface state pertains to the condition of a NW surface as identified by its physical, chemical, and structural properties. In the case of Si NWs, the surface state is commonly observed to be an amorphous silicon dioxide, or native oxide, layer covering Si core [Nasr Esfahani et al., 2022]. Native oxide is known to have significant effects such as reducing both the stiffness and strength [Pakzad et al., 2023b, Pakzad et al., 2024]. The formation of native oxide is also reported to generate substantial intrinsic tensile stresses within Si core up to 1.2 GPa [Nasr Esfahani et al., 2022]. A recent study highlighted the substantial impact of the combined effects of surface state and surface crystal anisotropy on the elastic properties and strength of Si NWs, which can be incorporated as the surface stress and surface elastic constants in Si NW nanomechanical modeling [Zare Pakzad et al., 2023c].

The implementation of such surface effects can be carried out through several analytical techniques. Core-surface [Zare Pakzad et al., 2023c, Gurtin and Ian Murdoch, 1975, Stan et al., 2008], core-shell (CS) [Miller and Shenoy, 2000, Chen et al., 2006a] and modified core-shell (M-CS) [Yao et al., 2012, Xu et al., 2016] models are extensively employed for this purpose. CS model utilizes a core with the modulus of the bulk material and a shell that is coaxial with the core, where the surface modulus is correlated to the reduction in surface bond lengths [Miller and Shenoy, 2000, Chen et al., 2006a]. CS model thus assumes an abrupt change of properties from the core to the surface. Hence, M-CS model was introduced to account for a gradual transition [Yao et al., 2012, Xu et al., 2016, Li et al., 2022]. So far, the surface state in M-CS approach has been utilized with unreconstructed Si only, thereby disregarding the presence of the native oxide surface [Yao et al., 2012, Xu et al., 2016, Li et al., 2022].

This study pursues the combination of M-CS model with molecular dynamics (MD) simulations in order to bridge the 10-nm CD gap between experimental and computational approaches mentioned above and thus provide a thorough understanding regarding the size-dependent elastic properties of Si NWs. By incorporating MD simulations, the surface effect, particularly due to the native oxide layer, will be captured, while M-CS model enables one to utilize this atomistic perspective beyond 10 nm. The need for such a multiscale modeling approach is clearly justified by recent compilation of data in review articles [Nasr Esfahani and Alaca, 2019, Yang et al., 2022].

### **8.3 Materials and Methods**

In this study, MD simulations are conducted using the modified Stillinger-Weber (m-SW) [Ganster et al., 2010] and Tersoff-Munetoh (TM) [Munetoh et al., 2007] interatomic potentials. Compared to other potentials utilized for the modeling of Si and oxygen interactions, these two were found to be optimum for capturing the elastic properties of Si NWs with a native oxide surface layer [Zare Pakzad et al., 2023c, Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2023a]. Si NWs in

different crystal orientations and with a diameter, ( $D$ ), in the range of 4 nm to 8 nm (as an indication of CD) are considered. In the remainder of this work, the native oxide layer with its amorphous structure will be denoted as aSiO<sub>2</sub>, and Si NWs with a native oxide layer (as opposed to those with an unreconstructed Si surface) are referred to as aSiO<sub>2</sub>-Si NWs.

The flowchart presented in Figure 8.1 outlines the computational methodology involving M-CS model combined with MD simulations. The M-CS model utilizes an exponential expression for the change of properties from bulk Si to the free surface of the native oxide layer for predicting the surface elasticity, where the surface modulus  $E_{aSiO_2}$  is expressed as a function of the surface radius,  $r$ , ranging from  $R_0$  to  $R_0 + t$ . Here,  $t$  denotes the native oxide thickness, while  $R_0$  represents the radius of the Si core. In this model, Equation 8.1 estimates the surface elasticity, with  $E_{aSiO_2}(r)$  representing the change of the elastic property across the surface layer, which is a function of the Si core modulus of elasticity, denoted as  $E_{Si}$ . The surface factor parameter  $\alpha$  establishes a relationship between the thickness,  $t$ , and a dimensionless constant  $\tilde{\alpha}$ , as  $\alpha = \tilde{\alpha}/t$ . The value of  $\tilde{\alpha}$  determines the level of inhomogeneity in the elastic properties for the transition between the bulk crystal and the oxide surface. Additionally, the sign of  $\tilde{\alpha}$  indicates whether the surface layer becomes stiffer (positive) or more compliant (negative) upon such transition.

$$E_{aSiO_2}(r) = E_{Si}e^{\alpha(r-R_0)} \quad R_0 \leq r \leq R_0 + t \quad (8.1)$$

After estimating the modulus of elasticity for the native oxide layer ( $E_{aSiO_2}$ ), the modulus of elasticity of the NW,  $E$ , can be calculated based on Equation 8.2 [Yao et al., 2012, Xu et al., 2016]. For further details on the M-CS model, interested reader is referred to the related literature [Yao et al., 2012, Xu et al., 2016].

$$E = E_{Si} \left[ \left(1 - \frac{2t}{D}\right)^2 + \frac{4t}{\tilde{\alpha}D} (e^{\tilde{\alpha}} - (1 - \frac{2t}{D})) - \frac{8t^2}{\tilde{\alpha}^2 D^2} (e^{\tilde{\alpha}} - 1) \right] \quad (8.2)$$

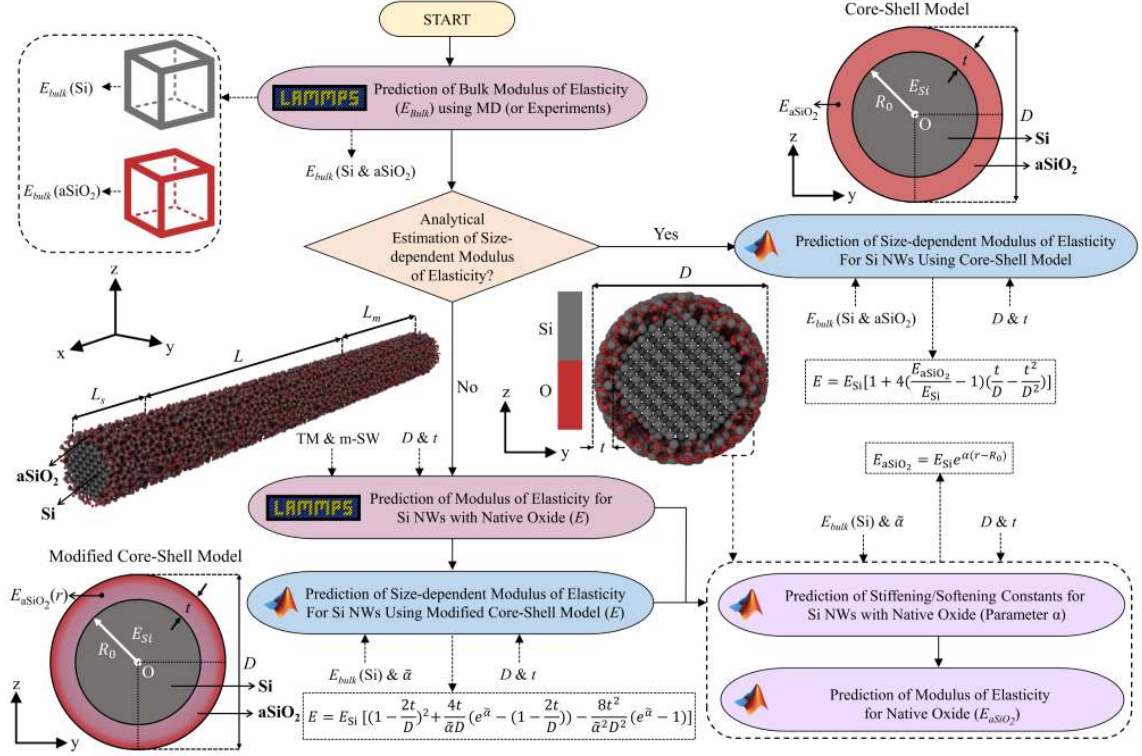


Figure 8.1: Flowchart depicting the methodology for the combination of Core-Shell (CS) and Modified Core-Shell (M-CS) models with Molecular Dynamics (MD) to implement the native oxide surface state in the calculation of the Si NW elastic properties. Both models consists of a Si crystal core with a bulk modulus of elasticity,  $E_{Si}$ . For CS model, the surface layer is composed of native oxide, (aSiO<sub>2</sub>), with a constant modulus,  $E_{aSiO_2}$ . For the M-CS model, the modulus, ( $E_{aSiO_2}(r)$ ), is evolving as a function of  $r$ . Si core and native oxide surface are depicted by grey and red colors, respectively, with the shaded grey layer in M-CS model indicating the transition between bulk and surface. The atomic configuration in MD simulations is represented over a circular cross-section of aSiO<sub>2</sub>-Si NWs with a critical dimension, CD, of  $D$  and a native oxide thickness,  $t$ . NW length ( $L$ ), support region length ( $L_s$ ), and movable region length ( $L_m$ ) are also shown. The grey and red spheres represent Si and O atoms, respectively. The fitting process in the M-CS model involves assigning geometric inputs in alignment with MD results and incorporating specific assumptions about core Si elasticity. The adjustment of the surface elasticity parameter during fitting reveals the level of inhomogeneity for particular configurations within the M-CS model. Consequently, M-CS curves are generated for two oxide thicknesses and three distinct assumptions regarding core Si elasticity.

## 8.4 Results

MD simulations are performed on aSiO<sub>2</sub>-Si NWs with the Si core along  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ , and  $\langle 112 \rangle$  crystal orientations using the LAMMPS code [Plimpton, 1995]. Circular NW cross-sections and an oblique view are depicted in Figure 8.1. Non-periodic boundary conditions are applied in all directions. To ensure the compatibility between MD simulations and the M-CS method, this study examines Si NWs with circular cross-section only. A length-to-diameter ( $L/D$ ) ratio of 10 is employed as a suitable limit for examining the elasticity of NWs through MD simulations [Pakzad et al., 2023b, Pakzad et al., 2024, Kang and Cai, 2007]. It should be noted that the common cross-sections of Si NWs are typically circular (mostly  $\langle 111 \rangle$ -Si and  $\langle 112 \rangle$ -Si NWs through bottom-up synthesis) or rectangular (mostly  $\langle 100 \rangle$ -Si and  $\langle 110 \rangle$ -Si NWs through top-down manufacturing) [Nasr Esfahani and Alaca, 2019, Pakzad et al., 2023b, Pakzad et al., 2024]. The influence of NW cross-sectional shape on elastic properties can be found elsewhere [Pakzad et al., 2024].

Initially, atoms are assigned an initial velocity with a Gaussian distribution at a finite temperature of 300 K, followed by an energy minimization using the conjugate gradient method. Subsequently, all NWs are relaxed at 300 K for 50 ps using a time step of 1 fs in a canonical NVT ensemble. During the relaxation step, the support and movable regions of length  $L_s$  and  $L_m$ , respectively, are held in a fixed configuration with both lengths set equal to one-eighth of the total length,  $L$ . This allows one to capture the initial stresses induced by the surface at the beginning of the stress-strain curves [Li and Gao, 2013]. In the next step, the tensile test is conducted by moving one end of the NW. To mitigate the shock wave resulting from high loading rates, a linearly varying constant velocity is applied along the longitudinal direction ( $x$ ), ranging from zero at the support to the maximum velocity applied at the movable boundary. In this regard, a velocity of 1.0 Å/ps at a temperature of 300 K is employed corresponding to a strain rate of  $\dot{\epsilon} \approx 1.0 \times 10^9 \text{ s}^{-1}$ . Such a strain rate falls within the usual range utilized in MD-based NW tensile tests

[Pakzad et al., 2023b, Pakzad et al., 2024, Pakzad et al., 2021, Kang and Cai, 2007]. Atomic stresses are determined by the virial theorem [Cormier et al., 2001]. Bulk elastic properties of Si,  $E_{Si}$ , and native oxide,  $E_{aSiO_2}$ , are first modeled via the m-SW and TM potentials. Results listed in Table 8.1 and Table 8.2 in the Supporting Information along with the corresponding experimental data [Nasr Esfahani and Alaca, 2019] are found to align well with previous theoretical and MD findings [Pakzad et al., 2023b, Ilinov and Kuronen, 2014, Park et al., 2005]. Guided by these MD results, M-CS model is then employed to observe the size dependence of NW elasticity,  $E$ .

Figures 8.2 and 8.3 demonstrate the change of  $E$  as a function of  $D$  obtained from the combined MD and M-CS model for Si NWs fabricated via top-down ( $\langle 100 \rangle$  and  $\langle 110 \rangle$ -oriented) and bottom-up ( $\langle 111 \rangle$  and  $\langle 112 \rangle$ -oriented) methods, respectively. The fitting procedure within the M-CS model is executed by allocating geometrical inputs in a fashion consistent with MD results, while adopting distinct assumptions regarding core Si elasticity. The tuning of the surface elasticity parameter during the fitting process reveals the degree of inhomogeneity for specific configurations within the M-CS model. In this respect, the M-CS curves are obtained for two oxide thicknesses and three distinct core Si elasticity assumptions. Plots also include extensive data from previous experimental measurements [Yang et al., 2022]. Lines in both Figures. 8.2 and 8.3 represent the results of the combined analytical-atomistic approach of this work, conclusively negating the existence of a 10-nm barrier. Specifically, results show a significant size-dependent  $E$  for aSiO<sub>2</sub>-Si NWs for  $D$  less than 10 nm. In this regard,  $E$  changes up to 28% as  $D$  increases from 4 nm to 8 nm for a native oxide thickness,  $t$ , of 0.5 nm (solid lines) (Figure 8.2). This change is very similar (about 32%) for bottom-up NWs (Figure 8.3) for both m-SW and TM potentials. The size effect becomes more noticeable with an increase of  $t$  to 1.0 nm (dashed lines), where the same increase in  $D$  from 4 nm to 8 nm leads to a 29% to 51% change in  $E$  for  $\langle 100 \rangle$  and  $\langle 110 \rangle$ , respectively (Figure 8.2). Similarly,  $\langle 111 \rangle$ -, and  $\langle 112 \rangle$ -oriented NWs exhibit a stiffening in the range of 42% to 66% over a similar size range (Figure 8.3).  $\alpha$  predicted by M-CS model for

both Figures. 8.2 and 8.3 is found to be within a very narrow range from -0.6 to -2.0, with the negative sign indicating the softening effect of the native oxide. Finally, TM potential is found to exhibit a higher degree of size-dependence compared to m-SW, although the trends are quite similar. Further details on the differences between the two potentials can be found elsewhere [Pakzad et al., 2023b].

Model findings are also compared with extensive amount of experimental data, where the combined analytical-atomistic model of this work is constructed using  $E_{Si}$  derived from experimental measurements [Nasr Esfahani and Alaca, 2019] in addition to MD simulations. For example, as no experimental report on  $\langle 100 \rangle$ -oriented Si NWs with  $D$  below 100 nm is available, scale-dependence is provided only based on MD results (Figure 8.2 (a)). In contrast, thanks to the large amount of experimental data available on  $\langle 110 \rangle$ -oriented Si NWs, a series of comparisons are provided in Figure 8.2 (b) [Zare Pakzad et al., 2021, Zhu et al., 2009, Li et al., 2003, Sadeghian et al., 2009, Tsuchiya et al., 2018, Hsin et al., 2008, Zhang et al., 2016, Han et al., 2007]. More specifically, when assigning experimental  $E_{Si}$ , the M-CS model aligns well with previous findings reported in experimental findings [Zhu et al., 2009, Tsuchiya et al., 2018, Hsin et al., 2008]. However, upon utilizing  $E_{Si}$  data from MD simulations, the M-CS model demonstrates a closer alignment with the reported  $E$  values from a separate series of experimental studies [Zare Pakzad et al., 2021, Li et al., 2003, Sadeghian et al., 2009, Zhang et al., 2016, Han et al., 2007]. The primary lesson from Figure 8.2 (b) is the absence of any critical dimensional barrier between computational and experimental findings. That means effective atomistic modeling can indeed provide the necessary guidance to an analytical approach, facilitating the capture of scale dependence across a wide range of dimensions.

The same methodology is then applied to  $\langle 111 \rangle$  and  $\langle 112 \rangle$  orientations as depicted in Figure 8.3.  $\langle 111 \rangle$  is another crystalline orientation for which a wealth of modulus data is available in experimental studies. The MD calculations of elasticity for  $\langle 111 \rangle$ -oriented aSiO<sub>2</sub>-Si NWs with follow-up M-CS predictions of different oxide layer thickness assumptions linking the atomistic predictions to experimental findings are elaborated further. Given M-CS estimations for  $\langle 111 \rangle$ -

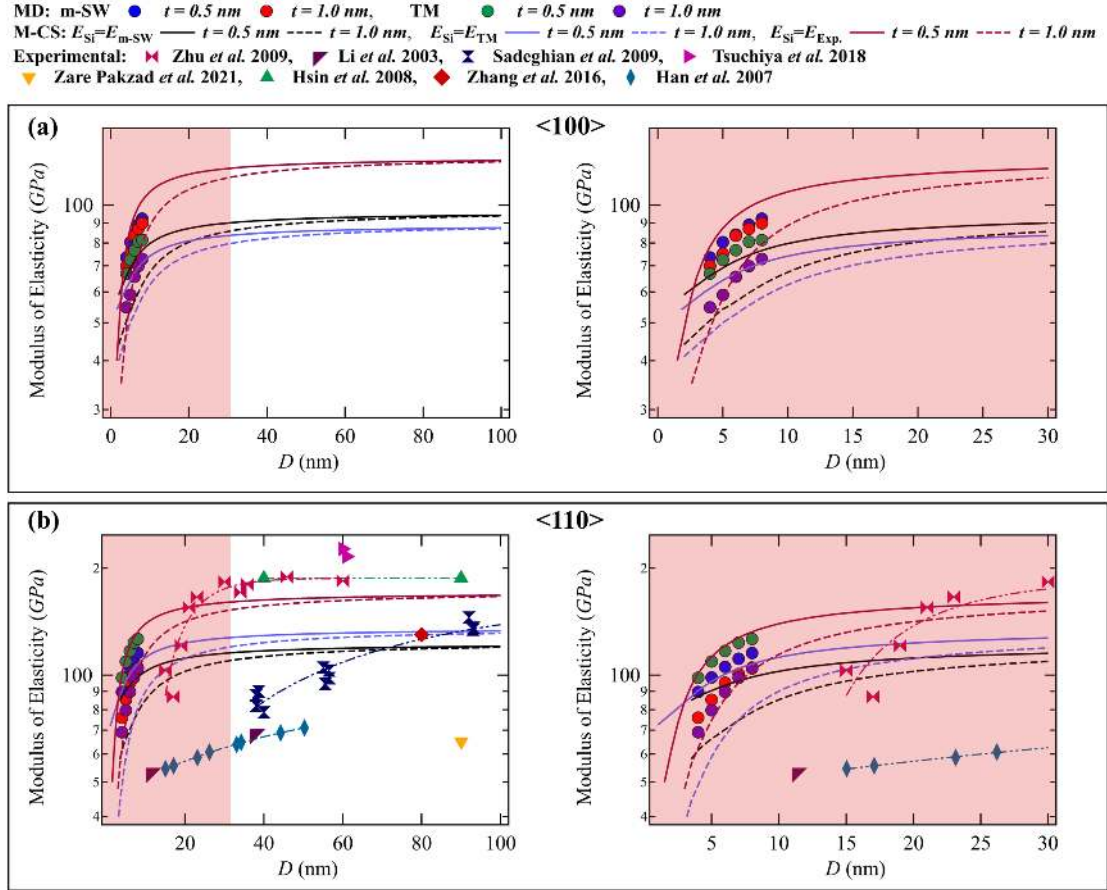


Figure 8.2: The modulus of elasticity,  $E$ , for aSiO<sub>2</sub>-Si NWs in (a)  $\langle 100 \rangle$  and (b)  $\langle 110 \rangle$  crystal orientations. MD simulations are used to predict the  $E_{Si}$  along with experimental values while combined with M-CS model of this work. Experimental data [Zhu et al., 2009, Li et al., 2003, Sadeghian et al., 2009, Tsuchiya et al., 2018, Zare Pakzad et al., 2021, Hsin et al., 2008, Zhang et al., 2016, Han et al., 2007] is plotted by extracting the modulus of elasticity ( $E$ ) from each respective study and utilizing it in the analysis of  $E$  as a function of  $D$ .



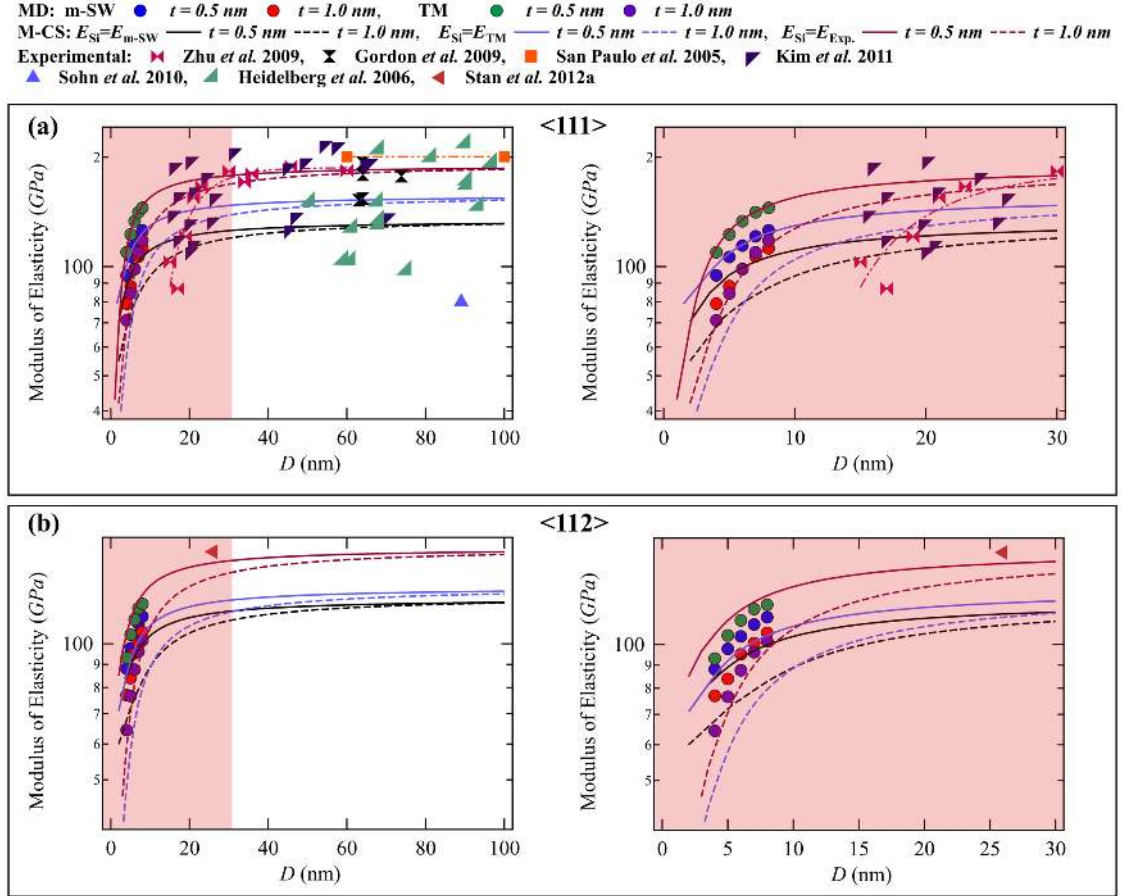


Figure 8.3: The modulus of elasticity,  $E$ , for aSiO<sub>2</sub>-Si NWs in (a)  $\langle 111 \rangle$  and (b)  $\langle 112 \rangle$  crystal orientations. MD simulations are used to predict the  $E_{Si}$  along with experimental values while combined with M-CS model of this work. Experimental data [Zhu et al., 2009, Gordon et al., 2009, San Paulo et al., 2005, Kim et al., 2011, Sohn et al., 2010, Heidelberg et al., 2006, Stan et al., 2012a] is plotted by extracting the modulus of elasticity ( $E$ ) from each respective study and utilizing it in the analysis of  $E$  as a function of  $D$ .

oriented Si NWs considering the observed deviations due to multiple  $E_{Si}$  and  $t$  assumptions align well with experimental predictions [Zhu et al., 2009, Gordon et al., 2009, San Paulo et al., 2005, Kim et al., 2011, Sohn et al., 2010, Heidelberg et al., 2006] given in Figure 8.3 (a). The M-CS model extends within both 100 nm and 30 nm ranges, as separately depicted in Figure 8.3 (b). Moreover, consistent with the findings of Zhu *et al.* [Zhu et al., 2009], the combined M-CS and atomistic methods reveal an increasing trend in  $E$  for  $\langle 111 \rangle$ -oriented Si NWs, further validating the accuracy of the M-CS model in capturing the size effect where experimental and computational trends are in proper agreement within the developed analytical-atomistic framework of this work. Given significant disparities between predicted experimental  $E$  for Si NWs, it is crucial to identify outliers within the established methodology, with Refs. [Sohn et al., 2010, Heidelberg et al., 2006] highlighting some of these outliers. For  $\langle 112 \rangle$ -oriented Si NWs of Figure 8.3 (b), M-CS model exhibits a good agreement with MD predictions as  $D$  increases. Despite the limited availability of experimental data for  $\langle 112 \rangle$ -oriented Si NWs [Stan et al., 2012a], the M-CS model, built upon experimental  $E_{Si}$ , offers a reliable trend, effectively addressing the transition from MD calculations to the experimental observations.

It should be emphasized that the limited available experimental data for  $\langle 100 \rangle$  and  $\langle 112 \rangle$  Si NWs leads to challenges in drawing definitive conclusions based on the findings depicted in Figure 8.2 (a) and Figure 8.3 (b). However, the observed size-dependent behavior of  $E$  for  $\langle 110 \rangle$  and  $\langle 111 \rangle$  Si NWs in Figure 8.2 (b) and Figure 8.3 (a) highlights the reliability of the proposed methodology to bridge the 10-nm barrier between computational and experimental findings and unite them forming a global trend. Unlike previous MD investigations on Si NWs with unreconstructed surfaces, which struggled to address computational and experimental reports on the size effect [Yang et al., 2022, Nasr Esfahani and Alaca, 2019], the present study successfully demonstrates the size-dependence in the modulus of elasticity of Si NWs. By incorporating the native oxide surface state, a direct connection is now established between the MD estimations and analytical methods.

Due to the importance of the insight obtained here regarding the role of the native

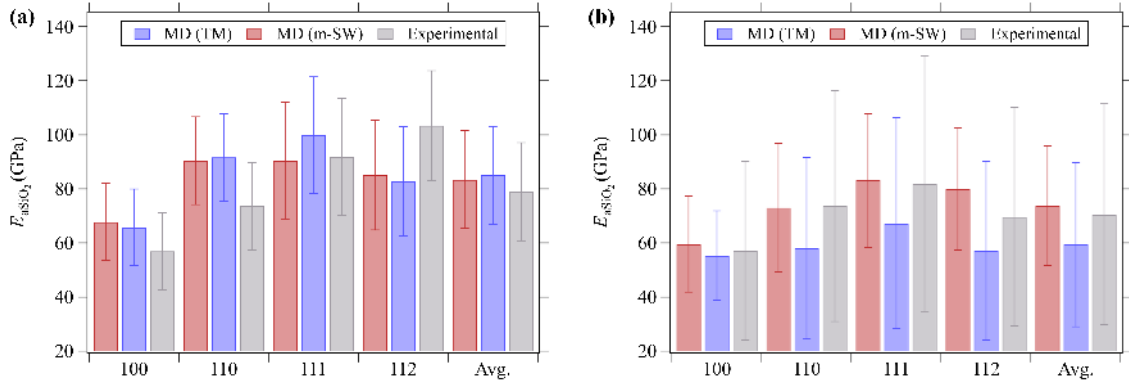


Figure 8.4: Modulus of elasticity of the native oxide ( $E_{aSiO_2}$ ) estimated using the M-CS model under two oxide thickness assumptions: (a)  $t = 0.5$  nm and (b)  $t = 1.0$  nm. Estimations are based on three approaches: MD predictions using the TM and m-SW potentials, as well as experimental calculations. Results are presented for four crystal orientations of core-Si, namely  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ , and  $\langle 112 \rangle$ , with the average value shown separately.

oxide in understanding the size effect in Si NW elastic behavior, the elasticity of the native oxide is studied in greater detail. Utilizing the M-CS formulation outlined in Equation 8.2, the estimation of  $E_{aSiO_2}$  is performed for various combinations of Si core crystalline orientation and  $t$  using Equation 8.1. This is achieved by linking the dimensionless constant calculation conducted earlier and utilizing Equation 8.1 to derive the elasticity for the native oxide layer. The corresponding results are presented in Figure 8.4 (a) and Figure 8.4 (b) for the case of  $t = 0.5$  nm and  $t = 1.0$  nm, respectively. Data are tabulated in Table 8.3 of the Supporting Information. Analysis of the findings reveals an average  $E_{aSiO_2}$  of  $75 \pm 28.6$  GPa, a finding in very good agreement with previous experimental reports on bulk aSiO<sub>2</sub> [Silva et al., 2006]. It is important to note that the limitations associated with the CS models in accurately capturing the actual changes in elasticity from the core to the shell region have been previously reported [Pakzad et al., 2023b]. Thus, it is observed that the M-CS model guided by proper MD estimations can generate more robust trendlines. This method not only reveals the size effect but also calculates the native oxide modulus at the nanoscale, marking the first instance of such calculation in the literature, to the best of our knowledge. The examination related to the CS model

is also carried out with detailed explanations and accompanying graphs provided in the Supporting Information.

## 8.5 Conclusion

In conclusion, this study comprehensively examines the size effect in Si NWs through the integration of atomistic and analytical methods. By establishing a connection between experimental observations and atomistic predictions for Si NWs of various orientations, the study successfully resolves the longstanding challenge of reconciling these two approaches, particularly across the 10-nm scale barrier. The combined use of atomistic and analytical methods yields valuable insights into the size-dependent characteristics of Si NWs, enhancing our understanding of their mechanical properties.

## 8.6 Supporting Information

The Supporting Information contains an in-depth discussion on the core-shell model, including its details, findings, and subsequent discussions given in Section 8.6.1. Additionally, detailed data tables and graphics are provided for MD simulations carried out on aSiO<sub>2</sub>-Si NWs, estimations of the bulk modulus of elasticity, and the estimation of the modulus of the native oxide using the M-CS model given in Section 8.6.2.

### 8.6.1 Core-shell Analysis

The CS model, illustrated in Figure 1, takes into account the distinct elastic properties of both the core and surface regions of the Si NW, as described in earlier research [Chen et al., 2006a, Stan et al., 2008]. In this regard,  $E$ , is determined through tensile testing and expressed as a function of the moduli of elasticity of the core Si ( $E_{Si}$ ) and the native oxide ( $E_{aSiO_2}$ ), as given in Equation 8.1, which is known as the CS model. The values of  $E_{Si}$  and  $E_{aSiO_2}$  are obtained through MD simulations, and a more comprehensive discussion on the specific methods and

techniques employed are provided in the Supporting Information. Further details on the formulation of the CS model can be found in relevant references [Chen et al., 2006a, Stan et al., 2008, Miller and Shenoy, 2000].

$$E = E_{Si} \left[ 1 + 4 \left( \frac{E_{aSiO_2}}{E_{Si}} - 1 \right) \left( \frac{t}{D} - \frac{t^2}{D^2} \right) \right] \quad (8.3)$$

In this context, the flowchart given in Figure 1 illustrates that the CS model relies on bulk modulus inputs for analytical estimations of  $E$  for Si NWs. A comparative analysis is conducted between the obtained results and previous experimental data using the CS model. Upon comparing the CS estimations provided in Figure 8.5 and Figure 8.6, it becomes apparent that this model exhibits inconsistent size estimations in comparison to the M-CS model. In this regard, the CS model, which utilizes atomistic bulk moduli, proves inadequate in accurately predicting the value of the parameter  $E$  for aSiO<sub>2</sub>-Si NWs with  $D$  below 8 nm.

#### 8.6.2 Atomistic and Analytical Data

Table 8.1 presents the obtained results for MD simulations conducted on aSiO<sub>2</sub>-Si NWs, while Table 8.2 contains the predictions for the bulk modulus for Si and aSiO<sub>2</sub> structures. Moreover, Table 8.3 provides the estimations for the modulus of elasticity of aSiO<sub>2</sub> using the M-CS model.

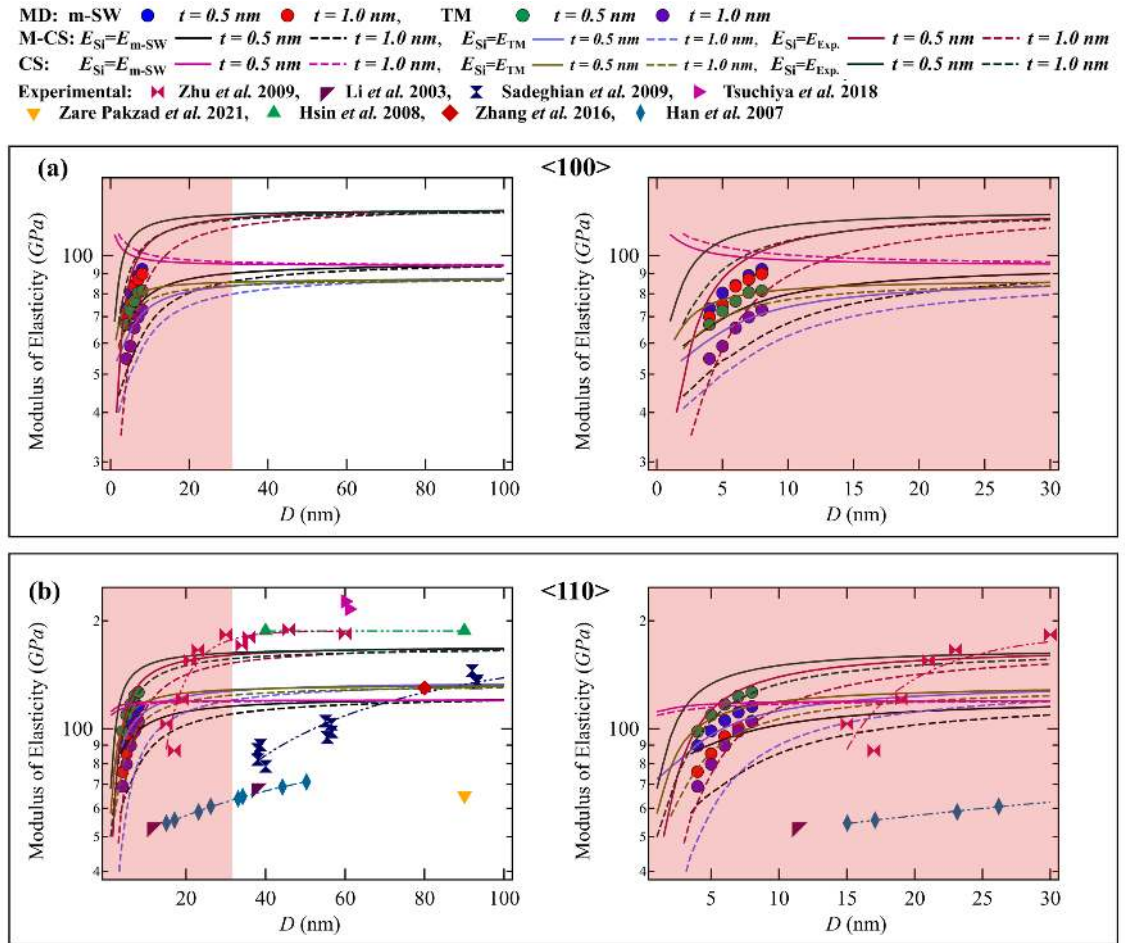


Figure 8.5: The modulus of elasticity estimations for aSiO<sub>2</sub>-Si NWs using the MD, CS, and M-CS methods with the core Si oriented along (a)  $\langle 100 \rangle$ , (b)  $\langle 110 \rangle$  are shown. The experimental  $E$  reported to the literature for each related crystal orientation is given.

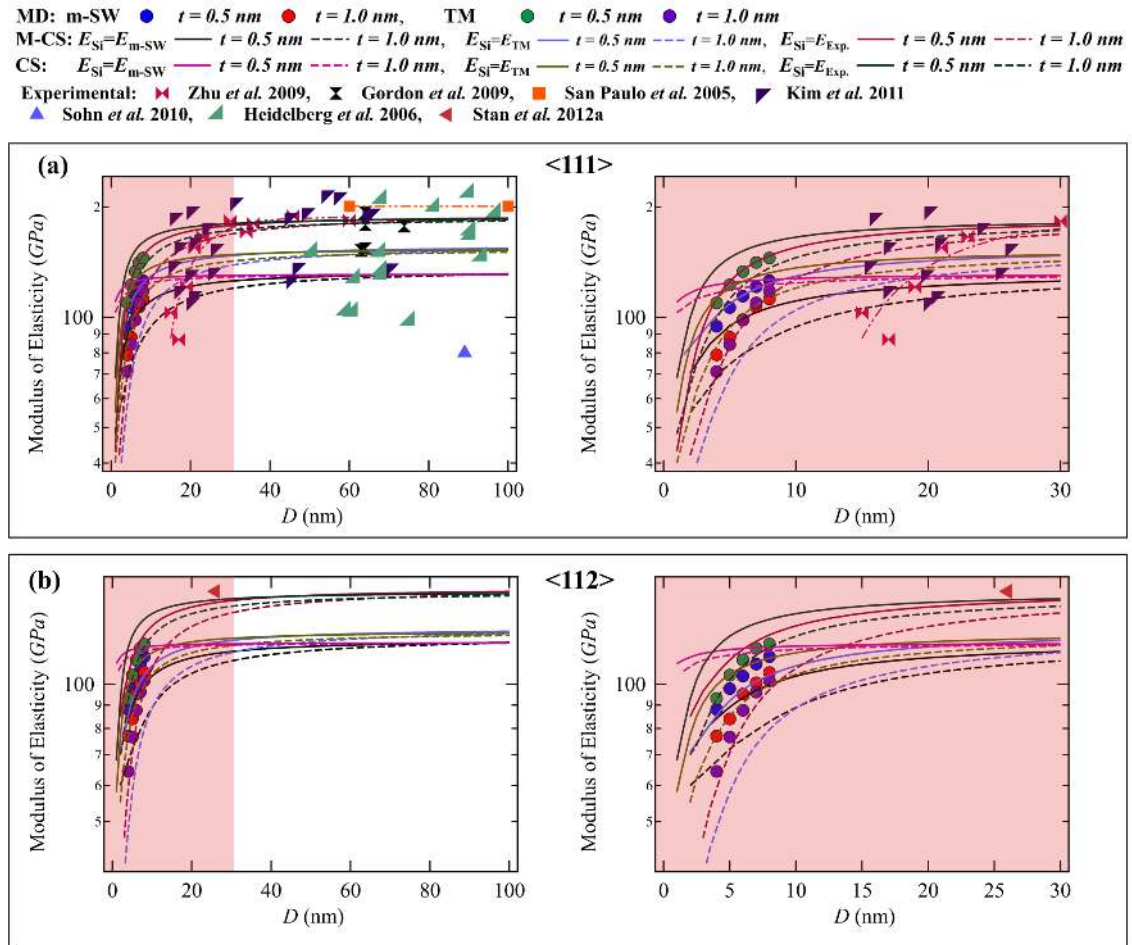


Figure 8.6: The modulus of elasticity estimations for aSiO<sub>2</sub>-Si NWs using the MD, CS, and M-CS methods with the core Si oriented along (a)  $\langle 111 \rangle$ , (b)  $\langle 112 \rangle$  are shown. The experimental  $E$  reported to the literature for each related crystal orientation is given.

Table 8.1: Modulus of elasticity ( $E$ ) estimations for aSiO<sub>2</sub>-Si NWs oriented along different crystal orientations are listed here. The NWs differ in their critical dimension ( $D$ ), oxide thickness ( $t$ ) and interatomic potential (m-SW and TM) used for the prediction of  $E$ .

| Si Orientation | $D$ (nm) | $E$ (GPa)    |              |              |              |
|----------------|----------|--------------|--------------|--------------|--------------|
|                |          | $t = 0.5$ nm | $t = 1.0$ nm | $t = 0.5$ nm | $t = 1.0$ nm |
|                |          | m-SW         | m-SW         | TM           | TM           |
| < 100 >        | 4        | 73.5         | 69.9         | 66.9         | 54.8         |
|                | 5        | 80.4         | 75.1         | 72.5         | 58.9         |
|                | 6        | 84.1         | 83.6         | 76.7         | 65.6         |
|                | 7        | 89.0         | 87.0         | 80.6         | 69.9         |
|                | 8        | 92.3         | 89.9         | 81.4         | 72.9         |
| < 110 >        | 4        | 89.7         | 75.9         | 98.3         | 69.1         |
|                | 5        | 98.6         | 85.4         | 109.3        | 79.7         |
|                | 6        | 105.6        | 95.2         | 117.0        | 89.8         |
|                | 7        | 111.2        | 100.8        | 123.4        | 98.4         |
|                | 8        | 115.5        | 105.0        | 126.4        | 104.6        |
| < 111 >        | 4        | 94.6         | 79.03        | 109.5        | 71.1         |
|                | 5        | 106.3        | 88.3         | 122.6        | 84.3         |
|                | 6        | 114.3        | 98.5         | 133.4        | 98.4         |
|                | 7        | 121.2        | 106.7        | 141.1        | 109.5        |
|                | 8        | 125.9        | 112.3        | 145.2        | 118.0        |
| < 112 >        | 4        | 88.1         | 77.0         | 93.2         | 64.4         |
|                | 5        | 97.9         | 83.9         | 104.8        | 76.7         |
|                | 6        | 104.3        | 95.2         | 113.2        | 87.7         |
|                | 7        | 110.8        | 100.8        | 119.9        | 96.1         |
|                | 8        | 115.0        | 106.2        | 122.6        | 101.8        |



Table 8.2: Modulus of elasticity of the bulk,  $E_{Si}$  and  $E_{aSiO_2}$ , calculated using MD simulations or obtained from prior experimental studies are listed here [Nasr Esfahani and Alaca, 2019].

| Method       | < 100 >-Si | < 110 >-Si | < 111 >-Si | < 112 >-Si | aSiO <sub>2</sub> |
|--------------|------------|------------|------------|------------|-------------------|
| MD (m-SW)    | 99.0       | 124.8      | 132.8      | 121.5      | 111.9             |
| MD (TM)      | 88.1       | 133.1      | 156.3      | 132.1      | 66.3              |
| Experimental | 131.0      | 169.0      | 188.0      | 160.0      | 70.0              |

Table 8.3: Modulus of elasticity of the native oxide (aSiO<sub>2</sub>) estimated via the M-CS model.

| Si Orientation | $t$    | $E_{aSiO_2}$ (GPa) |             |              |
|----------------|--------|--------------------|-------------|--------------|
|                |        | MD(m-SW)           | MD(TM)      | Experimental |
| < 100 >        | 0.5 nm | 67.8 ± 14.2        | 65.8 ± 11.8 | 57.0 ± 33.1  |
| < 110 >        |        | 90.5 ± 16.2        | 91.7 ± 21.9 | 73.7 ± 42.7  |
| < 111 >        |        | 90.6 ± 21.6        | 99.9 ± 28.2 | 81.9 ± 47.5  |
| < 112 >        |        | 85.1 ± 20.3        | 82.9 ± 24.6 | 103.5 ± 29.2 |
| Average        |        | 83.5 ± 18.1        | 85.1 ± 21.6 | 79.0 ± 38.2  |
| < 100 >        | 1.0 nm | 59.6 ± 17.7        | 55.4 ± 16.5 | 57.1 ± 33.1  |
| < 110 >        |        | 73.1 ± 23.9        | 58.0 ± 33.6 | 73.7 ± 42.7  |
| < 111 >        |        | 83.2 ± 24.7        | 67.3 ± 39.1 | 81.9 ± 47.5  |
| < 112 >        |        | 79.9 ± 22.6        | 57.1 ± 33.1 | 69.7 ± 40.4  |
| Average        |        | 73.9 ± 22.2        | 59.4 ± 30.6 | 70.6 ± 40.9  |

## Chapter 9

# MECHANICAL PROPERTIES OF SILICON NANOWIRES WITH NATIVE OXIDE SURFACE STATE

### 9.1 Overview

Silicon nanowires have attracted considerable interest due to their wide-ranging applications in nanoelectromechanical systems and nanoelectronics. Molecular dynamics simulations are powerful tools for studying the mechanical properties of nanowires. However, these simulations encounter challenges in interpreting the mechanical behavior and brittle to ductile transition of silicon nanowires, primarily due to surface effects such as the assumption of an unreconstructed surface state. This study specifically focuses on the tensile deformation of silicon nanowires with a native oxide layer, considering critical parameters such as cross-sectional shape, length-to-critical dimension ratio, temperature, the presence of nano-voids, and strain rate. By incorporating the native oxide layer, the article aims to provide a more realistic representation of the mechanical behavior for different critical dimensions and crystallographic orientations of silicon nanowires. The findings contribute to the advancement of knowledge regarding size-dependent elastic properties and strength of silicon nanowires.

### 9.2 Introduction

Nanowires (NWs) have gained significant attention due to their applications in high-performance devices across various fields, including nanoelectromechanical systems (NEMS) [Bachtold et al., 2022], nanoelectronics [Li et al., 2023, Zhang et al., 2021], energy harvesting [Nehra et al., 2020], and electromechanical/biochemical sensors [Alaca and Karimzadehkhoei, 2023, Akbari-Saatlu et al., 2020]. Silicon (Si) NWs

have been extensively utilized in various applications, including NEMS for mass spectrometers [Liu et al., 2022], gate-all-around transistors [Singh et al., 2023], and photodetectors/solar cells [Wang et al., 2021]. As the size of Si NWs decreases, the surface contribution becomes more significant, leading to a size-dependence in the mechanical behavior of the NWs [Nasr Esfahani and Alaca, 2019]. The investigation of size-dependent mechanical properties in NWs involves both experimental and modeling approaches where both disciplines encounter distinct difficulties [Nasr Esfahani and Alaca, 2019, Wang et al., 2017]. Precise study of the scale-dependence in Si NWs through experimental studies poses challenges in sample fabrication, device calibration, high-resolution measurements, NW alignment, modeling methods, and integration with microscale structures [Dasgupta et al., 2014, Zhu, 2017, Elhebeary and Saif, 2017b]. Theoretical and computational approaches, such as molecular dynamics (MD) simulations, first-principle methods, and Monte Carlo simulations, are powerful for investigating the mechanical properties of NWs [Nasr Esfahani and Alaca, 2019, Momeni et al., 2020]. However, the study of the elastic properties and strength of Si NWs using MD simulations faces inherent complexities and substantial challenges in interpreting their mechanical behavior. [Pakzad et al., 2021, Zare Pakzad et al., 2023c, Pakzad et al., 2023b, Nasr Esfahani and Alaca, 2019]. The challenges primarily arise from the surface effects, which include factors such as the surface state (native oxide vs. unreconstructed surface) and surface properties like surface energy, surface stress, and surface elastic constants [Pakzad et al., 2021, Pakzad et al., 2023b, Zare Pakzad et al., 2023c]. The utilization of the unreconstructed surface condition in MD modeling of the mechanical properties of Si NWs has given rise to discrepancies between computational and experimental findings [Yang et al., 2022, Nasr Esfahani and Alaca, 2019, Pakzad et al., 2023b, Zare Pakzad et al., 2023c]. Furthermore, comprehending the computational parameters, such as selecting suitable interatomic potentials, determining modeling details like time step and thermodynamic ensembles, as well as defining boundary conditions (B.C.s) and incorporating defects in MD simulations, has become increasingly challenging [Nasr Esfahani and Alaca, 2019, Pakzad et al., 2023b, Pakzad

et al., 2021, Zare Pakzad et al., 2023c]. In this context, the presence of native oxide, specifically amorphous silicon dioxide, as a vital component of the Si NW surface has a significant impact on the NW structure by introducing defects or other interfaces [Nasr Esfahani et al., 2022, Pakzad et al., 2023b, Zare Pakzad et al., 2023c]. Recent MD studies demonstrate that the modulus of elasticity of Si NWs can be reduced by up to 40% due to the native oxide surface condition compared to the unreconstructed surface state [Pakzad et al., 2023b]. Additionally, a similar reduction of up to 20% is estimated in the ultimate strength [Pakzad et al., 2023b]. Other structural aspects such as finite deformation and intrinsic stresses have to be modeled for mechanical consistency and relevance with respect to experimental conditions. A recent study has brought attention to the tensile intrinsic stresses in Si NWs that can reach up to 1.2 GPa when native oxide forms under ambient conditions [Nasr Esfahani et al., 2022]. The clear reduction observed in the mechanical properties of Si NWs highlights the need for further detailed examination, particularly considering the minuscule variations in the thickness of the native oxide layer and the cross-sectional shape [Zare Pakzad et al., 2021, Pakzad et al., 2023b, Pakzad et al., 2021, Zare Pakzad et al., 2023c].

Despite its significant importance, there are still several unresolved issues concerning the mechanical behavior of Si NWs [Minor et al., 2005]. One such topic is brittle-to-ductile transition (BDT), which lacks detailed *in-situ* thermomechanical testing and computational modeling at the nanoscale [Cheng et al., 2019, Kang and Cai, 2007]. There is growing evidence indicating that ductile behavior is observed in reduced-size Si NWs at much lower temperatures [Han et al., 2007, Cheng et al., 2019]. For instance, BDT is observed for Si NWs under tension at a critical dimension of 20 nm and a temperature as low as 90°C, whereas in bulk Si, BDT typically occurs at much higher temperatures, such as 540°C [Cheng et al., 2019]. Limited literature exists regarding bending, where BDT has also been identified as a scale-dependent and non-intrinsic property [Zheng et al., 2009]. In this respect, a recent bending study at 400°C reported activation of  $\langle 110 \rangle \{111\}$  dislocations at a much larger scale (2-5 mm) with multiple dislocation nucleation sites appear-

ing on the high-stress surface [Elhebeary et al., 2020]. Numerical modeling studies have explored the BDT phenomenon in Si NWs at the atomic level, yielding varying results. Some studies investigated the fracture behavior of Si NWs through MD simulations [Kang and Cai, 2010, Liu and Shen, 2012, Guénolé et al., 2011, El Nabi et al., 2015, Godet et al., 2015, Jeng et al., 2005, Xu, 2020, Kuo et al., 2014]. For instance, MD simulations conducted on Si NWs with diameters ranging from 2-8 nm found a clear size and temperature dependency, with only NWs below 4 nm exhibiting ductility at low temperatures [Kang and Cai, 2010]. Another study demonstrated through MD simulations that the competition between surface facet effect and axial orientation controls Si NW BDT, leading to different failure modes like dislocation emission, crystal-amorphous transition, or cleavage [Liu and Shen, 2012]. The existence of both brittle and ductile behavior at 10 K indicates a potential shift in the transition size at low temperatures, as indicated by experimental trends [Liu and Shen, 2012]. Regarding this matter, a constraint in BDT studies conducted using the MD method lies in their assumption of an unreconstructed surface state. This limitation makes the comparison between computational and experimental results difficult, as the experimental conditions may involve different surface states [Nasr Esfahani et al., 2022]. Moreover, numerous MD studies have shown significant variation in the predicted fracture mechanisms. Some studies have identified dislocation slip as the dominant mechanism [Godet et al., 2009, Yang et al., 2009], while others have suggested that the initiation of amorphization is energetically favorable around the crack tip [Han et al., 2007, Huang et al., 2009, Buehler et al., 2007]. To address this, failure probability formulations that integrate the ductile/brittle fracture mechanism into MD studies have been developed [Xu and Kim, 2019, Kang and Cai, 2007, Pakzad et al., 2023b].

Moreover, the examination of mechanical properties of Si NWs as a function of temperature using MD method has also been limited to the unreconstructed surface conditions [Kang and Cai, 2007, Xu and Kim, 2019, Jing et al., 2009a, Park et al., 2005, Jing et al., 2009b]. Another fundamental difference between experiments and atomistic simulations dedicated to the study of mechanical properties is the time

scale difference which leads to the use of different strain rates that are often several orders of magnitude higher than real experiments [Kang and Cai, 2010, Xu and Kim, 2019, Pakzad et al., 2023b]. In this respect, studies dedicated to analysis of strain rate effect of elastic properties and strength of Si NWs are common. A recent study exhibited deviations up to 10 % and 15 % for the modulus of elasticity and fracture strength of Si NWs with native oxide surface conditions [Pakzad et al., 2023b]. With the exception of a single study [Pakzad et al., 2023b], other studies investigating the strain rate effect on Si NWs using the MD method have also benefited from the unreconstructed surface assumption. This combination, along with the selection of interatomic potential and critical dimension of Si NWs, has led to the observation of diverse effects [Kang and Cai, 2010, Xu and Kim, 2019]. Moreover, the geometrical effects of Si NWs such as length to critical dimension ratio [Pakzad et al., 2023b] and the shape of cross-section [Jing et al., 2009b, Liu et al., 2015, Vogl et al., 2021] has been the topic of MD studies through tensile and bending tests reporting significant effects on mechanical behavior of Si NWs. The presence of flaws and defects can alter the properties of Si NWs and pose a critical issue in terms of atomic structure arrangement leading to changes in elastic properties and strength of NWs [Samykano, 2021, Elhebeary et al., 2020]. To comprehend the impact of such imperfections on the mechanical properties of NWs, extensive investigations are conducted on various forms of deficiencies, including point defects, vacancy clusters, defective surfaces, surface steps, and nano-voids [Huang et al., 2011, Liu et al., 2015, Katakam and Yedla, 2022, Cheng et al., 2015].

Motivated by the discrepancies observed between computational and experimental findings on the mechanical properties of Si NWs, this study focuses on investigating the tensile deformation of Si NWs. To tackle this issue, the present MD study on Si NWs with a native oxide surface state incorporates several critical parameters mentioned earlier. The subsequent sections of this article provide detailed information regarding the simulation methodology used to model the tensile response of Si NWs with native oxide surface state. The tensile simulations aim to investigate the influence of various factors, including cross-sectional shape, length to critical

dimension ratio, temperature, the presence of nano-voids, and strain rate on the mechanical behavior of Si NWs with different sizes and crystalline orientations. The objective of this article is to bridge the existing discrepancies between atomistic studies and experimental investigations by considering the more realistic surface state of native oxide in Si NWs.

### 9.3 Materials and Methods

Tensile simulations are performed on Si NWs with a native oxide surface state using the MD method [Thompson et al., 2022]. Figure 9.1 (a) and Figure 9.1 (b) depict the initial atomic configurations of Si NWs with two different cross-sectional shapes: circular and square, respectively. The critical dimension, denoted as  $D$ , ranges from 4 nm to 8 nm, representing the diameter for circular NWs and the width/height for square NWs. The native oxide layer, characterized by an amorphous structure, is referred to as  $\text{aSiO}_2$ , and Si NWs with native oxide are denoted as  $\text{aSiO}_2$ -Si NWs throughout the remainder of this work. For the  $\text{aSiO}_2$ -Si NWs in this study, a native oxide layer thickness ( $t$ ) of 0.5 nm is defined. The length ( $L$ ) of the  $\text{aSiO}_2$ -Si NWs remains constant with a length-to-critical dimension ( $L/D$ ) aspect ratio (AR) of 10, except for the tests conducted to examine the AR effect. Figure 9.1 (c) illustrates a Si NW with its length denoted as  $L$ , where the support and movable boundaries are labeled as  $L_s$  and  $L_m$ , respectively. Specifically, the boundary lengths  $L_s$  and  $L_m$  are set to one-eighth of the NW length ( $L$ ). By maintaining an AR of 10 across different critical dimensions of  $\text{aSiO}_2$ -Si NWs, any potential length-related effects are effectively eliminated [Pakzad et al., 2023b]. MD simulations are conducted on  $\text{aSiO}_2$ -Si NWs oriented along  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ , and  $\langle 112 \rangle$  crystal orientations. Non-periodic B.C.s are applied along all directions ( $x$ ,  $y$ , and  $z$ ) to account for the finite size of the system. In order to ensure consistency in cross-section designs and to thoroughly examine the effect of surface state, it is common to observe rectangular or square geometries in top-down fabricated Si NWs with crystal orientations  $\langle 100 \rangle$  and  $\langle 110 \rangle$  [Nasr Esfahani and Alaca, 2019]. Conversely, circular cross-sections are frequently encountered in bottom-up

fabricated Si NWs with crystal orientations  $\langle 111 \rangle$  and  $\langle 112 \rangle$  [Nasr Esfahani and Alaca, 2019]. Therefore, this study models aSiO<sub>2</sub>-Si NWs by considering both cross-sectional shapes and four crystal orientations of Si.

Atoms are initially assigned an initial velocity with a Gaussian distribution at a finite temperature. Afterward, an energy minimization is performed using the conjugate gradient method. Following this, the NW is relaxed at a constant temperature for 50 ps, employing a time step of 1 fs in a canonical NVT ensemble. During the relaxation step, the support and movable regions connected to the NW are held in a fixed configuration. In the subsequent step, a tensile test is performed by fixing one side of the NW ( $L_s$ ) while allowing the other end ( $L_m$ ) to move. To prevent the occurrence of shock waves due to high loading rates, a linearly increasing constant velocity is applied along the longitudinal direction ( $x$ -direction). This velocity starts from zero at the support and gradually reaches its maximum value at the movable boundary. In this regard, a velocity of 1.0 Å/ps is utilized at a constant temperature, corresponding to a strain rate of  $\dot{\epsilon} \approx 1.0 \times 10^9 \text{ s}^{-1}$ . This strain rate is considered appropriate for conducting tensile tests on NWs using MD simulations, as supported by previous studies [Kang and Cai, 2007, Pakzad et al., 2023b, Pakzad et al., 2021]. In this work, the modified Stillinger-Weber (m-SW) potential [Ganster et al., 2010], which has shown promising results in modeling Si NWs with native oxide, is employed. The specific expressions and coefficients for the m-SW potential can be found in the associated reference [Ganster et al., 2010]. Within this study, various parameters such as critical dimension, crystallographic orientation, AR, strain rate, and temperature are examined for aSiO<sub>2</sub>-Si NWs. Additionally, the impact of nano-voids, including their number and placement, on the mechanical properties of the NWs is investigated. Figures 9.1 (d-g) display atomic snapshots of aSiO<sub>2</sub>-Si NWs with different nano-void configurations: single (1), two centered (2-C), two surface (2-S), and four (4) nano-voids placed along the NWs. The diameter of the spherical voids is regarded as  $1/4^{th}$  of  $D$  for NWs of different sizes. The surface-based nano-voids (2-S) are positioned near the crystalline Si core and the native oxide surface layer, allowing for potential comparisons with the



centered (2-C) nano-voids given in Figure 9.1 (f) and Figure 9.1 (e), respectively.

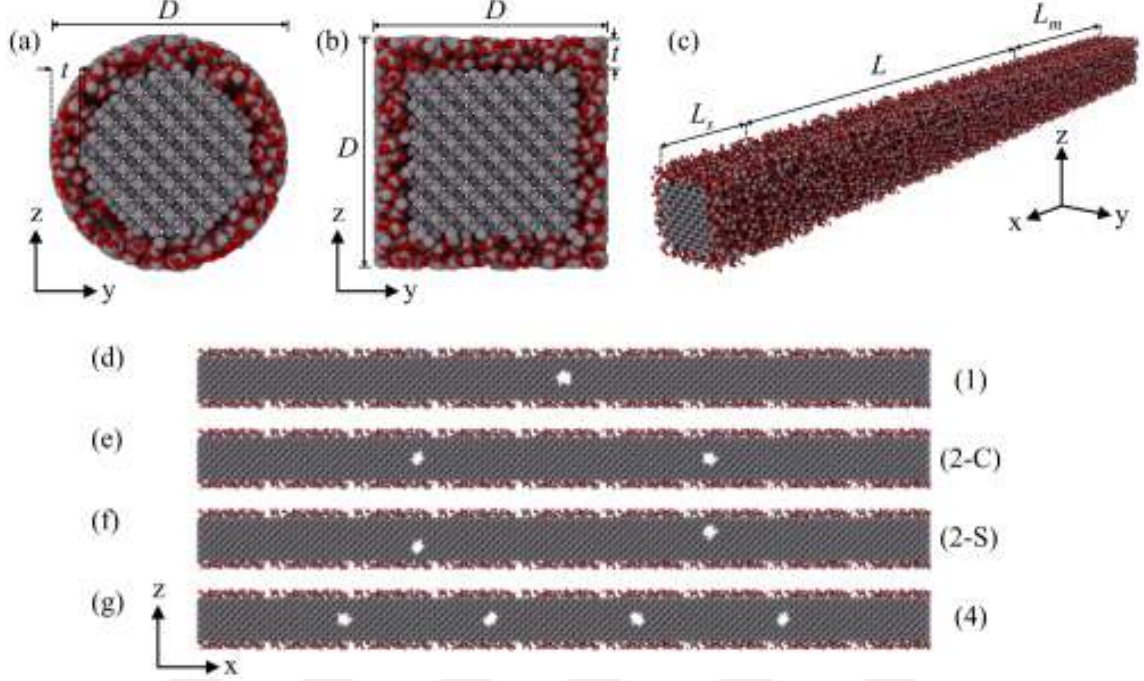


Figure 9.1: Atomic configurations of aSiO<sub>2</sub>-Si NWs with different cross-sectional shapes. (a) Circular cross-section and (b) square cross-section, where the critical dimension,  $D$ , and native oxide thickness,  $t$ , are indicated. (c) Representative view of an aSiO<sub>2</sub>-Si NW, illustrating the lengths: NW length ( $L$ ), support region length ( $L_s$ ), and movable region length ( $L_m$ ). Si and O atoms are represented by grey and red spheres, respectively. Side-views of aSiO<sub>2</sub>-Si NWs with various nano-void configurations: (d) single (1), (e) two centered (2-C), (f) two surface (2-S), and (g) four (4) nano-voids distributed along the NWs.

The stress state,  $\pi_{ij}$ , of the associated aSiO<sub>2</sub>-Si NWs is determined using the virial theorem [Zimmerman et al., 2004], as given in Equation 9.1. Here,  $\Omega_0$  represents the atomic volume in the undeformed system, with  $N$  being the total number of atoms. The atomic volumes for Si and aSiO<sub>2</sub> are obtained through the relaxation of the corresponding structures, and further details can be found in Ref. [Pakzad et al., 2021]. The atomic distances between atoms  $\alpha$  and  $\beta$  are denoted as  $r^{\alpha\beta}$ . The position of atom  $\alpha$  along the  $j$  direction is represented by  $v_j^\alpha$ , and the difference in positions between atoms  $\alpha$  and  $\beta$  is given as  $v_j^{\alpha\beta} = v_j^\alpha - v_j^\beta$ . The interatomic potential is represented by  $V$ .

$$\pi_{ij} = \frac{1}{2\Omega_0} \left[ \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \frac{1}{r^{\alpha\beta}} \frac{\partial V(r^{\alpha\beta})}{\partial r} (v_i^{\alpha\beta} v_j^{\alpha\beta}) \right] \quad (9.1)$$

## 9.4 Results

The section begins by establishing the stress-strain curves for different critical dimension and cross-sectional shapes of Si NWs for four crystallographic orientation of core-Si given in Section 9.4.1. Furthermore, the elastic properties and strength of Si NWs are studied as a function of AR (Section 9.4.2), temperature (Section 9.4.3), nano-void effects (Section 9.4.4), and strain rate (Section 9.4.5).

### 9.4.1 Cross-sectional Shape Effects

Figure 9.2 displays the stress-strain curves for aSiO<sub>2</sub>-Si NWs with circular and square cross-sections and critical dimensions of 4 nm, 6 nm, and 8 nm. The NWs are oriented along  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ , and  $\langle 112 \rangle$  crystal orientations given in Figure 9.2 (a), (b), (c), and (d), respectively. The design of the aSiO<sub>2</sub>-Si NWs includes an AR of 10 and a native oxide thickness of 0.5 nm, enabling a comprehensive examination of the combined effects of crystal orientation and cross-sectional shape. In the elastic regime, characterized by small strains, the stress-strain relationship is linear, allowing for the direct prediction of the modulus of elasticity ( $E$ ). As the stress increases, the relationship becomes non-linear until it reaches the ultimate strength ( $S$ ). Subsequently, the stress starts to decrease due to necking and fracture of the NWs. The ultimate strength is determined as the maximum stress achieved during the tensile deformation. The stress-strain curves presented in Figure 9.2 are utilized to measure the modulus of elasticity and ultimate strength for various crystal orientations and cross-sectional shapes. The results are summarized in Table 9.1. The findings demonstrate that as the critical dimension increases, the modulus of elasticity and ultimate strength of the NWs also increase. This comparison was made while maintaining the AR and  $t$  constant. Specifically, the modulus of elasticity shows a significant change, ranging from 25% for  $\langle 100 \rangle$  and

$\langle 110 \rangle$  crystal orientations to 30% for  $\langle 111 \rangle$  and  $\langle 112 \rangle$  crystal orientations when comparing  $D = 4$  nm to  $D = 8$  nm. Moreover, there is an observed increase of up to 40% in the ultimate strength of aSiO<sub>2</sub>-Si NWs with the increment in  $D$ . The influence of cross-sectional shape on the predicted properties, summarized in Table 9.1, results in deviations of up to 2.5 GPa and 1 GPa for the modulus of elasticity and ultimate strength estimations, respectively. The deviation between the shape-dependent modulus of elasticity and ultimate strength of aSiO<sub>2</sub>-Si NWs becomes more significant as the critical dimension decreases. The results presented in Section 9.4.1 are obtained at a temperature of 1 K and a strain rate of  $\dot{\epsilon} \approx 1.0 \times 10^9$  s<sup>-1</sup>, while maintaining a constant AR of 10. Further details regarding different ARs for aSiO<sub>2</sub>-Si NWs are discussed in Section 9.4.2. The subsequent discussions on the effects of temperature, nano-void, and strain rate can be found in Section 9.4.3, Section 9.4.4 and Section 9.4.5, respectively.

#### 9.4.2 Length to Critical Dimension Effect

To further investigate the size-dependent elastic properties and strength of aSiO<sub>2</sub>-Si NWs, the modulus of elasticity and ultimate strength of NWs with varying ARs are examined. Tensile tests are performed on aSiO<sub>2</sub>-Si NWs with similar  $D$  and crystal orientations as described in Section 9.4.1, with AR values ranging from 7 to 25. Figure 9.3 illustrates the relationship between the modulus of elasticity and the AR for aSiO<sub>2</sub>-Si NWs oriented along crystal orientations  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ , and  $\langle 112 \rangle$ , as shown in Figure 9.3 (a), (b), (c), and (d), respectively. The results indicate that there is a negligible size effect on the modulus of elasticity of aSiO<sub>2</sub>-Si NWs across all crystal orientations when the AR exceeds 12. Additionally, the findings demonstrate that NWs with smaller AR exhibit higher modulus of elasticity, and this trend is consistent across all crystal orientations for NWs with  $D$  of 4 nm and 6 nm. For NWs with  $D = 4$  nm, the modulus of elasticity predictions show more variation depending on the shape of the cross-section, whereas for NWs with larger  $D$ , the shape effect becomes insignificant for AR values greater than 10. Another observation regarding the shape effect is that NWs with a square cross-section ( $D =$

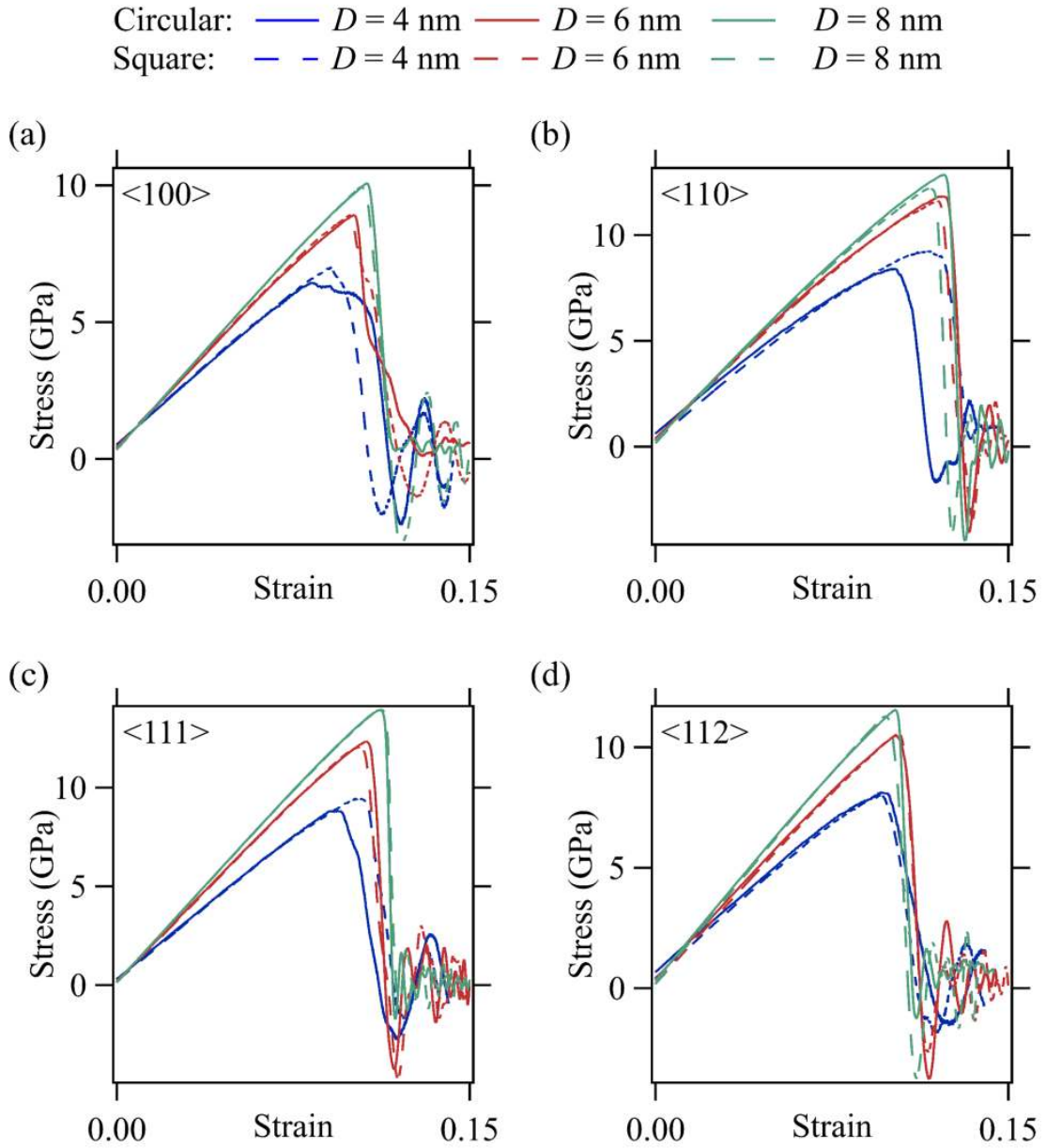


Figure 9.2: Stress-strain curves of aSiO<sub>2</sub>-Si NWs of different critical dimensions with an AR of 10. The curves correspond to NWs oriented along (a)  $\langle 100 \rangle$ , (b)  $\langle 110 \rangle$ , (c)  $\langle 111 \rangle$ , and (d)  $\langle 112 \rangle$  crystal orientations. Solid lines represent NWs with circular cross-sections, while dashed lines correspond to NWs with square cross-sections.

Table 9.1: The table presents the crystallographic orientations and dimensions of aSiO<sub>2</sub>-Si NWs with circular and square cross-sections, along with their corresponding modulus of elasticity ( $E$ ) and ultimate strength ( $S$ ).

| NW Orientation        | $D$ (nm) | $E$ (GPa) |        | $S$ (GPa) |        |
|-----------------------|----------|-----------|--------|-----------|--------|
|                       |          | Circular  | Square | Circular  | Square |
| $\langle 100 \rangle$ | 4        | 75.5      | 77.4   | 6.5       | 7.0    |
|                       | 6        | 90.8      | 90.9   | 8.9       | 8.9    |
|                       | 8        | 95.5      | 95.8   | 10.1      | 10.0   |
| $\langle 110 \rangle$ | 4        | 93.3      | 95.7   | 8.4       | 9.3    |
|                       | 6        | 112.6     | 112.9  | 11.9      | 11.6   |
|                       | 8        | 117.9     | 118.8  | 12.9      | 12.2   |
| $\langle 111 \rangle$ | 4        | 99.1      | 99.7   | 8.8       | 9.5    |
|                       | 6        | 122.2     | 122.0  | 12.3      | 12.1   |
|                       | 8        | 129.1     | 129.8  | 13.9      | 13.9   |
| $\langle 112 \rangle$ | 4        | 88.8      | 90.2   | 8.2       | 8.0    |
|                       | 6        | 107.9     | 108.0  | 10.5      | 10.6   |
|                       | 8        | 118.4     | 119.0  | 11.6      | 11.3   |

8 nm) at an AR of 7 exhibit a modulus of elasticity similar to higher ARs, while NWs with a circular cross-section demonstrate a higher modulus of elasticity. This could be attributed to the influence of shape effects and surface stresses when modeling NWs under free surface conditions and non-periodic B.C.s. Comparing these findings with previous literature, MD studies on the bending response of Si NWs with unreconstructed surface state indicate a slight decrease in the modulus of elasticity as the AR of the Si NWs increases from 10 to 25 [Nasr Esfahani and Jabbari, 2020]. Another recent MD study comparing the tensile properties of unreconstructed Si NWs and Si NWs with a native oxide revealed an insignificant effect of AR ranging from 7 to 40 when NWs were assumed as part of an infinite NW with periodicity applied along the NW dimension during modeling [Pakzad et al., 2023b]. However, the present study addresses the length factor by applying non-periodic B.C. along the NW, thereby simulating the length and subsequent AR effect under fixed B.C. When comparing the estimations of the modulus of elasticity with different ARs to experimental findings, the results show reliable agreement, with increased AR accurately reflecting experimental Si NWs, and the estimated values of  $E$  falling within the range of prior estimations for different orientations of Si NWs [Nasr Esfahani and Alaca, 2019].

Figure 9.4 presents the correlation between the ultimate strength and the AR for aSiO<sub>2</sub>-Si NWs oriented along crystal orientations  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ , and  $\langle 112 \rangle$ , as shown in Figure 9.4 (a), (b), (c), and (d), respectively. The results demonstrate slight variations in the ultimate strength for different ARs of aSiO<sub>2</sub>-Si NWs, influenced by factors such as cross-sectional shape and crystal orientation effects. Moreover, NWs with larger critical dimensions exhibit higher ultimate strength, ranging from 8-9 GPa for  $D$  of 4 nm to 10-14 GPa for  $D$  of 8 nm. The cross-sectional shape effect on the ultimate strength predictions is influenced by the combined effects of crystal orientation,  $D$ , and AR of the NWs. Previous works on partially oxidized Si NWs have reported an ultimate strength of approximately 10 GPa, which aligns with the findings depicted in Figure 9.4 [Xu, 2020]. Another recent study on the tensile properties of Si NWs with native oxide has demon-

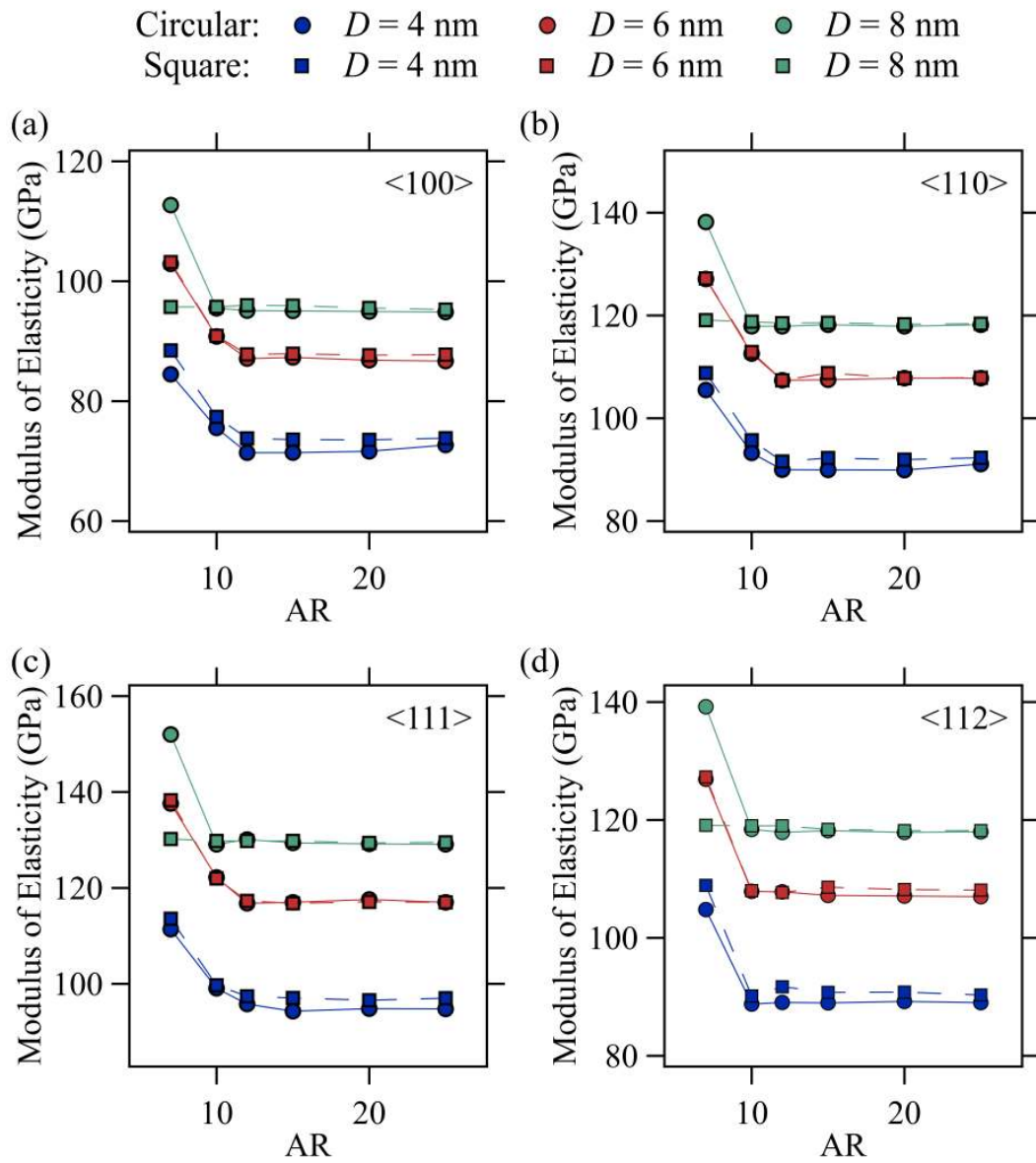


Figure 9.3: The modulus of elasticity as a function of AR for aSiO<sub>2</sub>-Si NWs oriented along (a)  $\langle 100 \rangle$ , (b)  $\langle 110 \rangle$ , (c)  $\langle 111 \rangle$ , and (d)  $\langle 112 \rangle$  crystal orientations.

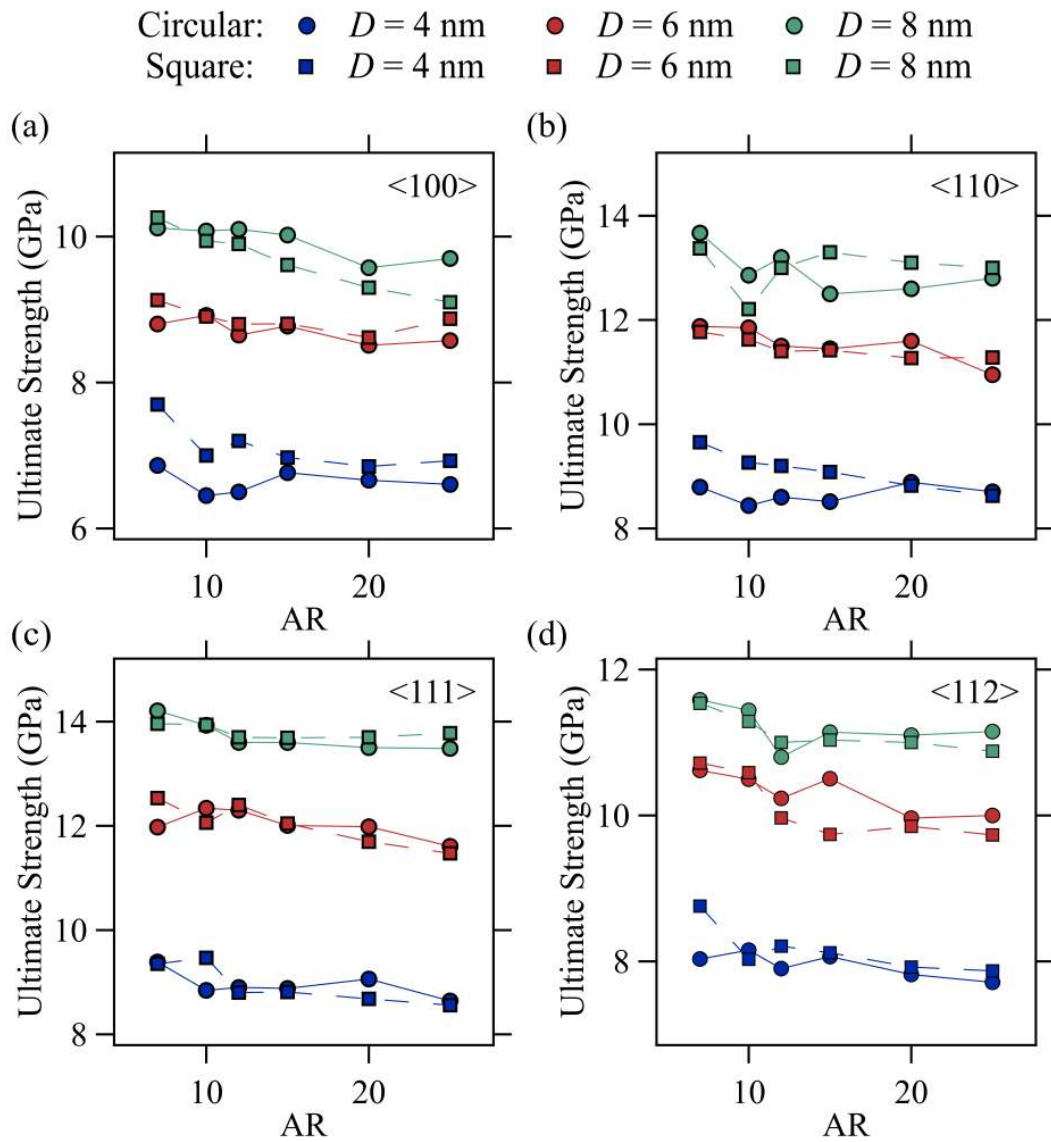


Figure 9.4: The ultimate strength as a function of AR for aSiO<sub>2</sub>-Si NWs oriented along (a)  $\langle 100 \rangle$ , (b)  $\langle 110 \rangle$ , (c)  $\langle 111 \rangle$ , and (d)  $\langle 112 \rangle$  crystal orientations.



strated a negligible AR effect when NWs are considered as part of an infinite NW [Pakzad et al., 2023b]. MD studies on unreconstructed Si NWs have reported ultimate strength ranging from 3 GPa to 15 GPa [Kang and Cai, 2007]. It is common to observe a wide range of predictions for the ultimate strength of Si NWs, particularly in experimental studies, where values up to 20 GPa have been reported in the literature [Nasr Esfahani and Alaca, 2019]. The findings presented here indicate that the assumption of a native oxide surface state and the accuracy of the m-SW potential contribute to good agreement with experimental results in estimating the strength of Si NWs.

#### 9.4.3 Temperature Effect

This section focuses on the predictions of the modulus of elasticity and ultimate strength for aSiO<sub>2</sub>-Si NWs with a particular emphasis on examining their temperature dependence. In the preceding sections of the paper, the tensile simulations for aSiO<sub>2</sub>-Si NWs were limited to 1 K. However, this section extends the temperature range from 1 K up to 1200 K to explore the temperature-dependent behavior of the NWs. The resulting predictions for the modulus of elasticity and ultimate strength are illustrated in Figure 9.5 and Figure 9.6, respectively. Figure 9.5 illustrates the modulus of elasticity for aSiO<sub>2</sub>-Si NWs as a function of temperature oriented along crystal orientations  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ , and  $\langle 112 \rangle$ , as depicted in Figure 9.5 (a), (b), (c), and (d), respectively. Regarding the modulus of elasticity predictions, a significant decrease of approximately 20-50 GPa is observed as the temperature increases for different crystal orientations. Specifically, the temperature rise from 1 K to 1200 K leads to a reduction in the modulus of elasticity from 80-120 GPa at 1 K to 50-100 GPa. To the best of our knowledge, no prior study has reported the temperature-dependent modulus of elasticity for Si NWs with a native oxide surface state. However, comparing our findings with previous MD studies on unreconstructed Si NWs tested under tensile [Kang and Cai, 2010, Xu and Kim, 2019] and buckling [Jing et al., 2009a] conditions, similar deviations in the modulus of elasticity can be observed, resulting in reductions due to temperature increases.

The reduction in the modulus of elasticity for unreconstructed Si NWs tested at 100 K and 1000 K is estimated to be up to 100 GPa. In this regard, aSiO<sub>2</sub>-Si NWs exhibit a lower temperature dependence compared to unreconstructed Si NWs [Xu and Kim, 2019].

Figure 9.6 shows the ultimate strength estimations as a function of temperature for NWs of different crystal orientations. The results are depicted for aSiO<sub>2</sub>-Si NWs oriented along crystal orientations  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ , and  $\langle 112 \rangle$ , as shown in Figure 9.6 (a), (b), (c), and (d), respectively. The results indicate a decrease in the ultimate strength as the temperature increases. The magnitude of this reduction varies depending on factors such as critical dimension, cross-sectional shape, and crystal orientation. Specifically, the ultimate strength decreases by up to 12 GPa when the temperature is increased from 1 K to 1200 K. For different  $D$  and crystal orientations, the ultimate strength, which ranges between 6-14 GPa at 1 K, decreases to 1-4 GPa at 1200 K. Deviation of up to 2 GPa is observed in the ultimate strength, emphasizing the significant impact of the cross-sectional shape on the strength of aSiO<sub>2</sub>-Si NWs. Prior MD studies on the buckling behavior of unreconstructed Si NWs have demonstrated a decreasing trend in the critical load with increasing temperature [Jing et al., 2009a]. Similarly, another MD study investigating the temperature effect on unreconstructed Si NWs under tensile testing reported a reduction in ultimate strength from 12-14 GPa to 4-5 GPa as the temperature increased from 10 K to 1200 K [Kang and Cai, 2010]. Furthermore, an MD study addressing the temperature impact on the ultimate strength of unreconstructed Si NWs found a reduction from 15 GPa to 5-10 GPa for different combinations of critical dimensions and interatomic potentials as the temperature increases from 100 K to 1000 K [Xu and Kim, 2019]. In this respect, the observed trend of reduction in ultimate strength for Si NWs with a native oxide surface state is consistent with that of unreconstructed Si NWs, exhibiting reductions that depend on the critical dimensions, crystal orientation, and cross-sectional shape of NWs.

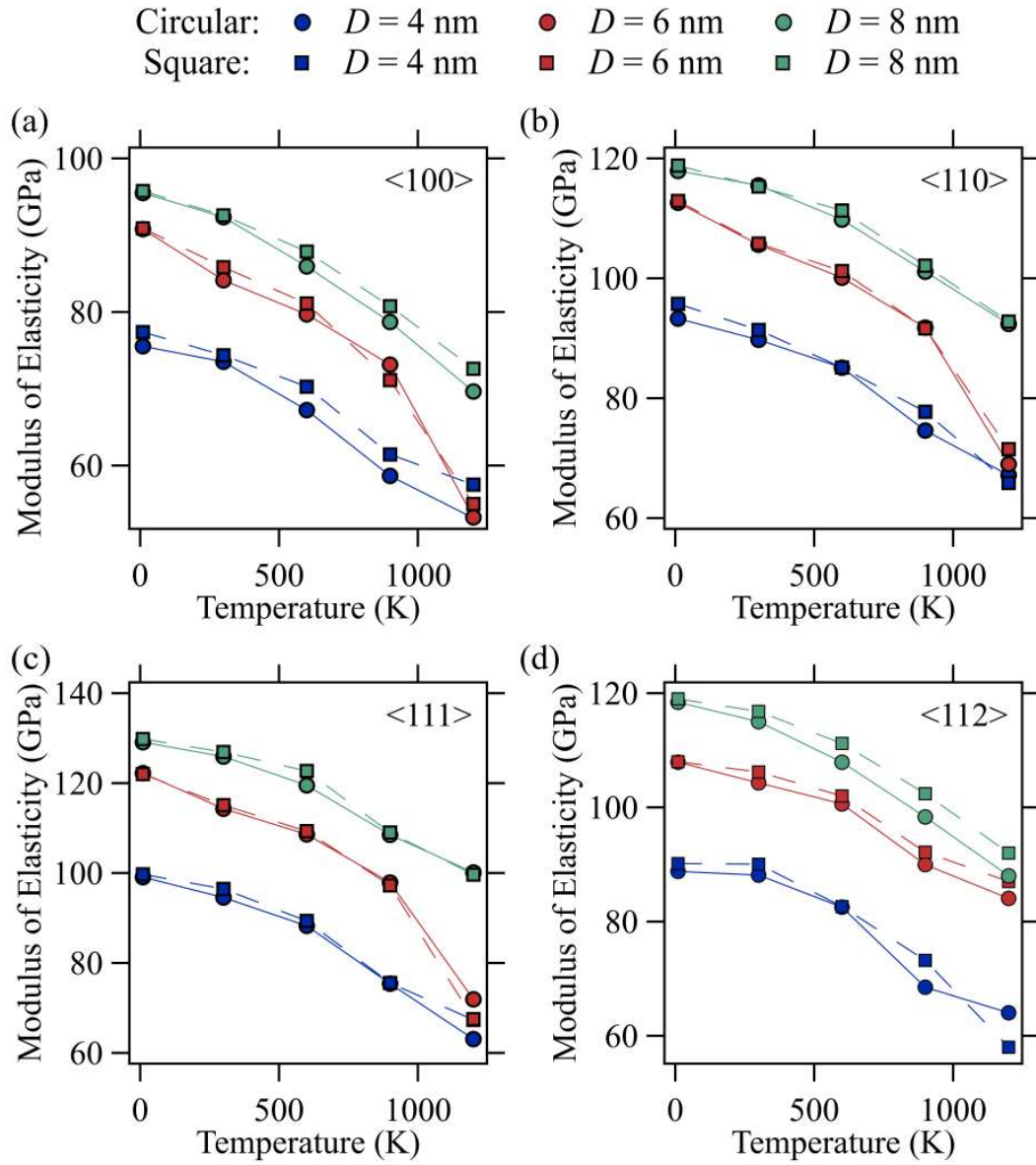


Figure 9.5: The modulus of elasticity as a function of temperature for aSiO<sub>2</sub>-Si NWs oriented along (a)  $\langle 100 \rangle$ , (b)  $\langle 110 \rangle$ , (c)  $\langle 111 \rangle$ , and (d)  $\langle 112 \rangle$  crystal orientations.

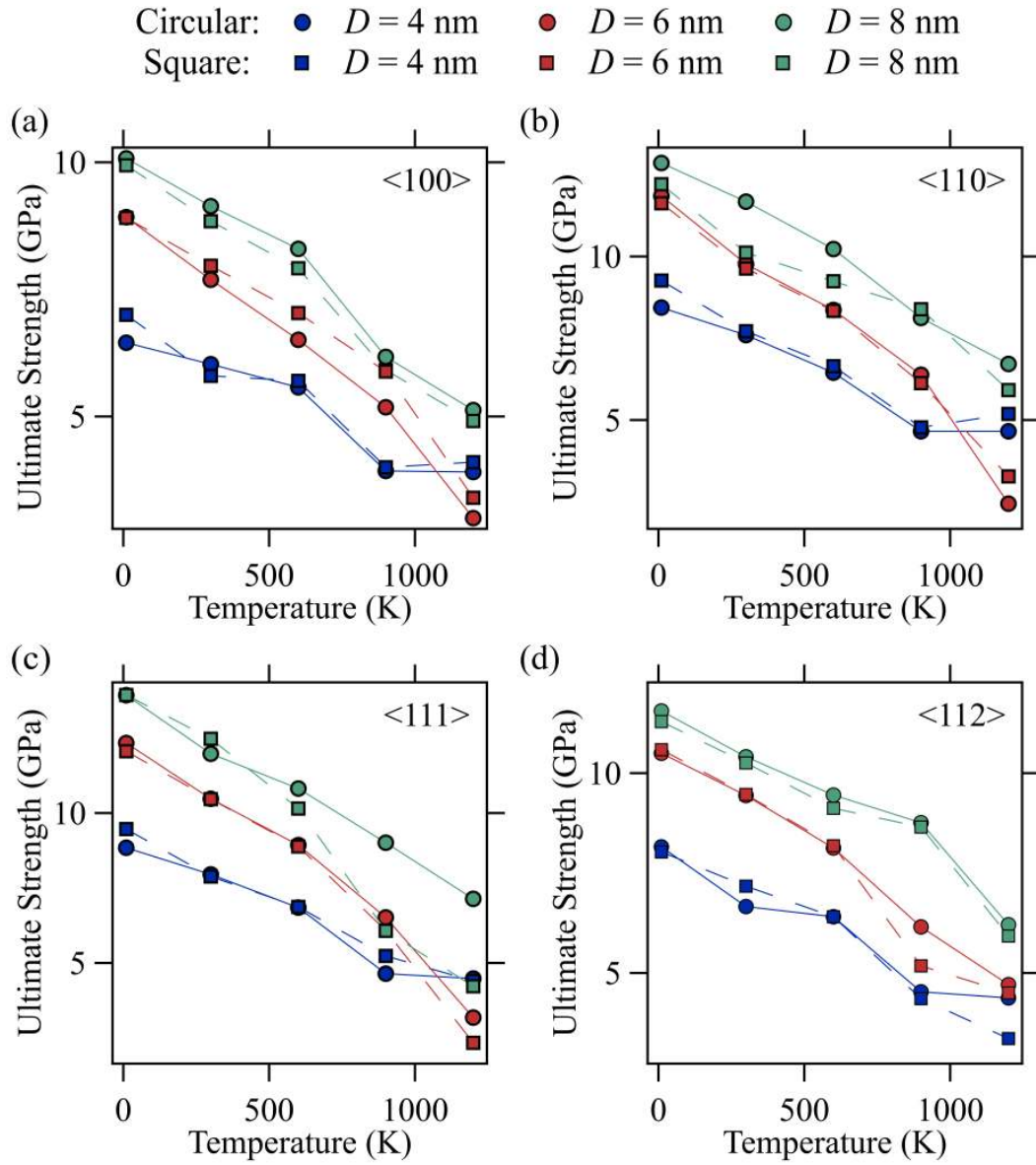


Figure 9.6: The ultimate strength as a function of temperature for aSiO<sub>2</sub>-Si NWs oriented along (a)  $\langle 100 \rangle$ , (b)  $\langle 110 \rangle$ , (c)  $\langle 111 \rangle$ , and (d)  $\langle 112 \rangle$  crystal orientations.

#### 9.4.4 Nano-void Effect

In order to assess the impact of nano-voids on the tensile properties of aSiO<sub>2</sub>-Si NWs, this study examines four distinct combinations placed along the NWs shown in Figure 9.7 (d). Figure 9.7 depicts the estimated modulus of elasticity for different nano-void combinations compared to the defect-free case in aSiO<sub>2</sub>-Si NWs oriented along crystal orientations  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ , and  $\langle 112 \rangle$ , as shown in Figure 9.7 (a), (b), (c), and (d), respectively. A slight decrease in the modulus of elasticity is observed in aSiO<sub>2</sub>-Si NWs as the number of voids increases from zero in the defect-free case to four nano-voids. This decrease becomes more negligible as  $D$  increases, indicating that defects have a more significant impact at smaller critical dimensions. More precisely, in the case of aSiO<sub>2</sub>-Si BWs with a  $D$  of 4 nm, the modulus of elasticity experiences a reduction of up to 5 GPa with the inclusion of four nano-voids. The reduction is estimated to be 1-4 GPa for NWs with  $D = 6$  nm and 1-2 GPa for NWs with  $D = 8$  nm. Comparing the location of nano-voids near the surface (2-S) to centered ones (2-C), a slightly lower modulus of elasticity is observed when the nano-voids are closer to the surface. Figure 9.8 illustrates the estimated ultimate strength for different nano-void combinations compared to the defect-free case in aSiO<sub>2</sub>-Si NWs oriented along crystal orientations  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ , and  $\langle 112 \rangle$ , as shown in Figure 9.8 (a), (b), (c), and (d), respectively. A decreasing trend in the ultimate strength of aSiO<sub>2</sub>-Si NWs, up to 2 GPa, is observed for different  $D$  and crystal orientations. The ultimate strength exhibits a clear decrease as the number of nano-voids increases. Additionally, for aSiO<sub>2</sub>-Si NWs with  $D$  of 6 nm and 8 nm, the location of the nano-voids also affects the ultimate strength, with a noticeable decrease observed for nano-voids located near the surface (2-S) compared to the centered ones (2-C). This impact of void location is evident for different crystal orientations. A recent study investigating the effect of nano-voids on the modulus of elasticity in NWs reported reductions of up to 10 GPa, depending on the number and size of the nano-voids [Katakam and Yedla, 2022].

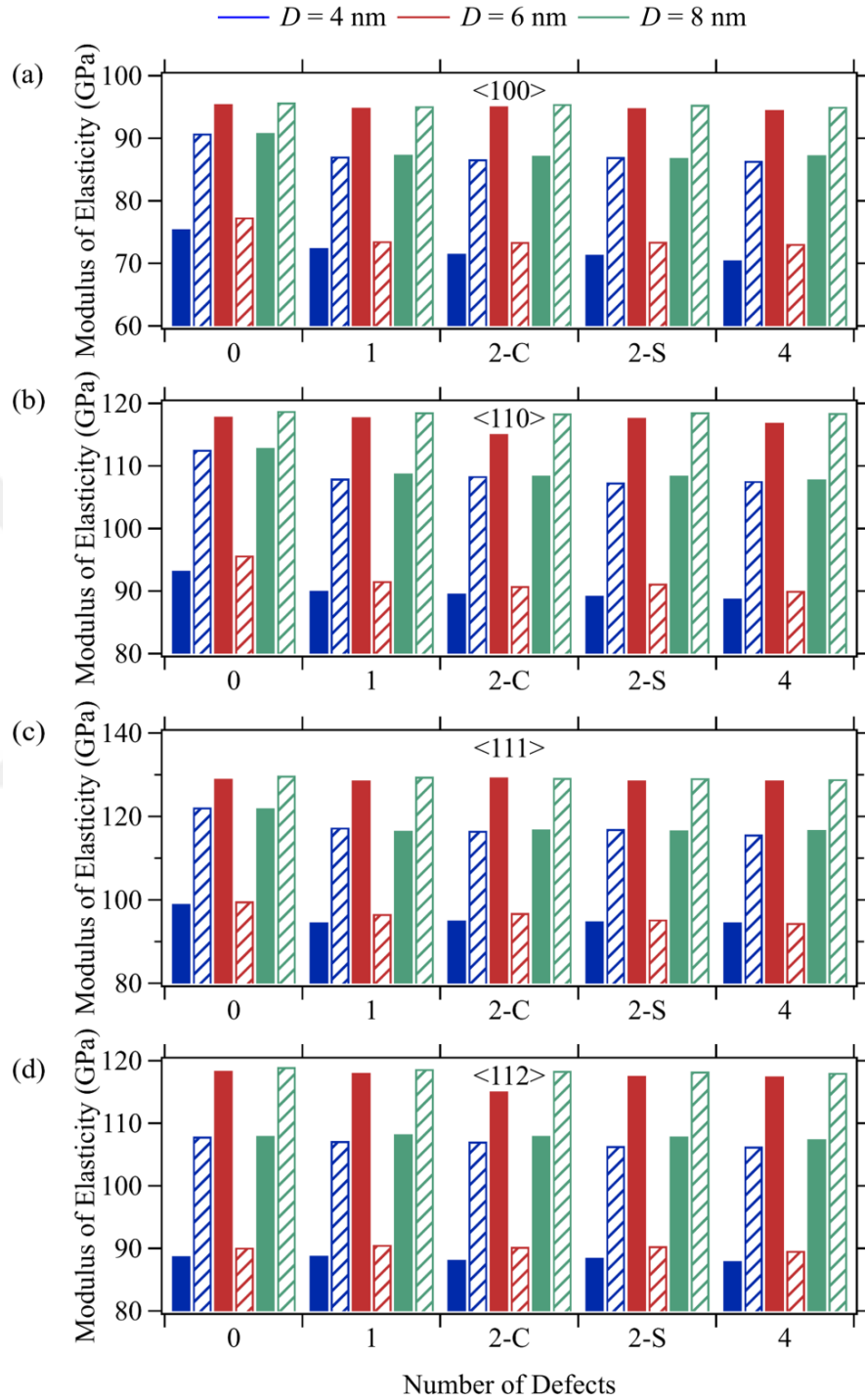


Figure 9.7: The modulus of elasticity as a function of defects distribution for aSiO<sub>2</sub>-Si NWs oriented along (a)  $\langle 100 \rangle$ , (b)  $\langle 110 \rangle$ , (c)  $\langle 111 \rangle$ , and (d)  $\langle 112 \rangle$  crystal orientations. The filled bars represent circular NWs, while the dashed bars correspond to square NWs.

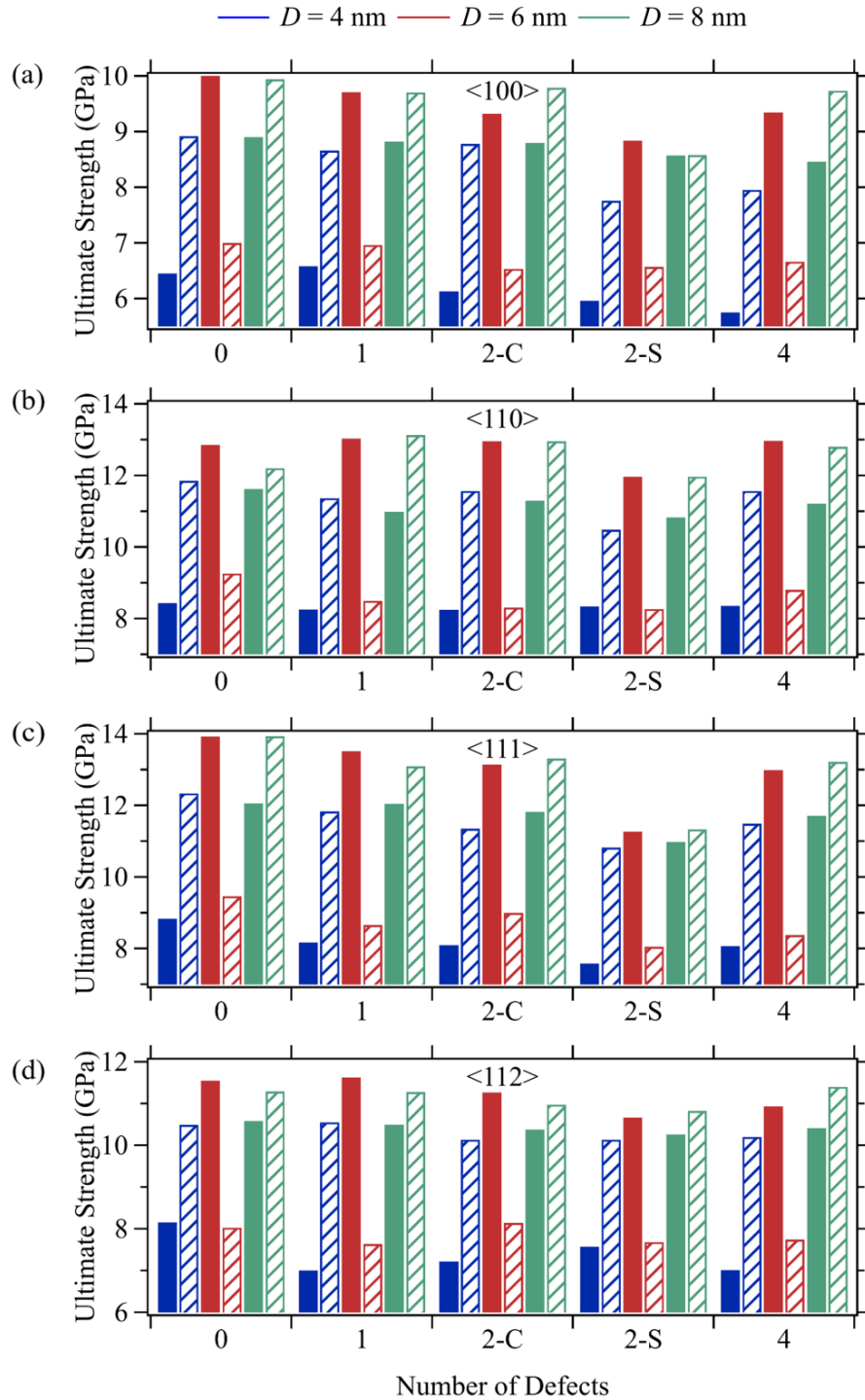


Figure 9.8: The ultimate strength as a function of defects distribution for aSiO<sub>2</sub>-Si NWs oriented along (a)  $\langle 100 \rangle$ , (b)  $\langle 110 \rangle$ , (c)  $\langle 111 \rangle$ , and (d)  $\langle 112 \rangle$  crystal orientations. The filled bars represent circular NWs, while the dashed bars correspond to square NWs.

#### 9.4.5 Strain Rate Effect

The strain rate during tensile testing is another significant factor affecting the elastic properties and strength of aSiO<sub>2</sub>-Si NWs. Figure 9.9 illustrates the estimated modulus of elasticity at different strain rates for NWs oriented along crystal orientations  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ , and  $\langle 112 \rangle$ , as shown in Figure 9.9 (a), (b), (c), and (d), respectively. Tensile tests are conducted on aSiO<sub>2</sub>-Si NWs using three strain rates:  $\dot{\epsilon} = 1 \times 10^9 \text{ s}^{-1}$ ,  $\dot{\epsilon} = 5 \times 10^9 \text{ s}^{-1}$ , and  $\dot{\epsilon} = 1 \times 10^{10} \text{ s}^{-1}$ . The results presented here, with minor variations due to the shape effect, indicate that the examined strain rates have an insignificant impact on the elastic properties of aSiO<sub>2</sub>-Si NWs. Additionally, Figure 9.10 displays the ultimate strength as a function of strain rate for NWs oriented along crystal orientations  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ , and  $\langle 112 \rangle$ , as shown in Figure 9.10 (a), (b), (c), and (d), respectively. The results reveal a slight increase in the ultimate strength of aSiO<sub>2</sub>-Si NWs when subjected to higher strain rates. Specifically, the ultimate strength of aSiO<sub>2</sub>-Si NWs tested at  $\dot{\epsilon} = 1 \times 10^{10} \text{ s}^{-1}$  is found to be 1-3 GPa higher compared to NWs tested at  $\dot{\epsilon} = 1 \times 10^9 \text{ s}^{-1}$ .

The investigation of strain rate effects on the tensile simulations of NWs is motivated by the need to assess the compatibility of interatomic potentials with the resulting elastic properties. An MD study employing the modified embedded-atom-method (MEAM) potentials reported negligible effects of strain rates spanning from  $\dot{\epsilon} = 5 \times 10^7 \text{ s}^{-1}$  to  $\dot{\epsilon} = 5 \times 10^8 \text{ s}^{-1}$  on the modulus of elasticity of unreconstructed Si NWs [Xu and Kim, 2019]. Another MD study on unreconstructed Si NWs, using the MEAM potential, found no significant influence of strain rates of  $\dot{\epsilon} = 5 \times 10^7 \text{ s}^{-1}$ ,  $\dot{\epsilon} = 5 \times 10^8 \text{ s}^{-1}$ , and  $\dot{\epsilon} = 5 \times 10^9 \text{ s}^{-1}$  on the tensile behavior of NWs [Kang and Cai, 2010]. Additionally, an MD study investigating the tensile response of unreconstructed Si NWs modeled with the SW potential determined that strain rates ranging from  $\dot{\epsilon} = 2 \times 10^8 \text{ s}^{-1}$  to  $\dot{\epsilon} = 2 \times 10^{10} \text{ s}^{-1}$  had no significant effect on the estimated modulus of elasticity [Jing et al., 2009a, Jing et al., 2009b]. In the case of Si NWs with a native oxide surface state, a recent study utilizing the m-SW and Tersoff-Munetoh potentials found no significant impact of strain rates ranging from



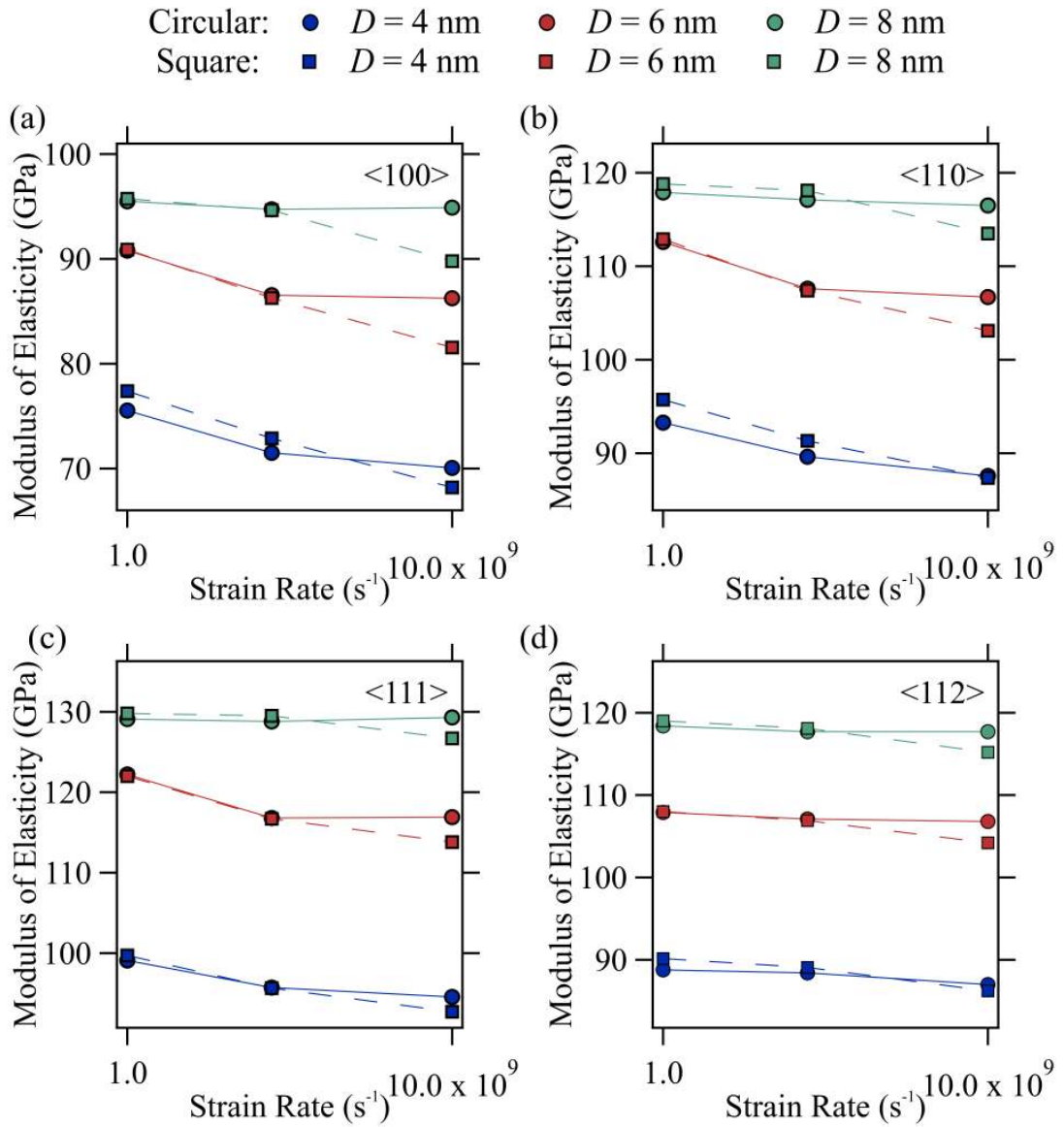


Figure 9.9: The modulus of elasticity as a function of strain rate for aSiO<sub>2</sub>-Si NWs oriented along (a) < 100 >, (b) < 110 >, (c) < 111 >, and (d) < 112 > crystal orientations.

$\dot{\epsilon} = 1 \times 10^8 \text{ s}^{-1}$  to  $\dot{\epsilon} = 5 \times 10^9 \text{ s}^{-1}$  on the elastic properties of the NWs [Pakzad et al., 2023b].

Regarding the ultimate strength of Si NWs with a native oxide surface state, a recent study using the m-SW potential reported deviations of up to 15% for strain rates ranging from  $\dot{\epsilon} = 1 \times 10^8 \text{ s}^{-1}$  to  $\dot{\epsilon} = 5 \times 10^9 \text{ s}^{-1}$  [Pakzad et al., 2023b]. Furthermore, the same study observed significant variations, up to 70%, in ultimate strength due to strain rate effects when employing the Tersoff-Munetoh potential, which is known to overestimate the ultimate strength [Pakzad et al., 2023b]. Another study on unreconstructed Si NWs reported that a slower strain rate leads to a lower critical buckling load, allowing for sufficient local deformations in the Si NWs [Jing et al., 2009a, Jing et al., 2009b]. Similarly, a study on unreconstructed Si NWs found an approximate decrease of 1 GPa in ultimate strength as the strain rate decreases while providing more time for defects to nucleate at lower stresses [Kang and Cai, 2010]. In the case of unreconstructed Si NWs modeled with modified MEAM potentials, no significant strain rate effects were observed for the ultimate strength when tested at  $\dot{\epsilon} = 5 \times 10^7 \text{ s}^{-1}$  and  $\dot{\epsilon} = 5 \times 10^8 \text{ s}^{-1}$  [Xu and Kim, 2019].

## 9.5 Conclusion

In this study, the mechanical properties of aSiO<sub>2</sub>-Si NWs are investigated by considering various factors such as crystallographic orientation, cross-sectional shape, critical dimensions, AR, temperature, and strain rate. Tensile tests are conducted on aSiO<sub>2</sub>-Si NWs with circular and square cross-sections using different critical dimensions to understand their stress-strain behavior. The results revealed that the modulus of elasticity and ultimate strength of the NWs increased as the critical dimension increased while maintaining a constant AR and native oxide thickness. The crystallographic orientation and cross-sectional shape also exhibit significant effects on the mechanical properties of Si NWs. Furthermore, the AR shows a negligible effect on the modulus of elasticity for values above 12, while NWs with smaller ARs demonstrate higher modulus of elasticity. The elastic properties and strength of Si NWs are analyzed by investigating various combinations of nano-voids positioned

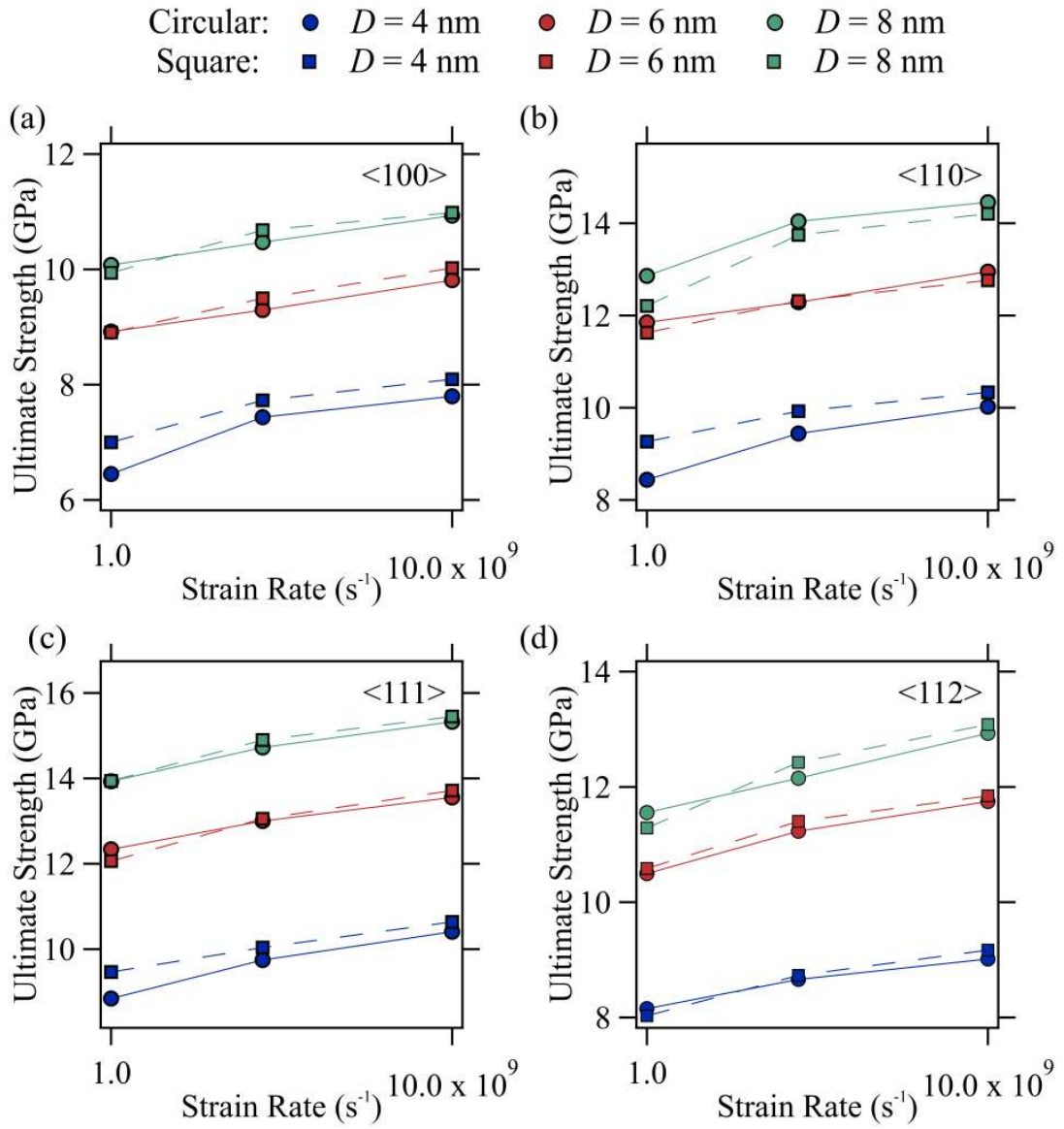


Figure 9.10: The ultimate strength as a function of strain rate for aSiO<sub>2</sub>-Si NWs oriented along (a)  $\langle 100 \rangle$ , (b)  $\langle 110 \rangle$ , (c)  $\langle 111 \rangle$ , and (d)  $\langle 112 \rangle$  crystal orientations.

along the NWs. The study also examines the influence of strain rate on the obtained results. Temperature dependence studies show decrease in the modulus of elasticity and ultimate strength with increasing temperature. The findings contribute to a better understanding of the mechanical behavior of aSiO<sub>2</sub>-Si NWs, highlighting the importance of considering native oxide surface conditions and appropriate modeling parameters. This study lays the groundwork for further research and optimization of aSiO<sub>2</sub>-Si NWs in various applications, providing insights for the design and development of high-performance Si NW-based devices.



## Chapter 10

# MACHINE LEARNING-DRIVEN ATOMISTIC ANALYSIS OF MECHANICAL BEHAVIOR IN SILICON NANOWIRES

### 10.1 Overview

This study explores the mechanical characteristics of silicon nanowires (Si NWs), with a specific focus on their modulus of elasticity. Employing a comprehensive methodology, the research integrates atomistic modeling through molecular dynamics simulations with advanced machine learning techniques. The molecular dynamics simulations yield a substantial dataset exceeding 3000 data points, exposing the mechanical response of Si NWs and highlighting the necessity for precise model calibration. The exploration of partial dependencies between surface state and crystal orientation presents a dependable means of estimating the modulus of elasticity in Si NWs. This study illustrates orientation-dependent elasticity using inverse pole figures, offering a mutually insightful approach. This endeavor not only enhances our comprehension of mechanical properties of Si NWs but also establishes a crucial link between computational and experimental research domains, building the framework for advancements in nanoelectromechanical applications.

### 10.2 Introduction

Nanowires (NWs) exhibit a significant potential as essential building blocks for the development of nanoelectromechanical systems (NEMS) [Bachtold et al., 2022, Karimzadehkhoei et al., 2023], nanoelectronics [Gao et al., 2022], and photonics [Quan et al., 2019, Bronstrup et al., 2010] with applications as highly sensitive sensors [Karimzadehkhoei et al., 2023, Zhang et al., 2023] and energy-related technolo-

gies [Panda et al., 2022, Nehra et al., 2020]. Significant advancements in fabrication techniques and the wider range of technological applications have generated increased interest in thoroughly characterizing NWs [Wang et al., 2016a, Zare Pakzad et al., 2023a, Zare Pakzad et al., 2023b]. The utilization of multi-scale modeling methods also contributes to this growing interest [Zare Pakzad et al., 2023c].

The surface contribution becomes more significant as a result of a size reduction in nanomaterials leading to different physical properties compared to the bulk counterpart [Wang et al., 2017, Mead et al., 2023]. The mechanical properties are found to be considerably size-dependent at nanoscale [Wang et al., 2017, Yang et al., 2022, Nasr Esfahani and Alaca, 2019]. Hence understanding the mechanical behavior of NWs is essential to embed them into NEMS devices [Karimzadehkhoei et al., 2023, Nasr Esfahani and Alaca, 2019, Park et al., 2009]. Various experimental methods are employed to investigate the impact of size reduction on the mechanical properties of NWs. This includes studying the modulus of elasticity, fracture strength, and brittle to ductile transition temperature, where considerable changes in the mechanical properties have been identified as a result of size reduction [Zare Pakzad et al., 2023c, Nasr Esfahani and Alaca, 2019, Zare Pakzad et al., 2021]. Thus nanomechanical modeling techniques have been developed as a means to explain such behavior in NWs. These approaches can be classified as continuum mechanics, analytical models, atomistic simulations and first principle methods providing in-depth analysis on the scale effect [Zare Pakzad et al., 2023c, Park et al., 2009, Sofiah et al., 2018, Momeni et al., 2020]. As the size decreases, the surface contribution becomes more prominent, leading to notable size-dependent properties of the NWs [Zare Pakzad et al., 2023c, Müller and Saúl, 2004, Pakzad et al., 2023b]. In this respect, understanding the scale effect becomes more challenging [Zare Pakzad et al., 2023c, Pakzad et al., 2023b, Nasr Esfahani et al., 2022].

Silicon (Si) NWs have been extensively investigated as fundamental components in semiconductor manufacturing due to their unique properties [Wang et al., 2017, Nasr Esfahani and Alaca, 2019, Ye et al., 2019, Ando and Namazu, 2023]. Although there have been numerous investigations into the size-dependent mechanical

properties of Si NWs, conflicting findings highlight the need for a more comprehensive analysis of the scale effect [Zare Pakzad et al., 2023c, Yang et al., 2022, Pakzad et al., 2023b]. A recent study highlights the necessity of adopting a multiscale theoretical framework to gain a comprehensive understanding of the size-dependent mechanical characteristics of Si NWs [Zare Pakzad et al., 2023c]. Furthermore, the importance of nanomechanical model selection is highlighted, where deviations of up to 85 GPa in elastic properties of Si NWs are attributed to the specific choice of the model [Zare Pakzad et al., 2023c]. In light of the existing challenges in fabrication, testing, and characterization, modeling continues to be a crucial element in precise interpretation of the findings [Zare Pakzad et al., 2023c, Zare Pakzad et al., 2021]. Additionally, the disparities between experimental and computational approaches concerning the scale effect present another significant challenge in this field [Yang et al., 2022, Nasr Esfahani and Alaca, 2019]. Molecular dynamics (MD) and density functional theory (DFT) play vital roles in revealing the size-dependent trends in the elastic properties of Si NWs [Pakzad et al., 2023b, Pakzad et al., 2021, Lee and Rudd, 2007, Pakzad et al., 2023a, Pakzad et al., 2024]. In line with this, MD simulations are used to subject Si NWs to tensile [Pakzad et al., 2024, Xu and Kim, 2019, Kang and Cai, 2007, Pakzad et al., 2023b], vibration [Kim et al., 2006, Park et al., 2005], and bending tests [Pakzad et al., 2023a, Zhuo and Beom, 2018, Ilinov and Kuronen, 2014], providing valuable insights into their mechanical properties. Thus, utilizing small-scale modeling methods can facilitate both analytical and experimental analyses to enhance the understanding of research outcomes.

The convergence between high-throughput computing and advanced machine learning (ML) algorithms has introduced a novel approach for enhancing the structural design and performance of nanomaterials [Jain et al., 2013, Curtarolo et al., 2013, Deringer et al., 2021, Catal et al., 2024]. This innovative approach has made a significant impact on the discovery of new materials [Deringer et al., 2019, Wang et al., 2023, Butler et al., 2018]. While atomic-scale modeling has made remarkable progress, they still face inherent limitations due to the substantial computational expenses associated with explicit methods like MD and DFT [Deringer et al.,

2019, Deringer et al., 2018]. Conversely, the field of NEMS design and industrial applications necessitate a more efficient and expeditious solution to address the size effect on the elasticity of Si NWs [Zare Pakzad et al., 2023c]. Given the current computational challenges encountered in investigating the size effect in Si NWs, ML presents an opportunity to streamline this process and inject a new level of realism into the field of material science and technology [Ramprasad et al., 2017, Erhard et al., 2023, Kulik et al., 2022]. Moreover, ML can function as a tool to offer enhanced understanding of material behavior at the nanoscale and to provide insights for the design purposes [Han et al., 2020]. Additionally, ML-based techniques are not only employed to explore material properties but are also harnessed for the creation of novel interatomic potentials for Si, offering a high degree of accuracy when compared to DFT references [Bartók et al., 2018, Dickel et al., 2021].

The current study addresses the size-dependent elastic properties of Si NWs using ML-driven atomistic simulations. The details associated with atomistic simulations are discussed in Section 10.3.1, while Section 10.3.2 addresses the specifics of ML modeling efforts. The results section offers an in-depth examination of atomistic findings given in Section 10.4.1 and ML-driven discoveries in Section 10.4.2. Ultimately, Section 10.4.3 provides an interpretation of the ML-based atomistic findings while exploring the potential for future expansion of the methodology introduced in this study. This work contributes valuable insights into the elastic properties of Si NWs, thereby enhancing our understanding of their mechanical characteristics at the nanoscale. The developed methodology has the potential to pave the way for comparing ML-based computational results to experimental findings, serving as the benchmark and validation measure for the quality of similar efforts [Zare Pakzad et al., 2023c, Nasr Esfahani and Alaca, 2019, Deringer et al., 2019, Kulik et al., 2022].

### **10.3 Methods and Materials**

This section covers the methodology of the study in two parts: the initial one discuss the computational aspects on the modeling of Si NWs using MD simulations,



while the subsequent section offers an extensive explanation of ML strategies. This includes discussions on data preparation, feature selection, and the algorithms employed within the framework of this article. An in-depth exploration of both approaches in Sections 10.3.1 and 10.3.2 are given, presenting a thorough analysis of the methods utilized.

### 10.3.1 Atomistic Simulations

This section offers a comprehensive account of modeling the tensile test of Si NWs using MD simulations. The two commonly employed boundary condition (B.C.) approaches for modeling the tensile behavior of NWs are examined: i) non-periodic and ii) periodic tensile. Sections in 10.3.1 are dedicated to discussing these two approaches individually. Furthermore, both sections delve into the specifics of various computational configurations, including the preparation of atomic configurations, interatomic potentials, and other relevant computational particulars.

#### *Non-periodic Tensile Simulation*

In this subsection, the atomistic methodology employed for the exploration of the tensile behavior of Si NWs utilizing a non-periodic B.C. along the NW is explained. MD simulations are conducted on Si NWs with unreconstructed surface states, utilizing the LAMMPS code [Thompson et al., 2022]. Figure 10.1 (a) illustrates the initial atomic configuration of Si NWs, emphasizing the geometric characteristics of the NW, which possesses a square cross-sectional shape. This representation includes the width, which serves as a representation of the critical dimension (CD) in Si NWs. Figure 10.1 (b) schematically describes the tensile modeling approach where the length ( $L$ ) of Si NW and the fixed and movable boundaries are labeled as  $L_f$  and  $L_m$ , respectively. The lengths  $L_f$  and  $L_m$  correspond to one-eighth of the NW length ( $L$ ). In this respect, the length to CD ratio ( $L/CD$ ) is termed as the aspect ratio (AR). Regarding the geometrical and computational details, Table 10.1 provides a complete description of input parameters. In this respect, the CD spans from 2 nm to 10 nm, while the predefined ARs are assigned as 7, 8, 9, 10, 12, 14, 16,

18, and 20. Si NWs having  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ , and  $\langle 111 \rangle$  crystal orientations are subjected to tensile test where the interactions between Si atoms are modeled using the Tersoff-T3 (TT3) [Tersoff, 1988] and Stillinger-Weber (SW) [Stillinger and Weber, 1985] potentials. Comprehensive details of the potential expressions and coefficients are available in the respective references [Tersoff, 1988, Stillinger and Weber, 1985].

Non-periodic B.C.s are imposed in all directions ( $x$ ,  $y$ , and  $z$ ) to account for a finite size. An energy minimization step is executed using the conjugate gradient method, followed by assigning an initial velocity distribution based on a finite temperature to all atoms. Subsequently, a relaxation process is carried out for 60 ps at a constant temperature, employing a 1 fs time step in the canonical NVT ensemble. During relaxation, the fixed and movable regions connected to the NW remain in fixed configurations. The subsequent tensile test involves fixing one end of the NW ( $L_f$ ) while allowing the other end ( $L_m$ ) to move. To mitigate shock wave generation due to rapid loading, a linearly increasing constant velocity is applied along the longitudinal direction ( $x$ ). The velocity starts from zero at the support and gradually increases to its maximum at the movable boundary. A velocity of  $1.0 \text{ \AA/ps}$  is applied at a constant temperature, corresponding to a strain rate of  $\dot{\epsilon} \approx 1.0 \times 10^9 \text{ s}^{-1}$ . This rate aligns with the strain rate employed in previous MD-based tensile tests on NWs [Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024, Kang and Cai, 2007]. The simulations are carried out at three distinct temperatures: specifically, 10 K, 300 K, and 600 K. The Virial theorem [Cormier et al., 2001] is employed for stress calculations given in Equation 10.1.

$$\pi_{ij} = \frac{1}{2\Omega_0} \left[ \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \frac{1}{r^{\alpha\beta}} \frac{\partial V(r^{\alpha\beta})}{\partial r} (v_i^{\alpha\beta} v_j^{\alpha\beta}) \right] \quad (10.1)$$

Here,  $\Omega_0$  represents the atomic volume in an undeformed system, where  $N$  denotes the total number of atoms. The distances between atoms  $\alpha$  and  $\beta$  are denoted as  $r^{\alpha\beta}$ . Furthermore,  $v_j^\alpha$  signifies the position of atom  $\alpha$  along the  $j$  direction, which can be expressed as  $v_j^{\alpha\beta} = v_j^\alpha - v_j^\beta$ . The term  $V$  corresponds to the interatomic

potential. The virial stress can be calculated by summing contributions from all atoms (and atom pairs) within the simulation cell, and subsequently dividing the result by the cell volume, which in this context corresponds to the volume of the NW.

### *Periodic Tensile Simulation*

This subsection outlines the MD approach used to investigate the tensile behavior of Si NWs with unreconstructed surfaces and periodic B.C.s applied along the NW. Similar to the Si NWs described in Section 10.3.1A, atomistic simulations are carried out on Si NWs with crystal orientations listed in Table 10.1, utilizing the LAMMPS code [Thompson et al., 2022]. In contrast to the Si NWs discussed earlier, periodic B.C.s are applied along the  $x$ -direction, while the  $y$ - and  $z$ -directions are constrained to model an infinitely long NW segment given in Figure 10.1 (c). The parameters such as CD, AR, interatomic potential, and temperature are repeated for Si NWs studied using this method. The MD simulations start with an energy minimization step using the conjugate gradient method, followed by the assignment of initial velocities based on a Gaussian distribution at the specified temperature. Subsequently, dynamic equilibration at the designated temperature is carried out for 60 ps, utilizing the Nose-Hoover isobaric-isothermal (NPT) ensemble with a time step of 1 fs. Following equilibration, the simulation cell undergoes longitudinal deformation at a strain rate of  $\dot{\epsilon} = 1 \times 10^9 s^{-1}$ , which falls within the suitable range for MD-based tensile testing [Pakzad et al., 2023b, Kang and Cai, 2007], as well as for Si NWs discussed in Section 10.3.1A. This ensures consistency in the deformation of Si NWs within the scope of this study. The stress-strain curves obtained for Si NWs are utilized to determine the modulus of elasticity, employing the formulation given in Equation 10.1.

Apart from Si NWs featuring unreconstructed surfaces modeled in this study, the comprehensive framework also encompasses Si NWs with native oxide surface states, as previously investigated by the authors [Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024]. In this regard, readers are encouraged to refer to the

provided references in Table 1 for computational details on modeling Si NWs with native oxide [Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024].

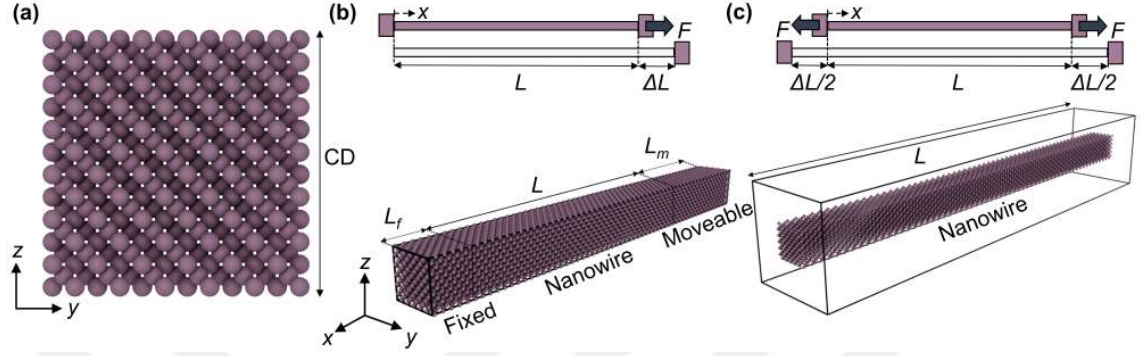


Figure 10.1: (a) Cross-sections of a Si NW with dimensional parameter defined as  $CD$ , representing NW width. (b) Non-periodic tensile simulation of Si NWs exhibited schematically (upper) and with atomic configuration (lower). The associated NW length ( $L$ ) and B.C.s regions are referred as fixed ( $L_f$ ) and movable boundaries ( $L_m$ ). (c) Periodic tensile simulation of Si NWs exhibited schematically (upper) and with atomic configuration (lower). The associated NW length ( $L$ ) and simulation box are shown. The force denoted by  $F$  schematically illustrates the direction of the tensile simulations.

### 10.3.2 Machine Learning

This section encompasses the intricacies related to data extraction from modeling Si NWs with unreconstructed surface states, as elaborated in Section 10.3.1, and draws upon information available in the literature for Si NWs with a native oxide surface state [Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024]. Further explanations regarding the data will be presented in Section 10.3.1A, while details pertaining to feature selection and the implementation of ML models will be discussed in Section 10.3.1B and Section 10.3.1C, respectively.

#### Data Preparation

Effective data preparation is crucial for developing a robust ML algorithm, where the relevance of data is as important as the quantity for successful predictions. To construct the dataset necessary for training the ML algorithms, two primary sources

of input are employed. The modeling efforts outlined in Section 10.3.1 generate tensile responses for Si NWs under different parameter sets, with a specific focus on Si NWs featuring the unreconstructed surface state. In light of three crystallographic orientations of Si, two distinct interatomic potentials, three designated testing temperatures, and nine differing Si NW CDs, coupled with nine distinct ARs modeled via non-periodic and periodic B.C.s, a comprehensive collection of 2916 Si NWs is established within this study. Additionally, data from previous research conducted by the authors on Si NWs with a native oxide surface state, as documented in relevant literature [Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024], are assimilated into the overall dataset.

The Si NWs featuring a native oxide surface state exhibit variations in critical dimension, native oxide layer thickness, applied B.C.s (non-periodic and periodic), temperature, and interatomic potentials (Tersoff-Munetoh (TM) [Munetoh et al., 2007] and modified Stillinger-Weber (m-SW) [Ganster et al., 2010]). Notably, two key distinctions arise upon integrating data from Si NWs with these distinct surface conditions. Firstly, the unreconstructed Si NWs maintain their original surface thickness without any native oxide layer, whereas the Si NWs with native oxide exhibit values that account for differing oxide layer thicknesses. Secondly, recognizing the structural deviations resulting from oxygen atom presence in Si NWs with native oxide surfaces, a consolidation is performed concerning the categorization of Tersoff and SW potentials. Consequently, TT3 and TM, as well as SW and m-SW, are grouped within the same potential family, and comparable values are attributed during dataset preparation. In this context, the Tersoff (TT3 [Tersoff, 1988] and TM [Munetoh et al., 2007]) and Stillinger-Weber (SW [Stillinger and Weber, 1985] and m-SW [Ganster et al., 2010]) represent two distinct families of interatomic potentials within the framework of this article. With the inclusion of the dataset pertaining to Si NWs with native oxide surface states, a total of 305 additional data points are appended to this study's collection. This extension elevates the overall number of data points to 3221, each representing the modulus of elasticity of a unique Si NW.

Certainly, acquisition a substantial number of data points stands as a primary

challenge in materials informatics, primarily due to the computational costs associated with acquiring materials and their corresponding target variables. Consequently, datasets frequently comprise a limited quantity of data points. Notably, to the best of our knowledge, the number of data points available for different Si NWs, specifically those investigating elasticity using MD (excluding those presented by the authors [Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024]), is currently less than 300. This circumstance might contribute significantly to the well-recognized discrepancies between elastic properties of Si NWs obtained via computational and experimental approaches [Yang et al., 2022, Nasr Esfahani and Alaca, 2019]. In this context, every data point within the dataset encompasses seven distinct features, as delineated in Table 10.1, along with a single target variable representing the modulus of elasticity of the Si NW. The tabulated features encompass crystallographic orientation (ORNT), CD, AR, interatomic potential (POT), temperature (T), BC (non-periodic and periodic), and surface state (SS). Each unique combination detailed in Table 10.1 for the unreconstructed surface condition is simulated, and the dataset is further enriched through the incorporation of Si NWs with native oxide surface states from pertinent literature [Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024]. In the context of ML applications, the intrinsic nature of predictors within the dataset might necessitate preprocessing to enhance the overall performance of the ML process. Specifically, variables within a dataset can exhibit non-normal distributions or disparate scales, all of which can adversely impact the efficacy of ML algorithms. Therefore, prior to training, an in-depth analysis of the dataset will be undertaken to comprehend the data distribution and subsequently implement suitable data transformation techniques. Through data transformation, the variables are normalized and scaled to ensure equitable treatment by ML algorithms. In this study, a z-score normalization (standardization) approach is employed to achieve standard scaling and normalization of features, ensuring a mean of zero and a standard deviation of one. The next section will cover the details associated with descriptors and feature selection for ML algorithms.

### *Feature Selection*

A meticulous feature selection process is conducted prior to crafting the dataset. Within this context, seven parameters outlined in the previous section, alongside their corresponding details as presented in Table 10.1, are identified as essentials for this task. In this regard, highly correlated features are excluded from this scheme, as they would redundantly convey a shared realm of information. For instance, this applies to combinations such as strain rate and time step within the context of tensile modeling of Si NWs. Despite the selection of seven features for this study, the assessment of correlation between these features is crucial, considering both linear and non-linear perspectives. To address the potential linear correlation, the Pearson's correlation coefficient (PCC) is calculated [Sedgwick, 2012]. To address broader correlation issues, the random forest (RF) method, renowned for its efficacy in classification and regression tasks, is also utilized for feature correlation study [Archer and Kimes, 2008]. In contrast to alternative feature selection methods, the RF method assigns importance scores to variables by ranking them based on their performance during model optimization. This approach allows for a comprehensive evaluation of feature correlations, facilitating enhanced interpretation of findings. Before implementing ML algorithms for data generation, the initial focus revolves around refining the dimensionality of the dataset by emphasizing the most pertinent features. From a modeling perspective, this entails considering factors like time step, cross-section shape, alternative testing methods such as bending or compression, and different types of interatomic potentials like the Modified Embedded Atom Method (MEAM) potential [Xu and Kim, 2019]. However, while this approach could enhance the dataset, it carries the risk of introducing an excessive number of input features, potentially leading to overfitting especially when dealing with a limited number of instances due to the problem's potential high degree of freedom or non-linearity. The following section will address the specifics pertaining to ML algorithms.

Table 10.1: Summary of input parameters used for modeling the tensile behavior of Si NWs.

| Definition             | Descriptor | Values                                                                                                                                                                                                                              |
|------------------------|------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Crystal Orientation    | ORNT       | $\langle 100 \rangle$ : $[100]$ - $x$ $[010]$ - $y$ $[001]$ - $z$<br>$\langle 110 \rangle$ : $[110]$ - $x$ $[001]$ - $y$ $[\bar{1}10]$ - $z$<br>$\langle 111 \rangle$ : $[111]$ - $x$ $[1\bar{1}0]$ - $y$ $[\bar{1}\bar{1}2]$ - $z$ |
| Critical Dimension     | CD         | 2, 3, 4, 5, 6, 7, 8, 9, 10 nm                                                                                                                                                                                                       |
| Length to Width Ratio  | AR         | 7, 8, 9, 10, 12, 14, 16, 18, 20                                                                                                                                                                                                     |
| Interatomic Potentials | POT        | Tersoff (TT3 [Tersoff, 1988] and TM [Munetoh et al., 2007]) & Stillinger-Weber (SW [Stillinger and Weber, 1985] and m-SW [Ganster et al., 2010])                                                                                    |
| Temperature            | T          | 10, 300, 600 K                                                                                                                                                                                                                      |
| Boundary Conditions    | BC         | Non-periodic and Periodic                                                                                                                                                                                                           |
| Surface State          | SS         | Unreconstructed and Native Oxide (Refs. [Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024])                                                                                                                           |



### Machine Learning Algorithms

The analysis of the dataset and associated features using ML algorithms occurs in a two-step process. Initially, the Regression Learner toolbox in MATLAB [Inc., 2022] is employed to assess various ML models. By training the toolbox's available models, which encompass RF, K-Nearest Neighbors (KNN), linear regression (LR), decision trees (DT), multi-layer perceptron (MLP), and support vector machines (SVM), the models exhibiting the most promising performance are identified. This preliminary stage facilitates the selection of appropriate models for a more in-depth exploration of ML algorithms. Within this context, MATLAB's models are leveraged, with 70% of the dataset allocated for training and 30% for validation, utilizing 10-fold cross-validation. The evaluation of ML models centers on their predictive accuracy with respect to the test dataset. Transitioning to the second stage of ML modeling, building upon the insights gained from the initial stage, various ML algorithms namely, RF, KNN, LR, DT, MLP, and SVR are assessed in their ability to forecast the target variable. Prior to model training, the original dataset is divided into training data, facilitating model optimization, and a test dataset, employed to gauge the models' predictive accuracy on unseen data. The evaluation of ML models is grounded in their predictive errors on the test dataset, measured by root mean squared error (RMSE), mean absolute error (MAE), and coefficient of efficiency ( $R^2$ ) as defined by Equations 2, 3 and 4, respectively. In this regard,  $y_i$  and  $\tilde{y}_i$  are true and predicted values, respectively. Here  $\bar{y}$  is the average of the predicted values and  $n$  is the total number of the samples. All computations are executed using the scikit-learn library within the Python programming language [Pedregosa et al., 2011]. Upon identifying the most effective models, additional optimization techniques, including hyperparameter tuning, are experimented with to determine optimal configurations. These optimizations are iterated to enhance the training process and mitigate the risk of overfitting given the current training dataset.

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \tilde{y}_i)^2} \quad (10.2)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \tilde{y}_i| \quad (10.3)$$

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \tilde{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (10.4)$$

## 10.4 Results

The section begins by presenting the particulars concerning the MD modeling, including the outcomes of atomistic assessments for predicting the modulus of elasticity in Si NWs as discussed in Section 10.3.1. It explores the intricacies of the dataset, furnishing additional insights into the data arrangement intended for the following phase of the results section (Section 10.4.1). Subsequently, the results of the ML approach, realized through two distinct stages carried out using MATLAB and Python (discussed in Section 10.3.2), are elaborated (Section 10.4.2). Finally, the interpretation of findings on the elastic properties of Si NWs will be carried out in Section 10.4.3.

### 10.4.1 Atomistic Results

Utilizing atomistic simulations, particularly MD, presents a viable approach for investigating the elastic properties of Si NWs. Despite an extensive literature examining factors like crystallographic orientation, critical dimension, cross-section shape, AR, testing method, strain rate, temperature, interatomic potential, surface condition, defects or flaws, and B.C.s, a consensus regarding the size effect in elasticity of Si NWs is still missing. This stems not only from disparities between computational and experimental efforts but also from significant deviations observed in atomistic findings due to variations in aforementioned parameter selection. Moreover, given the extensive applications of Si NWs in future electronics and NEMS, there is an imperative need for a rapid and precise exploration of elasticity concerning size effects. In this context, the integration of ML algorithms with computational approaches

has the potential to streamline this process. This section presents the outcomes of MD simulations conducted within the scope of this paper, as well as previous data points from studies published by the authors. Within this framework, the modulus of elasticity of Si NWs is derived from stress-strain curves as the output parameter. This comprehensive analysis includes data from 2916 Si NWs modeled in this study, along with an additional 305 data points extracted from prior research by the authors [Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024]. This accumulation results in a dataset comprising 3221 data points, each representing the modulus of elasticity for a unique Si NW.

Given the computational demands associated with modeling Si NWs with a native oxide layer due to the increased number of atoms involved, the primary focus of modeling efforts is directed toward unreconstructed Si NWs. Specifically, all possible combinations of Si NWs with unreconstructed surface states, accounting for the nine different CDs, nine various ARs, three distinct temperatures, two types of B.C.s, and two types of interatomic potentials are simulated. This extensive dataset serves as a valuable resource for ongoing and prospective studies, considering its unique size and composition. The dataset presented within this section will undergo examination and analysis through the utilization of ML models in two distinct stages given in Section 10.4.2.

#### *10.4.2 Machine Learning Results*

This section provides a detailed analysis of the findings derived from the application of ML models in a two-stage process. Initially, the available models within the Regression Learner toolbox of MATLAB are trained to conduct an initial assessment of the data. The outcomes are visualized in Figure 10.2, showcasing the RMSE and MAE for the testing datasets. This assessment is conducted using a 70% training dataset and a 30% testing dataset, with a 10-fold cross-validation approach. In this context, a range of models including RF, KNN, DT, MLP, LR, and SVR-based, each with different hyperparameters or kernels, are examined. The results depicted in Figure 10.2 clearly highlight that linear models such as LR and SVR with linear

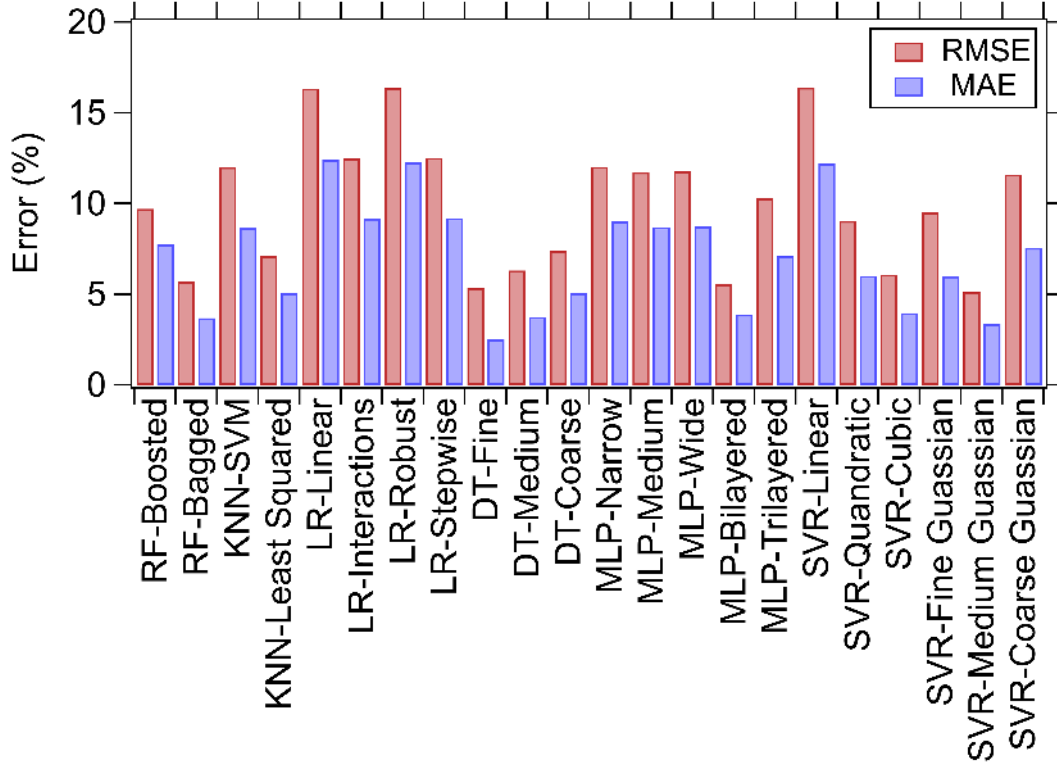


Figure 10.2: RMSE and MAE on test errors for different ML algorithms employed via Regression Learner toolbox in MATLAB.

designations exhibit the highest errors. This observation underscores the anticipated presence of non-linearity within the problem domain. However, the disparities in error rates based on varying model hyperparameters and their impact on errors emphasize the need for a more thorough investigation of the models, involving precise parameter calibration and kernel selection.

Following the initial data set examination within the context of ML algorithms, the Python scikit-learn library is employed to conduct a more detailed investigation of elasticity in Si NWs. This analysis involves the assessment of various ML algorithms, namely RF, KNN, LR, DT, MLP, and SVR while different training data percentages, ranging from 30% to 90% with 10% intervals, are used in this evaluation. Given the size of dataset in this study, it is important to split the data

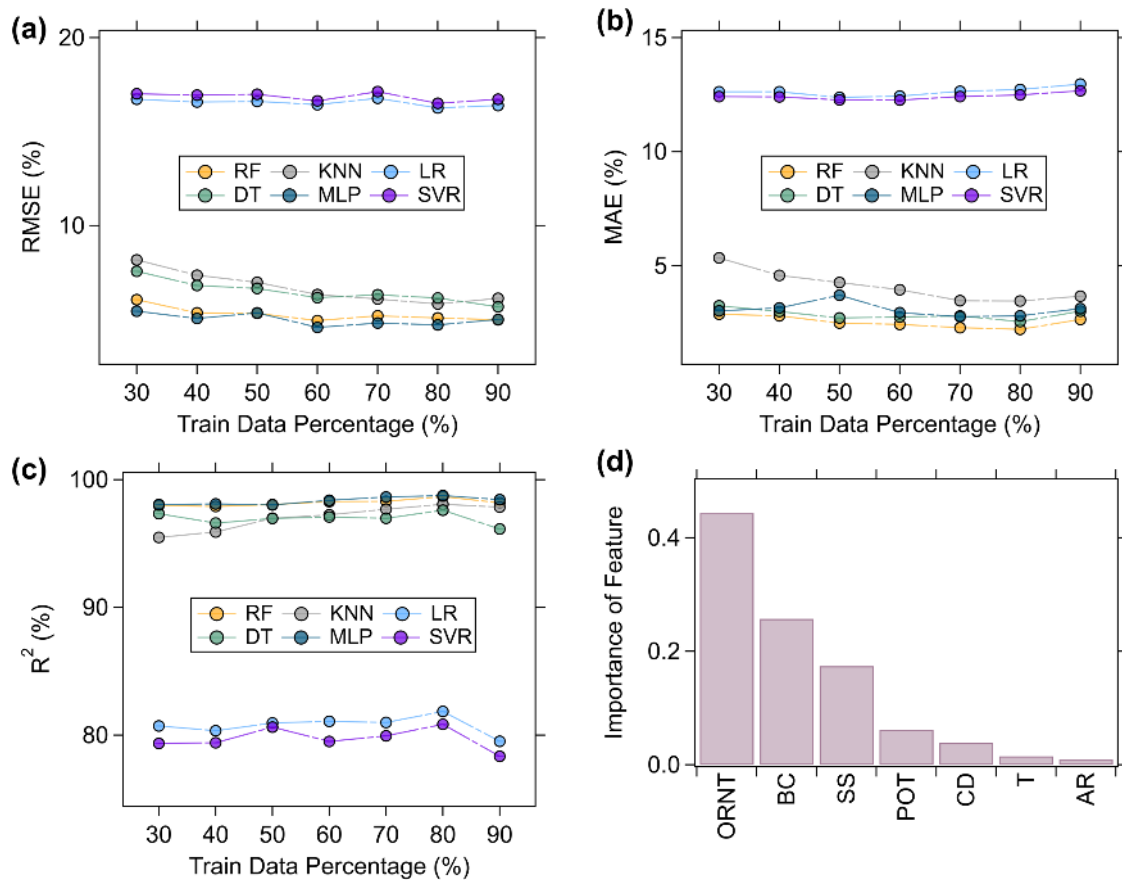


Figure 10.3: The evolution of (a) RMSE, (b) MAE, and (c)  $R^2$  on test dataset with changing training dataset proportions for the RF, KNN, LR, DT, MLP, and SVR algorithms. (d) The relative feature importance for input variables based on their performance obtained via the RF method.

thoughtfully, aiming for a balanced distribution in both the training and test datasets to avoid overfitting. To ensure robustness, the random assignment of the data set for this analysis is repeated across 100 trials. The ML models are evaluated based on their prediction errors on the test dataset. Subsequently, calculations of RMSE, MAE, and  $R^2$  are performed, with their respective standard deviations presented in Figures 10.3 (a), (b), and (c), respectively. When considering RMSE as the most critical performance evaluation parameter in the context of ML algorithms, a clear distinction emerges in the errors obtained. Specifically, four models – RF, KNN, MLP, and DT – report RMSE values below 10%, while LR and SVR, which both employ linear kernels in this study, exhibit higher RMSE values. This emphasizes

the non-linearity of the problem when examining the elasticity of Si NWs. Furthermore, MAE, a common measure of forecast error in time series analysis, confirms the findings from the RMSE analysis, showing a greater dependence on the training data percentage for smaller data subsets. In this context, the calculation of  $R^2$  provides an additional quantitative assessment of the observation of non-linearity. Linear models exhibit a degree of correlation of approximately 80% within the context of prediction and target values, while the remaining four models (RF, KNN, MLP, and DT) demonstrate more than 95% coefficient of efficiency, underscoring their suitability for this task.

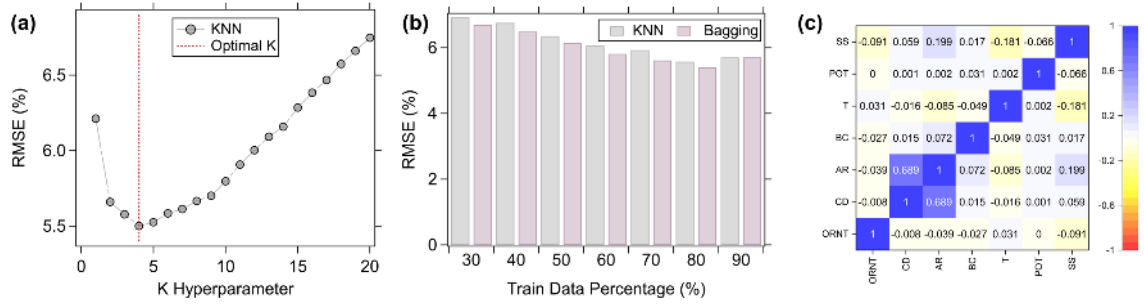


Figure 10.4: (a) The change in RMSE with increasing  $K$  hyperparameter for KNN algorithm. (b) Estimation of RMSE with bagging method while compared with KNN algorithm. (c) The heatmap of PCCs for associated features discussed in Table 10.1, The higher color intensities exhibit the enhanced correlation between the two features while the blue and red colors indicate positive and negative correlation, respectively.

Upon initial examination of the performance of ML models on the dataset, the significance of features becomes more pronounced. The RF method, which utilizes a forest of numerous trees, is particularly adept at this task. One notable advantage of RF is its ability to provide feature importance, making it an appealing tool for potential follow-up analyses, such as partial dependence analysis between features. The feature importance results obtained from the RF algorithm in this study are depicted in Figure 10.3 (d). Among these features, the crystallographic orientation, ORNT, the boundary condition definition during testing, BC, and surface state, SS, emerge as the most crucial parameters, showcasing the highest impor-

tance within the context of this problem. Conversely, the numerous simulations conducted on geometric properties, including CD and AR, exhibit lower importance when compared to the previously mentioned features. This observation is consistent with earlier research, which emphasizes the significant impact of surface effects and crystal orientation on the mechanical properties of Si NWs [Zare Pakzad et al., 2023c, Zare Pakzad et al., 2021, Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2023a, Pakzad et al., 2024].

Following the discussion on error analysis, a subsequent examination and discussion of algorithms are carried out using a 30% test data percentage, which corresponds to optimal error rates observed for the majority of the trained models. Furthermore, the performance of the KNN algorithm hinges on the value of the hyperparameter  $K$ , which defines the number of closest neighbors considered from the training dataset when making predictions for a new data point. This provides an opportunity for further improvement of the KNN model where the  $K$  hyperparameter can be fine-tuned. Lower values of  $K$  such as those close to 1, result in predictions that closely resemble the patterns in the training data, reducing flexibility but potentially increasing generalization capabilities. In contrast, higher values of  $K$  introduce more diversity in the neighbor selection process. In this context, Figure 10.4 (a) displays the RMSE across a range of  $K$  hyperparameter values, spanning from 1 to 20. The optimal value of  $K$  is identified as 4, corresponding to the minimum error achieved. Furthermore, the paper explores the application of the bagging ensemble technique to enhance the stability and accuracy of the KNN model. The reduction in RMSE percentages for various training data percentages is illustrated in Figure 10.4 (b), demonstrating the benefits of this technique in improving model performance.

Furthermore, Figure 10.4 (c) displays a heatmap illustrating the PCCs among the input variables. Notably, the parameters representing dimensionality, specifically CD and AR, exhibit the highest correlation, reaching approximately 0.7. This correlation represents the strongest linear relationship among all the features. However, it's essential to acknowledge the limitations of the PCC method, as it disregards

model performance variations and overlooks non-linear relationships among variables. Consequently, reliance on importance calculations based on the RF method is considered to be more reliable. In this context, it is important to note that the BC (second most importance feature given in Figure 10.4 (d)) pertains to the computational methodology employed and is unrelated to the physical interpretation of properties in Si NWs.

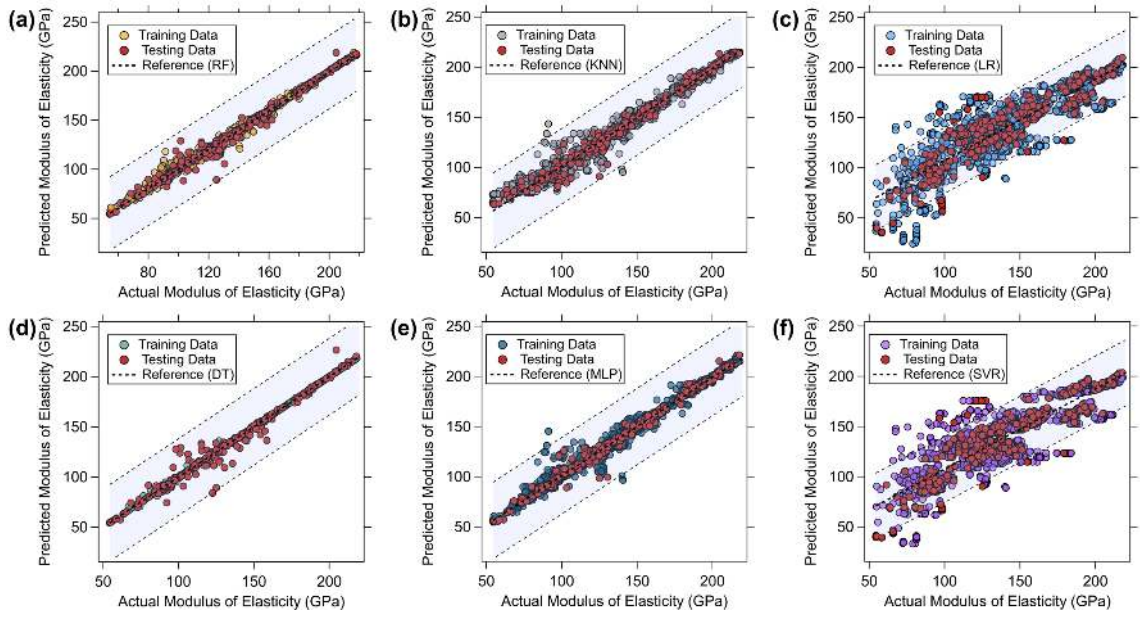


Figure 10.5: Performance of (a) RF, (b) KNN, (c) LR, (d) DT, (e) MLP, and (f) SVR algorithms in predicting modulus of elasticity as a function of actual modulus of elasticity available in the testing set. The line of references, along with their corresponding standard deviations, is also provided for each model.

As depicted in Figure 10.5, the performance of six algorithms in predicting the modulus of elasticity of Si NWs, as a function of the actual modulus of elasticity obtained via MD simulations, is showcased. Given the performance disparities among various ML models, particularly when excluding the linear models (LR and SVR) from consideration within the scope of this study, it becomes essential to conduct a more detailed examination of these models. To ensure robustness and prevent overfitting, a ten-fold cross-validation approach is employed. Among these algorithms, the RF and DT models emerge as the top performers, followed by KNN and MLP. In



contrast, LR and SVR with linear kernels exhibit the least favorable performance. Further examination of the best-performing models involves hyperparameter tuning, particularly for the RF model. This fine-tuning is implemented to control the maximum depth of individual trees, mitigating the risk of overfitting, while also governing the minimum sample leaf and minimum sample split parameters. Through this process, the following hyperparameter values are determined for the RF model: a maximum depth of 10, a minimum sample leaf of 1, and a minimum sample split of 5. This optimization results in a notable improvement, with a 0.3% reduction in RMSE, a 0.2% reduction in MAE, and a 0.2% increase in  $R^2$ . Similarly, a detailed analysis of hyperparameters for the DT model is carried out, leading to the selection of the following values: a maximum depth of 10, a minimum sample leaf of 3, and a minimum sample split of 5. This hyperparameter tuning results in a 0.6% reduction in RMSE, a 0.1% reduction in MAE, and a significant 0.8% increase in  $R^2$ . These findings underscore the importance of hyperparameter tuning in optimizing the performance of ML models, particularly for decision tree-based algorithms like RF and DT. Given this, a more thorough analysis of the two most important features – crystallographic orientation (ORNT) and surface state (SS) – is necessary. Section 10.4.3 of the paper will present the results of such analysis based on the feature importance.

#### 10.4.3 Interpretation of Results

This section is dedicated to interpreting the outcomes of the ML-based analysis of the MD simulations conducted on Si NWs, with a particular focus on the areas where ML can address existing gaps in the literature. As previously discussed, the size-dependent behavior of the modulus of elasticity remains an ongoing research challenge, lacking a definitive answer regarding the size effect. Considering various effective parameters, crystal orientation, dimensionality, and surface state prove to be notably challenging. One crucial aspect of the analysis presented here is the interpretation of partial dependence between the surface state and crystal orientation of Si NWs. These two features stand out as the most impactful, disregarding the

influence of BC, which mainly mirrors computational methodology and does not directly represent the modulus of elasticity in Si NWs. Furthermore, once ML algorithms achieve a reliable level of performance, they can serve as efficient tools for predicting the surface state and Si NW orientation, facilitating the rapid estimation of the modulus of elasticity. Focusing on four models, specifically the KNN, MLP, DT, and RF, which have demonstrated superior performance in this study, this section explores the partial dependence of surface state on three crystal orientations of Si NWs. These relationships are visualized in Figures 10.6 (a), (b), (c), and (d), respectively. It is noteworthy that each model exhibits a distinct trend in prediction, influenced by the level of non-linearity, spanning across the three crystal orientations and the provided range of surface states. Rather than identifying a single, most successful model, the results depicted in Figure 10.6 offer a valuable and prompt method for estimating the modulus of elasticity for Si NWs. In light of the discrepancies between experimental findings and computational results when addressing the size effect in the elastic properties of Si NWs, Figure 10.6 serves as an initial step towards a more informed interpretation of the elastic response in Si NWs. It provides a promising foundation for an intelligent roadmap towards understanding the behavior of Si NWs in terms of their modulus of elasticity. To the best of our knowledge, such an approach has not been reported previously.

Given the significance of crystal orientation in Si NWs, as indicated in prior literature and in the context of this study, the common approach for characterizing the orientation of crystalline materials in a spatially resolved manner is through techniques like electron backscatter diffraction (EBSD) [Hielscher and Schaeben, 2008, Purcek et al., 2012, Li et al., 2019]. This study focuses on the utilization of inverse pole figure (IPF) coloring to assess the influence of crystal orientation on the modulus of elasticity of Si NWs. IPF offers a set of visual representations that enable the transformation of arbitrarily scattered pole figure data, a task that involves considerable mathematical and computational challenges. To address the relationship between crystal orientation and the modulus of elasticity of Si NWs, a detailed analysis based on the partial dependence calculations of four successful ML

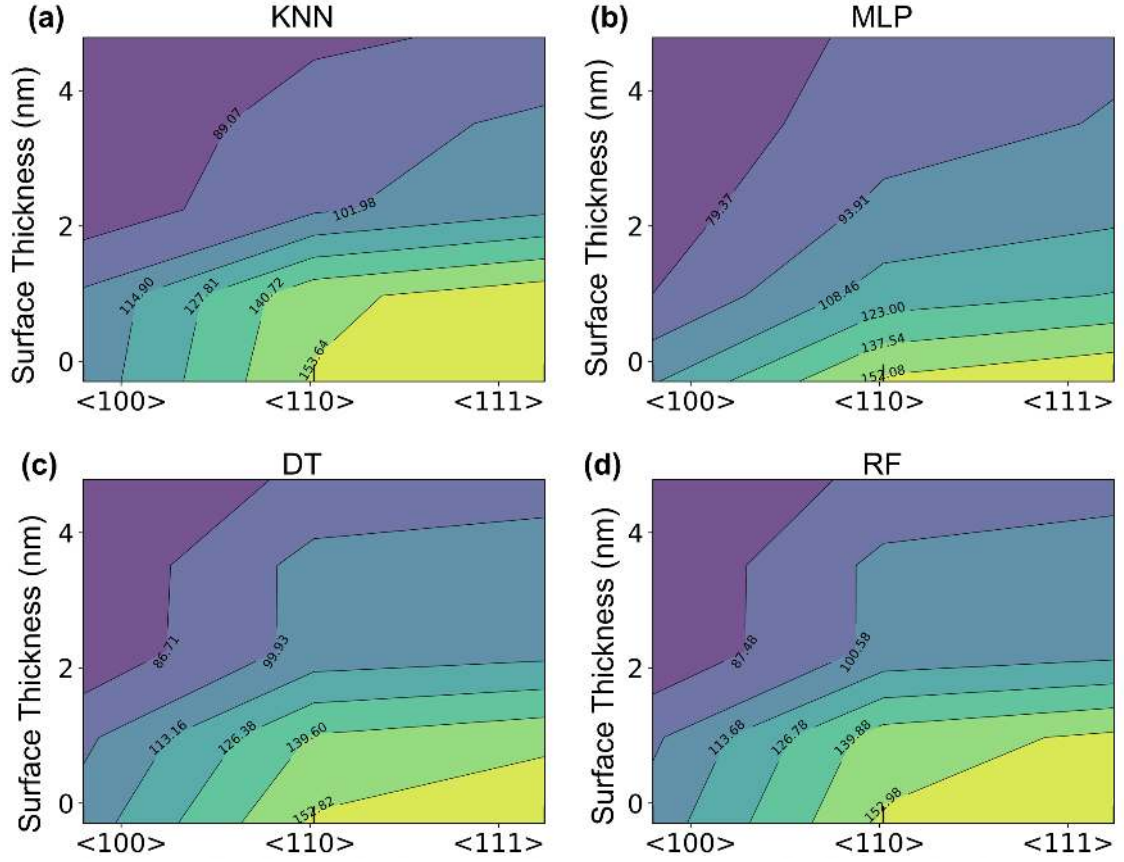


Figure 10.6: Partial dependence of elasticity between surface thickness and crystallographic orientation of Si NWs studied using (a) KNN, (b) MLP, (c) DT, and (d) RF models.

models is conducted, given in Figure 10.7. In this regard, the IPF visualizations for the modulus of elasticity with a constant surface thickness are presented for the KNN, MLP, DT, and RF models in Figures 10.7 (a), (b), (c), and (d), respectively. The shapes displayed in these figures represent stereographic projections of specific directions situated at the three corners, which correspond to the directions within the Si NWs investigated here. The various shades in the IPFs indicate varying degrees of stiffness in relation to the different orientations of Si NWs. This analysis on the orientation-dependent modulus of elasticity for Si NWs is carried out based on partial dependence analysis while maintaining a constant surface thickness, enabling the observation of variations between different ML models as different crystal orientations are examined. Considering the uncertainties associated with size dependent

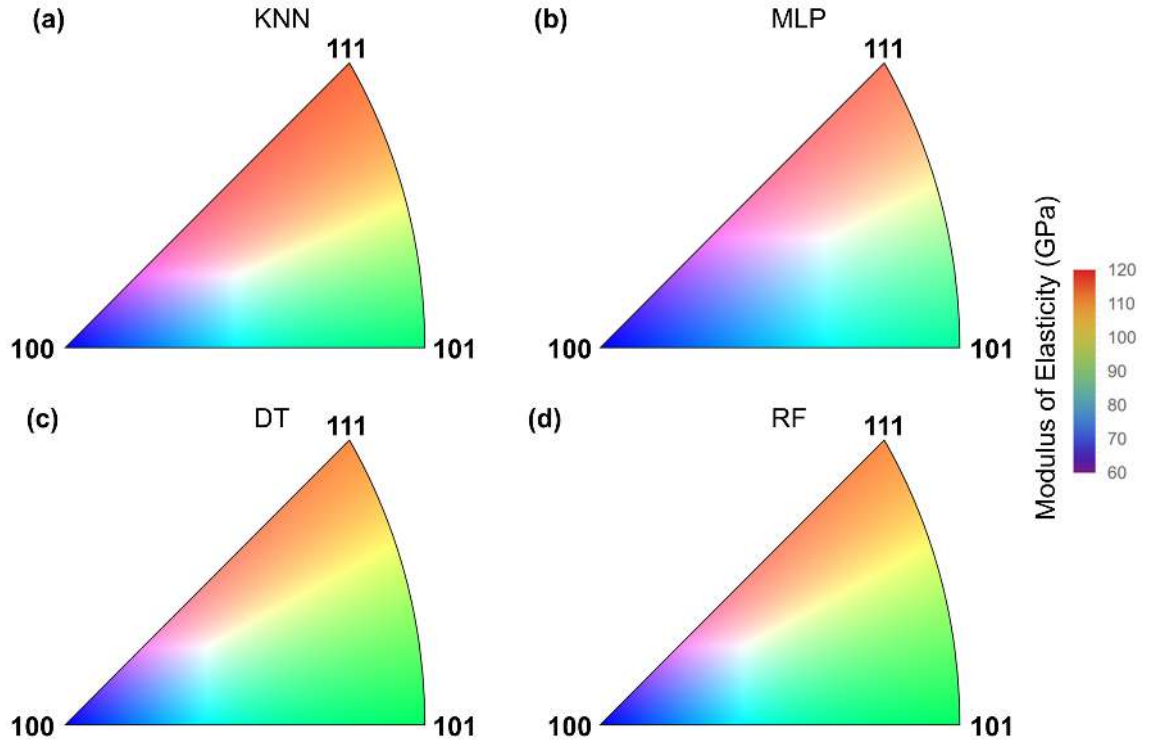


Figure 10.7: Crystal orientation dependence of modulus of elasticity visualized using IPF for Si NWs using (a) KNN, (b) MLP, (c) DT, and (d) RF models.

elastic properties of Si NWs in the literature, Figure 10.7 is, to the best of our knowledge, the first representation of orientation dependence within the context of elastic properties of Si NWs. In this regard, Figure 10.7 demonstrates the significance of scale effect while the deviations between the ML models remain negligible.

### 10.5 Conclusion

In conclusion, this study has studied the mechanical properties of Si NWs through a comprehensive analysis that integrated atomistic modeling and ML techniques. The MD simulations provided valuable data encompassing various parameters, offering insights into the elastic properties of Si NWs. This dataset, comprising over 3000 data points, has unveiled the non-linear and multifaceted nature of mechanical behavior of Si NWs, emphasizing the need for precise model calibration. The ML phase of study further expanded our understanding by revealing the size dependency

in mechanical response of Si NWs. Through meticulous hyperparameter tuning and model optimization, the improved accuracy in predicting the modulus of elasticity is achieved. Additionally, the investigation into partial dependencies between surface state and crystal orientation offers an efficient and intelligent approach to estimate modulus of elasticity as a function of parameters with high feature importance. The analysis of partial dependence is extended via IPF for detailed orientation dependent representation of elastic properties in Si NWs. Overall, this study underscores the potential for synergizing computational and experimental efforts in the realm of NWs. This work paves the way for more accurate predictions and a better grasp of the size-dependent mechanical properties of Si NWs, with implications for advancements in various fields, including nanoelectromechanical systems and nanoelectronics.

## Chapter 11

# SIMPLIFIED TOP-DOWN FABRICATION OF SUB-MICRON SILICON NANOWIRES

### 11.1 Overview

Silicon nanowires are among the most promising nanotechnology building blocks in innovative devices with numerous applications as nanoelectromechanical systems. Downscaling the physical size of these devices and optimization of material functionalities by engineering their structure are two promising strategies for further enhancement of their performance for integrated circuits and future-generation sensors and actuators. Integration of silicon nanowires as transduction elements for inertial sensor applications is one prominent example for an intelligent combination of such building blocks for multiple functionalities within a single sensor. Currently, the efforts in this field are marred by the lack of batch fabrication techniques compatible with semiconductor manufacturing. Development of new fabrication techniques for such one-dimensional structures will eliminate the drawbacks associated with assembly issues. The current study aims to explore the limits of batch fabrication for a single nanowire within a thick Si layer. The objective of the current work goes beyond the state of the art with significant improvements to the recent viable approach on the monolithic fabrication of nanowires, which was based on a conformal side-wall coating for the protection of the nanoscale silicon line followed by deep etch of the substrate transforming the protected layer into a silicon nanowire. The newly developed fabrication approach eliminates side wall protection and thereby reduces both process complexity and process temperature. The technique yields promising results with possible improvements for future micro and nanofabrication processes.

## 11.2 Introduction

Nanowires (NWs) are crucial building blocks of emerging optoelectronic and nanoelectromechanical systems (NEMS) [Karimzadehkhoei et al., 2023, Alaca and Karimzadehkhoei, 2023, del Moral et al., 2021, Bachtold et al., 2022]. Further miniaturization opportunities in CMOS integration [Waldrop, 2016] indicate NWs can provide significant improvements in NEMS [He et al., 2005, De Marchi et al., 2014, Boodhoo et al., 2015, Esfahani et al., 2017b, Tran et al., 2018, Tasdemir et al., 2016, Xu et al., 2022]. With device dimensions shrinking to quantum limits, the fabrication or synthesis techniques of nanoscale features become increasingly challenging [Nasr Esfahani and Alaca, 2019, McIntyre and i Morral, 2020, Zafar et al., 2018]. In addition to NEMS, microelectromechanical systems (MEMS) also benefit from downscaling for the development of on-chip integration of miniaturized smart sensors [Karimzadehkhoei et al., 2023, Alaca and Karimzadehkhoei, 2023]. This leads to products with more intelligence and relatively low power consumption [Karimzadehkhoei et al., 2023, Alaca and Karimzadehkhoei, 2023, Verma et al., 2021, Zhang et al., 2020]. A number of candidate materials emerged in response to the available challenges, among which silicon (Si) NWs constitute a major subset due to compatibility with semiconductor manufacturing processes [Karimzadehkhoei et al., 2023, Alaca and Karimzadehkhoei, 2023, Nasr Esfahani and Alaca, 2019]. Thanks to their piezo resistivity and increased sensitivity to strain associated with reduced dimensions, Si NWs exhibit a promising potential in miniaturized inertial sensors [Alaca and Karimzadehkhoei, 2023, Tasdemir et al., 2016, Meng and Li, 2020, Kon et al., 2007, Esfahani et al., 2018]. Despite their immense potential as essential building blocks in NEMS, mechanical behavior of Si NWs is still under examination for a complete understanding [Zare Pakzad et al., 2021, Pakzad et al., 2023b, Pakzad et al., 2021, Zare Pakzad et al., 2023c, Pakzad et al., 2023a, Pakzad et al., 2024]. Moreover, Si NWs could facilitate the combined functionalities within a single sensor, such as an accelerometer [Miani et al., 2022], pressure sensor [Lou et al., 2012] and gyroscope [Gadola et al., 2021], operating in multiple degrees of

freedom.

Silicon-based inertial sensors are generally comprised of basic blocks: a NW as transducing element and a shuttle with a certain stiffness [Tasdemir et al., 2016, Allain et al., 2012, Yilmaz et al., 2017]. A major challenge encountered in the fabrication of these sensors is obtaining a deterministic assembly of the Si NW with a microscale device such as the shuttle [Karimzadehkhoei et al., 2023, Alaca and Karimzadehkhoei, 2023, Tasdemir et al., 2016, Allain et al., 2012, Yilmaz et al., 2017, Fain et al., 2018]. Among the fabrication approaches of such structures, different techniques have been proposed [Karimzadehkhoei et al., 2023, Alaca and Karimzadehkhoei, 2023]. Formation of the Si NW in a thin silicon-on-insulator (SOI) substrate with subsequent deposition of thick polysilicon film for the formation of structural layer dedicated to MEMS has lead to successful fabrication results [Allain et al., 2012, Robert et al., 2009, Ollier et al., 2012]. Such monolithic method involves a high-temperature deposition step where Si NW is directly patterned within the device layer and is buried at the bottom of a thick polysilicon deposition [Alaca and Karimzadehkhoei, 2023, Robert et al., 2009]. Nevertheless, in principle, accessing the Si NW for the doping, contact formation or other surface processes remains impractical [Alaca and Karimzadehkhoei, 2023, Tasdemir et al., 2016, Yilmaz et al., 2017, Tasdemir et al., 2018]. The high-temperature deposition and etching processes could also amplify the generation of residual stresses in the Si NWs [Nasr Esfahani et al., 2022, Dolabella et al., 2020]. There exists another Si NW fabrication method with a variation of single-crystal reactive etching and metallization (SCREAM) process used with thicker device layer and is based on sidewall passivation and subsequent etching [Tasdemir et al., 2016, Tasdemir et al., 2018, Wollschläger et al., 2016, Chen and MacDonald, 2004, Kim et al., 2019, Park et al., 2010, Tsuchiya et al., 2016, Kilinc et al., 2020, Zou et al., 2017]. Among recent uses of this method, a monolithic fabrication approach allows the integration of Si NWs both with MEMS and NEMS where the process utilizes a high-resolution lithography and two-step etching technology [Tasdemir et al., 2016, Zare Pakzad et al., 2023c, Zare Pakzad et al., 2021, Yilmaz et al., 2017, Nasr Esfahani et al.,



2022, Tasdemir et al., 2018, Wollschläger et al., 2016, Kilinc et al., 2020]. The successful demonstration of up to 40  $\mu\text{m}$  of etch depth where Si NWs retain their mechanical integrity was demonstrated [Esfahani et al., 2018]. With the increasing importance of strain engineering, the characterization of embedded stresses in Si NWs fabricated via the aforementioned approaches has become important [Zare Pakzad et al., 2023c, Zare Pakzad et al., 2021, Nasr Esfahani et al., 2022, Dola-bella et al., 2020, Spejo et al., 2020]. Thus, the reduction in the number of processes and associated complexity of each step integrated with low-temperature fabrication techniques has emerged as a technological demand in NEMS [Nasr Esfahani et al., 2022, Zare Pakzad et al., 2023c].

The protection of NWs upon fabrication and the subsequent generation of residual stresses during etching steps are significant tasks encountered in the process development of nanoscale features integrated into micro or mesoscale structures [Tasdemir et al., 2016, Tasdemir et al., 2018, Nasr Esfahani et al., 2022, Zare Pakzad et al., 2023c]. For instance, the SCREAM process which involves the initial definition and etching of precursor line in the form of a protrusion on the surface faces similar challenges [Tasdemir et al., 2016, Tasdemir et al., 2018]. The difficulties are related to the subsequent isotropic plasma etching steps for the generation of an undercut of adequate extent for the release of free-standing elements [Shaw et al., 1993, Shaw et al., 1994, Zhang et al., 2004]. In this study, a monolithic fabrication method is presented that would allow the fabrication of Si NWs integrated with Si-based MEMS and NEMS. The developed process resembles the SCREAM technique and relies on deep etching steps for the generation and release of Si NWs. The reduction in the number of processes with immense attention given to the utilization of low-temperature processes has been the major emphasis towards the modification of the prior monolithic methods [Tasdemir et al., 2016, Tasdemir et al., 2018, Wollschläger et al., 2016, Chen and MacDonald, 2004, Kim et al., 2019, Park et al., 2010, Tsuchiya et al., 2016, Kilinc et al., 2020, Zou et al., 2017]. The developed approach requires the creation of a well-defined nanoscale pattern with subsequent etching steps for the generation of nanoscale protrusion on the substrate surface and subsequent release

of the NW. In the remainder of this article, the monolithic fabrication technology with reduced process complexity is explained in detail. This is followed by a structural and dimensional analysis of the resulting Si NWs in relation to the specific process steps. A comparison with alternative technologies is provided.

### **11.3 Fabrication Method and Process Development**

The process begins with a p-type,  $\langle 100 \rangle$  Si wafer of 100 mm diameter, 525  $\mu\text{m}$  thickness, and a resistivity range of 0.1–100  $\Omega\text{cm}$ . The surface of the wafer is primed in an oxygen plasma system with a power of 350 W and  $\text{O}_2$  flow rate of 400 sccm for 5 min. As the photoresist (PR), 1- $\mu\text{m}$ -thick AZ MIR 701 is spin-coated at 3000 rpm. The exposure for the definition of sub-1- $\mu\text{m}$ -thick PR lines is carried out in Heidelberg laser writer (DWL66+). The pattern linewidths,  $w$ , between 600 nm – 1  $\mu\text{m}$  are introduced parallel to  $\langle 110 \rangle$ -direction of the Si wafer (Figure 11.1 (a)). After the exposure power calibration, the optimum power is found to be 30 mW with 40-70% of intensity resulting in the proper dose selection for the patterning step. Following the exposure, the wafer is developed in AZ 726 MIF and rinsed in water. This step defines both the critical in-plane dimension of the NW pattern,  $w$ , and the orientation of the Si NW to be formed during the subsequent steps. Following the patterning step, the photoresist layer is treated in an initial fluorine-based plasma resembling that of the deep reactive ion etching (DRIE) process. This enhancement increases the selectivity of the photoresist as an etch mask. This enhancement increases the selectivity of the photoresist as an etch mask. The formation of the precursor line is then followed by the first etching step in the fluorine-based plasma indicated by the isotropic etch step of Figure 11.1 (b). The initial etching process given in Figure 11.1 (b) occurs in accordance with the parameters established for the subsequent etching step. In this respect, a DRIE recipe is developed to produce an ample scallop size allowing the release of Si NW, at the end of the first cycle of etching (Figure 11.1 (c)). During this step, the microscale features will be formed, while the Si NW is released. The developed recipe includes alternating steps of plasma etching and passivation using a Sentech SI 500C with associated parameters

Table 11.1: Deep reactive etching recipe

| Step | Process gas | Flow rate (sccm) | Pulse duration (seconds) | Power (W) |
|------|-------------|------------------|--------------------------|-----------|
| 1    | $C_4F_8$    | 150              | 6                        | 1000      |
| 2    | $SF_6$      | 240              | 11                       | 1000      |

given in Table 11.1. The temperature read-out during the DRIE step is within the range of 30 °C to 40 °C, categorizing the developed recipe as an ambient temperature process. Further etching cycles are carried out to obtain a single Si NW over the desired trench depth of  $h$ . The NW linewidth,  $w'$ , is reduced continuously due to etching from the sidewalls. The pulse duration of  $SF_6$  in the recipe is tuned to produce an ample scallop size allowing the release of Si NW. The extent of the undercut is adjusted while considering the patterned width of the Si protrusion. It takes approximately 180 seconds to complete a 8  $\mu\text{m}$  deep etch under the conditions provided in Table 11.1. Finally, the etch mask is removed by  $O_2$  plasma etching (Figure 11.1 (d)).

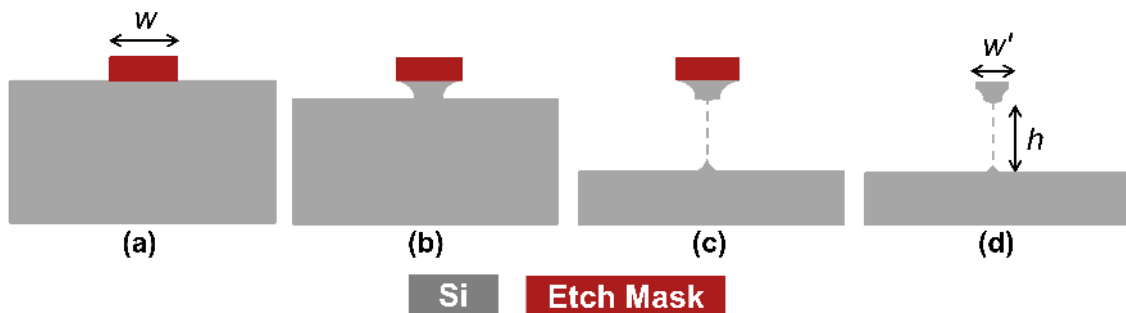


Figure 11.1: Process flow for a single suspended Si NW. (a) Lithography step through laser beam writer with pattern linewidth of  $w$  with PR serving as etch mask. (b) First isotropic Si etching step forming the surface protrusion, the precursor line for the future Si NW. (c) DRIE step with an ample undercut to release the Si NW, while attacking it from the unprotected bottom and side surfaces. (d) Removal of etch mask. The resulting NW linewidth and etch depth are indicated by  $w'$  and  $h$ , respectively.

### 11.4 Results

An array of Si NWs with  $h$  of 8  $\mu\text{m}$ ,  $w$  ranging between 600 nm – 1000 nm, and length ( $L$ ) ranging between 6-25  $\mu\text{m}$  is shown in Figure 11.2. The NW width,  $w'$ , ranging between 300 to 900 nm is obtained. In this context, sub-micron Si NW structures are created using the developed methodology. Consequently, throughout the rest of this work, these structures are denoted as Si NWs. The etch depth of  $h = 8 \mu\text{m}$  is achieved by assigning 6 cycles of DRIE to pattern NWs connected to the support pillars. Some examples for the length to patterning width ( $L/w$ ) ratio denoted as aspect ratios (AR) equal to 10, 15, 20, and 25 are given in Figure 11.2. Figure 11.2 also exhibits the close-up views of Si NWs with  $w$  of 900 nm and ARs of 10, 15, 20, and 25, where  $w'$  is calculated as 500 nm irrespective of the AR of the NW. The difference between the patterning width,  $w$ , and Si NW width,  $w'$ , is due to unprotected sidewalls etched during DRIE steps with associated parameters given in Table 11.1. Despite doubling the AR of the patterned Si NW with similar  $w$  shown in Figure 11.2,  $w'$  remains identical. The developed process flow demonstrates a notable level of repeatability, resulting in a 90% process yield while working within the specified range of widths spanning from 600 nm to 1000 nm given in Figure 11.2. However, it is worth emphasizing that additional investigation is necessary to fine-tune the yield calibration, particularly when dealing with smaller NW dimensions, where a decrease in yield is anticipated. In this respect, a 90% yield is maintained for the size scale depicted in Figure 11.2. The yield data obtained pertains to the repeatability of the process flow when using a maximum substrate size of  $15 \times 15 \text{ mm}^2$ . Additional calibration is required to accommodate various substrate sizes and types. The obtained  $w'$  with respect to the patterned  $w$  is a function of  $h$  where due to unprotected sidewalls, thinner NWs can be fabricated upon executing more etching cycles.

To characterize the boundaries that define the cross-section of the Si NWs, the mid-span of the Si NW is cut with the focused gallium ion beam (FIB) at 30 kV in a triple-beam FIB (HITACHI NX5000) and follow-up scanning electron

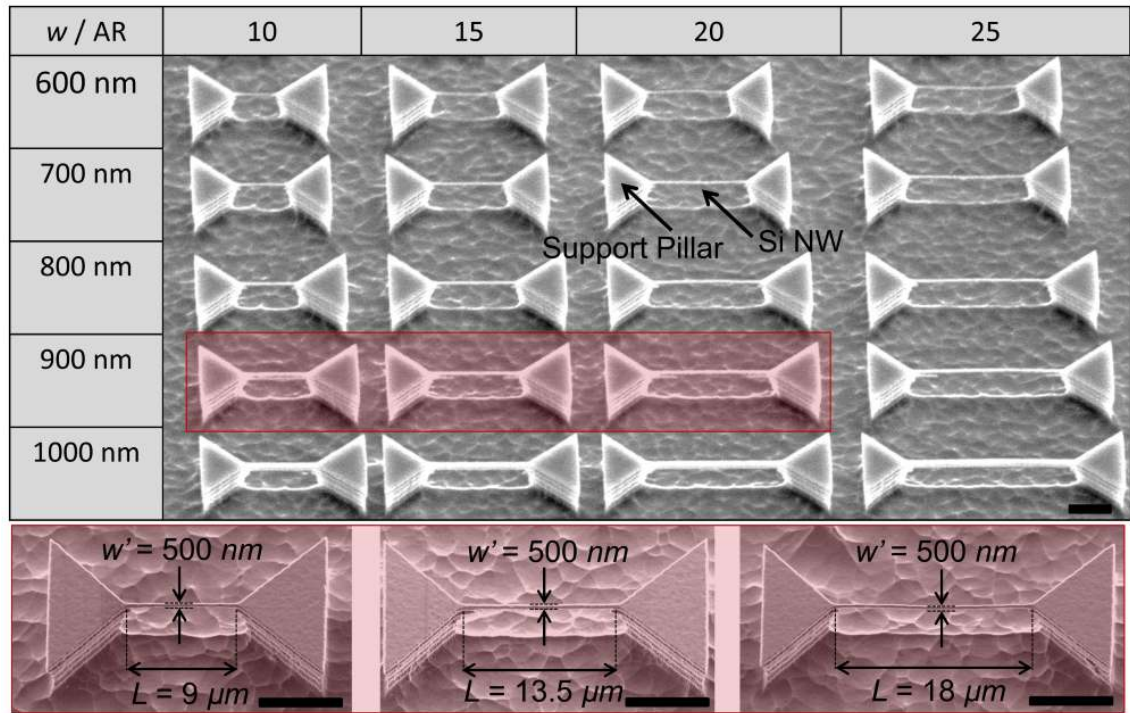


Figure 11.2: A set of Si NWs anchored between two 8- $\mu\text{m}$ -thick, triangular supports with similar  $w$  and ARs of 10, 15, 20, and 25 are shown. The close-up micrographs show the highlighted Si NWs with tilted views with associated  $w' = 500$  nm and different ARs. The scale bars in all micrographs correspond to 6  $\mu\text{m}$ .

microscopy (SEM) imaging of the remaining Si NW and connected anchors. Figure 11.3 (a) shows an isometric view of a Si NW connected to support anchors. Figure 11.3 (b)-(e) exhibit the micrographs of the Si NW subjected to back-to-back FIB millings. The final cross-section observed confirms the possible expected shape depicted schematically in Figure 11.3 (d). The sequential imaging attempts also display the consistency of the fabrication method in successful generation of Si NW with identical cross-section shape while regions from the middle or end parts of the NW are compared.

Figure 11.4 shows the relation between the patterned width,  $w$ , versus the Si NW width,  $w'$ , by taking the size reduction due to sidewall etching into account. Figure 11.4 (a) and Figure 11.4 (b) demonstrate Si NWs with moderate and deep trench depths of 8 and 16  $\mu\text{m}$ , respectively. The results in Figure 11.4 (c) exhibit

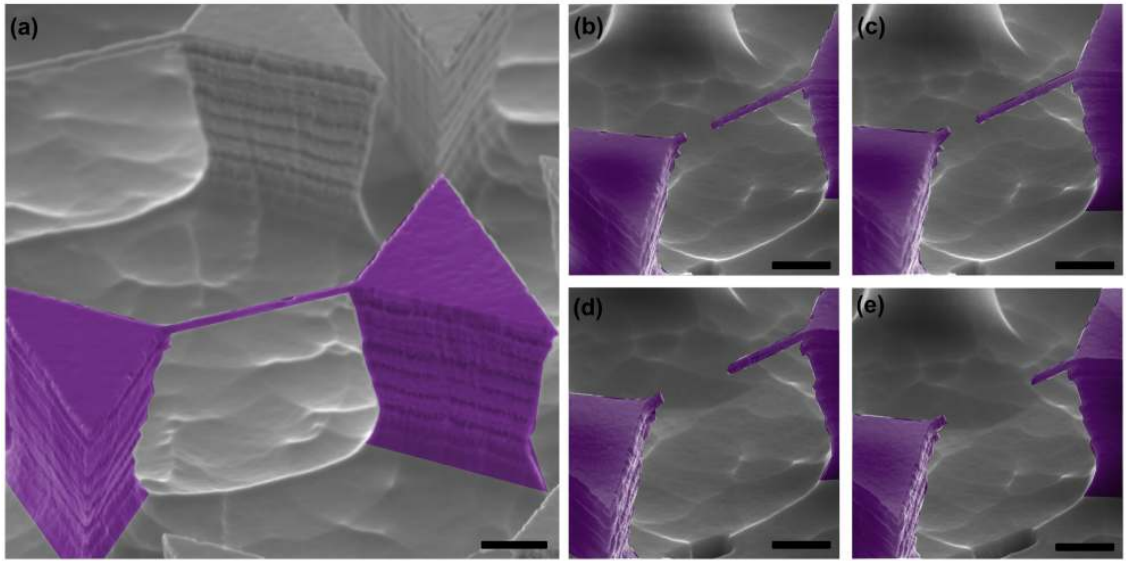


Figure 11.3: (a) A Si NW ( $w' = 500$  nm and  $L = 9$   $\mu$ m) with the highlighted part being subject to the FIB milling process. (b)-(e) FIB cuts near the midsection of the NW with indications on the longitudinal integrity of the Si. The scale bars in all micrographs correspond to 3  $\mu$ m.

a reduction of up to 50% observed by increasing the trench depth by a factor of 2. For proper statistical treatment, the measurements are carried out on three identical NWs of the same size. The results obtained for NWs with a deeper trench show a lower chance of survival for Si NWs with lower critical dimensions with an identical etching recipe. A possible solution can be modifications of etching parameters, such as tuning the pulse duration of  $\text{SF}_6$ . This could alter the scallop size with a higher chance of Si NW survival upon fabrication with lower dimensions at higher trench depths. This can also affect the total process yield for various applications [Esfahani et al., 2017b]. Despite dissimilarity observed for the survival of NWs with different trench depths, the relation between  $w$  and  $w'$  remains almost linear. It is crucial to highlight that the critical dimensions of Si NWs are directly impacted by both the number of DRIE cycles and the initial pattern width. Nevertheless, it is evident that there is an almost linear reduction in the sidewall dimensions. This provides a guideline for possible integration of the etching recipe for different applications with proven capability of the approach for the delivery of a specific combination of NW

size and trench depth. The recipe can be modified further for extreme trench depth applications [Esfahani et al., 2017b], as well as facilitate the integration of MEMS and NEMS devices into multiscale architectures [Ali et al., 2023, Tiwari et al., 2022].

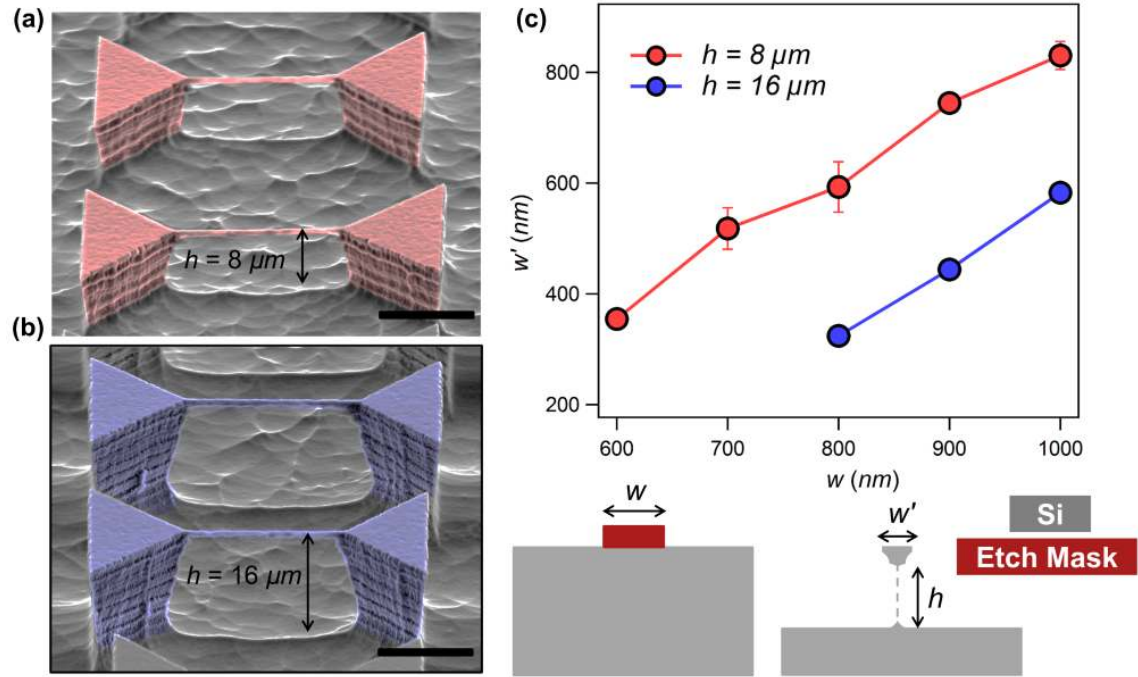


Figure 11.4: Si NWs fabricated with  $h$  of (a)  $8 \mu\text{m}$  and (b)  $16 \mu\text{m}$ . The scale bars in micrographs correspond to  $6 \mu\text{m}$ . (c) Relation of  $w$  to  $w'$  revealing the linear dependence between the patterned nanoscale features and fabricated Si NWs. The reduction in width is a direct outcome of unprotected sidewalls upon fabrication. Each data point corresponds to three NW samples.

Compared to similar approaches, the proposed technique in this study has the capability of generating Si NWs at lower temperatures ( $< 30\text{-}40^\circ\text{C}$ ), and hence, it has the potential of minimizing fabrication-induced residual stresses in NWs [Nasr Esfahani et al., 2022]. Such stresses are commonly addressed as a critical factor in the electromechanical response of Si NWs [Nasr Esfahani et al., 2022, Zare Pakzad et al., 2023c]. The exclusion of processes with higher temperatures for the creation of MEMS features also helps with the uniformity of the generated structures compared to previous approaches with thick polysilicon deposition upon MEMS fabrication [Allain et al., 2012]. Prior demonstrations on modulation of  $\text{SF}_6$  pulse



duration for the previous monolithic method [Tasdemir et al., 2016, Wollschläger et al., 2016] exhibits possible improvements of current technology with controllable undercut definition for fabrication of a stack of Si NWs. There are two major differences observed between the two monolithic fabrication approaches introduced here and the prior version [Esfahani et al., 2017b, Tasdemir et al., 2016, Zare Pakzad et al., 2021, Tasdemir et al., 2018, Wollschläger et al., 2016, Nasr Esfahani et al., 2022, Zare Pakzad et al., 2023c]. First, further removal of processes and the total complexity in back-to-back steps could potentially introduce further stresses in Si NWs. Second, the unprotected side surfaces in current technology compared to the well-controlled Si protrusion protection from both sides in the prior approach [Tasdemir et al., 2016, Tasdemir et al., 2018, Wollschläger et al., 2016] could be a determining parameter for specific applications. This could potentially alter the critical dimension, trench depth, and possible microscale feature integration designs. Having outlined the capabilities of the proposed technology while compared to the prior version [Esfahani et al., 2017b, Tasdemir et al., 2016, Zare Pakzad et al., 2021, Tasdemir et al., 2018, Wollschläger et al., 2016, Nasr Esfahani et al., 2022, Zare Pakzad et al., 2023c], one can now consider the alternatives used for the combination of MEMS with NWs [Kaestner and Rangelow, 2020, Hofmann et al., 2020]. Similar to prior examples [Tasdemir et al., 2016, Tasdemir et al., 2018], the current technology also delivers the location of Si NW fabricated on the surface opposing other monolithic technologies [Allain et al., 2012] with NW placed at the bottom of the MEMS layer. With the current method, the Si NW remains accessible for further processes such as contact formation, mechanical testing, and doping attempts [Zare Pakzad et al., 2023b]. The successful control on the location and orientation of Si NW demonstrates the reliability of the developed method for follow-up fabrication steps while compared to opposing bottom-up techniques [Wagner and Ellis, 1964].

The introduced method facilitates the scale-up integration of Si NWs with larger microscale features while compared to prior examples in the literature. One such example could be the inertial sensors comprised of separated layers as the NW and MEMS structures. Further enhancements to the current approach could alleviate



challenges in the pick-and-place assembly of NWs [Nasr Esfahani and Alaca, 2019, Ali et al., 2022]. One such challenge commonly encountered in serial pick-and-place techniques is the uncertainties associated with the alignment and interface properties of NWs. The current method also helps with the elimination of further post processes such as soldering to fix the NW. On the contrary, the new method is predominantly based on thick SOI technology, where the microscale features are co-fabricated with nanoscale structures such as NWs. The trench depth of  $16\text{ }\mu\text{m}$  is another significant outcome of the current method where most microelectromechanical systems have a relevant thickness at this scale [B Spejo et al., 2023]. Additionally, modifications of the etching recipe could strengthen the possibility of NW survival with deeper etch depths. The controllable location and orientation of NWs upon fabrication is another achievement of current technology while compared to other bottom-up alternative methods.

### **11.5 Conclusion**

The current study has shown the successful demonstration and implementation of a monolithic multiscale fabrication approach, where Si NWs are obtained with reduced process complexity at lower temperature processes. The present technology enables access to Si NWs as active components beside other microscale features connected to the nanoscale features. Incorporation of fast lithography tools and etching processes exhibits state-of-art mechanical precision, where a two-order-of-magnitude difference between Si NW and the microscale anchor components is achieved. The current method has also yielded a noteworthy result, with a trench depth measuring  $16\text{ }\mu\text{m}$ . The technique yields promising results which can be improved further by process optimization for future MEMS and NEMS applications.

## Chapter 12

# INNOVATIVE MEMS STAGE FOR AUTOMATED MICROMECHANICAL TESTING

### 12.1 Overview

This study introduces a comprehensive methodology for designing, fabricating, and testing a MEMS stage integrated into a commercial testing device, with a focus on enabling automated testing of multiple samples under in-plane loading conditions. Drawing inspiration from recent innovative MEMS stage designs, a new approach is developed to integrate micromanipulator tips into a commercial micro-mechanical testing machine, allowing for automated one-directional loading of micro-scale samples. To address challenges related to handling and alignment, a co-fabrication technique is employed, enabling the simultaneous fabrication of the micro-sample and MEMS stage within a single process flow. A novel fabrication method utilizing a silicon-on-insulator substrate is utilized. The calibration of testing method is conducted using both analytical and experimental methods to ensure accurate measurement of force and deflection within the in-plane testing protocol. The released micro-beam structures undergo repetitive loading to evaluate bending deformation. The developed approach is extended to multiple testing attempts on MEMS stage–micro-sample, combinations co-fabricated within a single chip, enabling precise statistical treatment of the measurements.

### 12.2 Introduction

The quest for worldwide connectivity and the rise of digital technologies and the Internet of Things (IoT) are intricately linked to the advancement of sensor miniaturization, made possible by microelectromechanical systems (MEMS) [Alaca and

Karimzadehkhoei, 2023, Karimzadehkhoei et al., 2023]. Conversely, the field of nanomechanics is also experiencing significant advancements through the utilization of MEMS technology and integrated microscale testing devices [Elhebeary and Saif, 2017b, Bhowmick et al., 2019, Zhu, 2023]. Conducting intricate characterization schemes that go beyond stress-strain analysis, such as fracture, fatigue, and wear testing, is possible [Bhowmick et al., 2019]. These tools not only facilitate the measurement of diverse mechanical properties but can also provide real-time or near-real-time inspection within electron microscopes [Espinosa et al., 2013]. While dynamic monitoring and analysis of microstructural evolution during *in-situ* testing offer significant advantages, the limitations associated with conducting such testing within confined chambers predominantly restricted to vacuum conditions have prompted researchers to explore alternative methods [Elhebeary and Saif, 2017b, Bhowmick et al., 2019, Zhu, 2023]. Approaches to address the limitations include the development of microfabricated flexural stages [Emon et al., 2021], the modification of micromanipulators to enable complex loading conditions [Acuna et al., 2021], exploring high-temperature testing conditions [Elhebeary et al., 2020], and on-chip solutions for environmental effects, such as testing under heavy ion-irradiation [Lapouge et al., 2017]. In this regard, microscale stages possess the capability to convert one form of motion into another, rendering them highly advantageous for conducting small-scale tests, particularly for nanowires (NWs), films structures, and biological samples [Elhebeary and Saif, 2017b, Acuna et al., 2021, Elhebeary et al., 2020, Elhebeary and Saif, 2018]. Picoindentors or actuators that employ push-to-pull techniques are also commonly used to generate the required forces and motions, leading to notable progress in NW testing [Guo et al., 2011]. In this context, the integration of commercial tools that can enable more sophisticated testing on MEMS stages could potentially play a pivotal role in the advancement of sensing and characterization technologies in the future [Bhowmick et al., 2019, Zhu, 2023]. Given the significance of characterization and testing techniques [Elhebeary and Saif, 2017b] and their critical role in precisely interpreting the properties of silicon (Si) NWs [Pakzad et al., 2023b, Nasr Esfahani et al., 2022, Pakzad et al., 2021, Zare Pakzad et al.,

2021], this area of research necessitates the development of innovative solutions. Understanding the effects of temperature on Si NWs and micro-wires is crucial for investigating size-dependent mechanical properties and the brittle-to-ductile transition [Elhebeary et al., 2020, Pakzad et al., 2024]. Furthermore, the use of manual joysticks or haptic devices by operators in micro or nano testing activities underscores the necessity for advancing semi- or fully automatic manipulation techniques [Zhang et al., 2022a, Barrios et al., 2023]. To achieve more accurate and efficient testing procedures, the adoption of innovative MEMS stages or imaging feedback techniques becomes crucial [Elhebeary and Saif, 2018, Zhang et al., 2022a].

The present study introduces a comprehensive methodology for the design, fabrication, and testing of a MEMS stage integrated into a commercial testing device. The main objective is to facilitate automated testing of multiple samples, with a specific focus on achieving in-plane loading conditions. Taking inspiration from recent novel designs for MEMS stages [Emon et al., 2021, Elhebeary et al., 2020, Elhebeary and Saif, 2018, Elhebeary and Saif, 2017b, Elhebeary and Saif, 2017c], an innovative design is developed to enable the integration of micromanipulator tips using a micro-mechanical testing machine. This integration aims to streamline the process of automated one-directional loading conditions. In order to tackle challenges related to handling and alignment, a co-fabrication technique is utilized, enabling the fabrication of both the micro-sample and the MEMS stage within a single process flow. The MEMS stage incorporates groups of beams that serve as frames or supports, allowing for the application of complex loading scenarios during in-plane testing of the micro-sample. The fabrication method employs a silicon-on-insulator (SOI) substrate, enabling the simultaneous creation of the micro-sample and MEMS stage, with the subsequent release of the final structure. To ensure reliable measurement of force and deflection within the in-plane module of the testing machine, a calibration process is conducted using analytical and experimental methods. In this regard, the released micro-beam structures undergo repetitive loading conditions to evaluate bending deformation under in-plane loading state. The obtained data is subjected to statistical analysis and compared to analytical linear estimation of

micro-beam stiffness. The developed approach is expanded to encompass multiple testing attempts conducted on several MEMS stage–micro-sample combinations co-fabricated within a single chip. This extension allows for precise statistical analysis of the obtained results. Details on design, fabrication, testing, and analytical calculations can be found in Section 12.3.2, while calibration and testing results are presented in Section 12.3.3.

### **12.3 Methods and Materials**

This section presents a novel MEMS stage specifically developed for enabling automated mechanical testing on co-fabricated micro-samples. The specific design aspects of the stage are elaborated in Section 12.3.1. Additionally, the fabrication process flow, encompassing the necessary steps for creating the MEMS stage, is detailed in Section 12.3.2. The experimental setup for conducting both single and automated multi-testing, along with the analytical procedure employed for testing calibration, are discussed in Section 12.3.3 and Section 12.3.4, respectively.

#### **12.3.1 MEMS Stage Design**

The primary objective of the MEMS stage design is to create a microflexural platform that enables push-to-bend testing of silicon micro-samples. The schematic representation of the design, depicted in Figure 12.1, illustrates the integration of a loading platform with one-directional testing capabilities. The stage consists of support, T-shape, backbone, sensing, axial, and frame beams connected to the micro-sample. The micro-sample in this study is a micro-wire structure anchored from both ends, allowing for bending deformation when the T-shape beam is pushed in the designated loading direction. The design is inspired by previous work on *in-situ* pure bending experiments on micro-wires, which demonstrated successful mechanical testing and examination of fracture behavior in micro-scale Si structures [Elhebeary et al., 2020]. The operation of the MEMS stage involves fabricating a micro-wire positioned transverse to the straining direction, enabling bending deformation when a load is applied in the  $x$ -direction at the upper support end, while

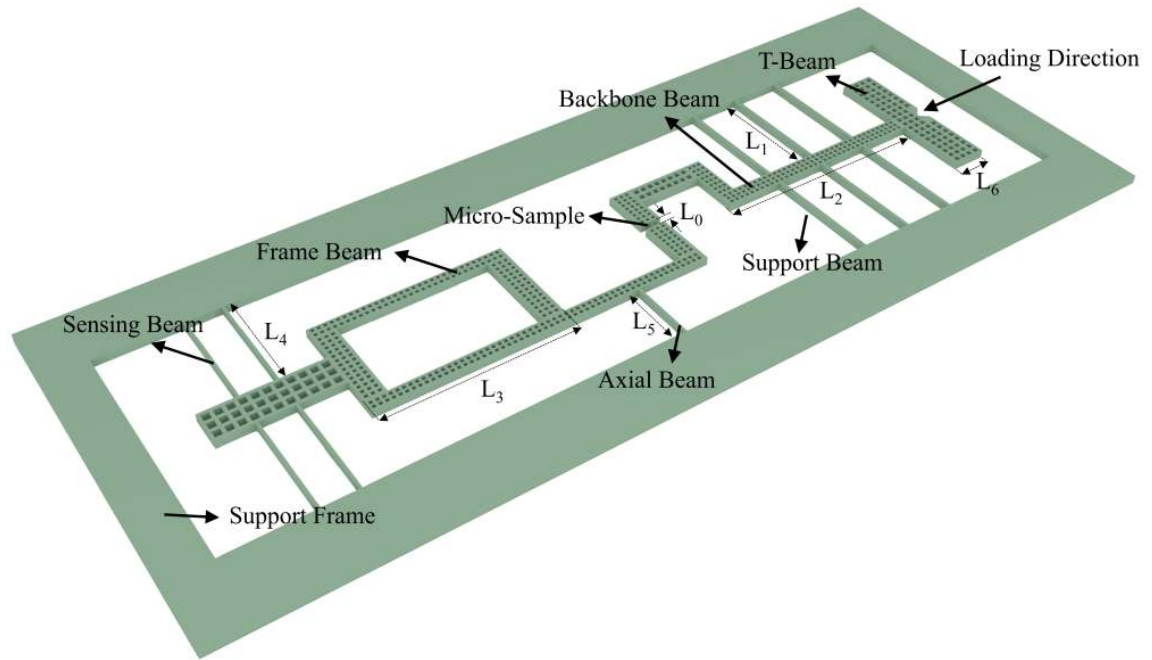


Figure 12.1: Schematic of the geometrical design, involving micro-sample-integrated MEMS testing stage. MEMS stage is anchored to a support frame with associated loading direction ( $x$ ).

the bottom support remains connected to the axial and frame beams, serving as a soft anchor for the sample. The rigid frame serves as a support region for the combined beams within the stage, providing high in-plane compliance to maximize the bending stress to uniaxial stress ratio in the micro-sample. The functionality of the stage is designed to induce bending stresses in the sample while limiting axial tensile stress. The frame beams act as strong supports, facilitating the transfer of motion to the micro-wire. The support beams that hold the T-beam prevent rotation at the anchors, ensuring the one-dimensional application of the load during the pushing process. In addition to the modified design, a novel co-fabrication technique is implemented to fabricate the sample and stage together with precise lithographic accuracy, addressing alignment and handling issues. The dimensions of the various beams and parts designed for the MEMS stage are listed in Table 12.3.1. Detailed information on the fabrication process and testing method of the MEMS stage will be provided in Section 12.3.2 and Section 12.3.3 of this article, respectively. Further

insights into the mechanism and analytical approach for interpreting the MEMS stage can be found elsewhere [Elhebeary and Saif, 2017a, Elhebeary and Saif, 2018].

Table 12.1: Geometrical dimensions of the beams comprising the MEMS stage and micro-sample with given labels in Figure 12.1.

| Beam     | Length ( $\mu\text{m}$ ) |      | Width ( $\mu\text{m}$ ) |     |
|----------|--------------------------|------|-------------------------|-----|
| Sample   | $L_0$                    | 40   | $w_0$                   | 1   |
| Support  | $L_1$                    | 650  | $w_1$                   | 20  |
| Backbone | $L_2$                    | 1260 | $w_2$                   | 100 |
| Frame    | $L_3$                    | 1100 | $w_3$                   | 75  |
| Sensing  | $L_4$                    | 600  | $w_4$                   | 15  |
| Axial    | $L_5$                    | 425  | $w_5$                   | 15  |
| T-shape  | $L_6$                    | 200  | $w_6$                   | 900 |

### 12.3.2 Fabrication Process

The fabrication process flow for the MEMS stage–micro-sample is illustrated in Figure 12.2, depicting the cross-section of the design in the  $x - z$  plane as shown in Figure 12.1. The fabrication begins with a double-sided polished SOI wafer, consisting of a device layer with a thickness of  $2 \mu\text{m}$  and a buried oxide (BOX) layer with a thickness of  $0.5 \mu\text{m}$ . In the first step (Figure 12.2 (a)), both sides of the wafer are coated with silicon nitride (SiN) using a plasma-enhanced chemical vapor deposition (PECVD) process. Afterward, dicing is conducted to generate small chips with dimensions of  $15 \times 15 \text{ mm}^2$  (not shown in the fabrication process). Subsequently, an etch mask is patterned to selectively etch the SiN layer (Figure 12.2 (b)). The next step (Figure 12.2 (c)) involves the selective removal of the SiN using patterned etch mask, with masked region protecting the SiN. After the selective SiN removal, etch mask is removed and the Si available on the device layer is selectively etched to define the MEMS stage and the micro-sample (Figure 12.2 (d)). Meanwhile, SiN acts as etch mask for the masked Si region during the selective Si etching process. A

slight amount of isopropyl alcohol (IPA) is also added to etch solution to minimize Si etch roughness during the process. The BOX layer underneath the device layer serves as etch stop and becomes visible once the Si etch in device layer is completed. The sample is cleaned with acetone and IPA, and washed with deionized water, followed by the removal of the BOX and the SiN layers to create a suspended MEMS structure with co-fabricated micro-sample for micromechanical testing (Figure 12.2 (e)).

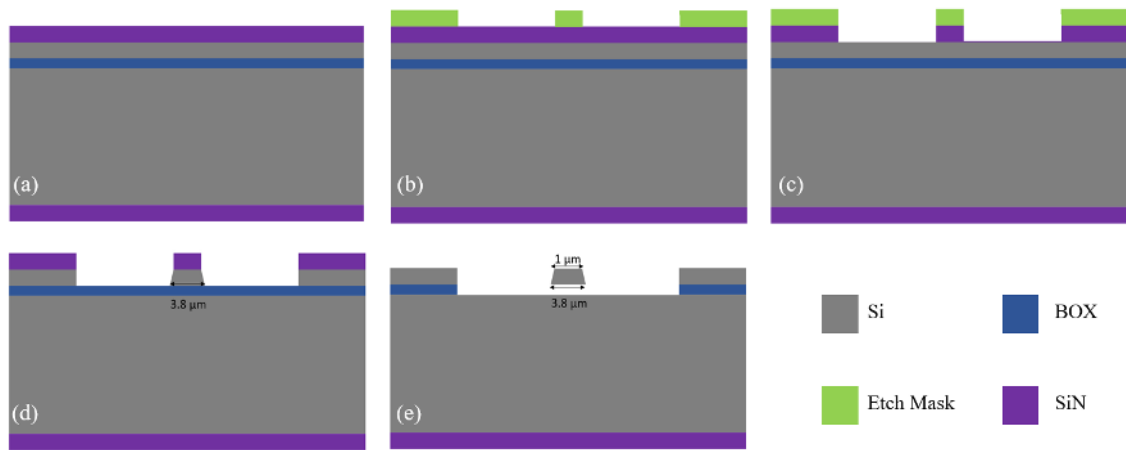


Figure 12.2: The fabrication process flow utilized for the co-fabrication of micro-sample and MEMS stage, (a) SiN coating via PECVD, (b) Etch mask patterning, (c) Dry etch of SiN, (d) Definition of MEMS stage via through-Si etch, (e) Release of the co-fabricated MEMS stage–micro-sample structure via etch of underneath BOX layer.

### 12.3.3 Mechanical Testing

The force-deflection response of the co-fabricated MEMS stage–micro-sample is obtained using a commercial micro-mechanical testing machine (FemtoTools, FT-MTA03) schematically shown in Figure 12.3 (a). To facilitate in-plane loading conditions, a sophisticated T-shape beam design and integrated micro-manipulator tip are employed during the testing process. The testing machine is positioned on a vibration isolation platform. In-plane testing is monitored using an optical microscope with a 180° rotation range and a 95 mm working distance, connected to a



3-megapixel CMOS digital camera. For precise positioning of the chip with multiple MEMS stage–micro-samples and long-range movements in the  $x-y-z$  directions, a 3-axis nanopositioning stage is utilized (see Figure 12.3 (b)). The 3-axis piezoscanner, equipped with capacitive encoders, enables continuous and fast movements. Additionally, a 2-axis microscope stage ensures proper alignment of the micromechanical testing module with respect to the optical microscope. The uniaxial loading of the MEMS stage is achieved using a MEMS-based capacitive sensing probe (FT-S20'000-2Axis-TP2) with maximum range and resolution of 20 mN and 100 nN, respectively (see Figure 12.3 (c)). The micro-manipulator system allows precise maneuvering along the  $x$ ,  $y$ , and  $z$  axes, with movement ability ordering three order of magnitude spanning from 0.1 nm to 29 mm. Two clamps on the positioning stage are used for sample mounting, while adjustable LED lights aid in accurate observation and calibration of the sample position. Prior to use, the micro-manipulator and each individual micro-force sensor undergo calibration by the manufacturer. To induce bending deformation in the micro-sample, the compression test module within the testing machine applies a pushing force to the T-shape beam in the  $x$ -direction. During the testing, force measurements are acquired at a rate of 25 data points per second (25 Hz). Continuous monitoring of force and position over time enables calibration and inspection of the noise level during the testing process. To ensure the reliability of the force-deflection responses, the calibration process involves conducting tests on released clamped-free beams using the in-plane compression module. The force-deflection graphs are analyzed to calculate the stiffness values, which are then compared with the analytical estimations described in Section 12.3.4. Following the calibration, the automated array measurements are performed using the micro-mechanical testing machine on multiple micro-samples co-fabricated within the same chip. The movement of the micro-probe tip between tests is designed with a speed of  $50\text{ }\mu\text{m/s}$ , with a testing speed of  $0.25\text{ }\mu\text{m/s}$ . The tests are conducted on a set of MEMS stage–micro-samples, with four samples placed in a single column, as illustrated in Figure 12.3 (d). This testing procedure allows for force-deflection measurements without modifying the assembly of the chip within the micro-mechanical

testing machine. The testing system has a displacement resolution of 0.1 nm and a force resolution of 100 nN. The multiple samples are equidistantly placed within the same chip, with a spacing of 4250 nm, enabling continuous measurements during array testing. Real-time video recordings of the testing process, capturing the force-deflection responses of all four samples, are discussed in detail in Section 12.3.3.

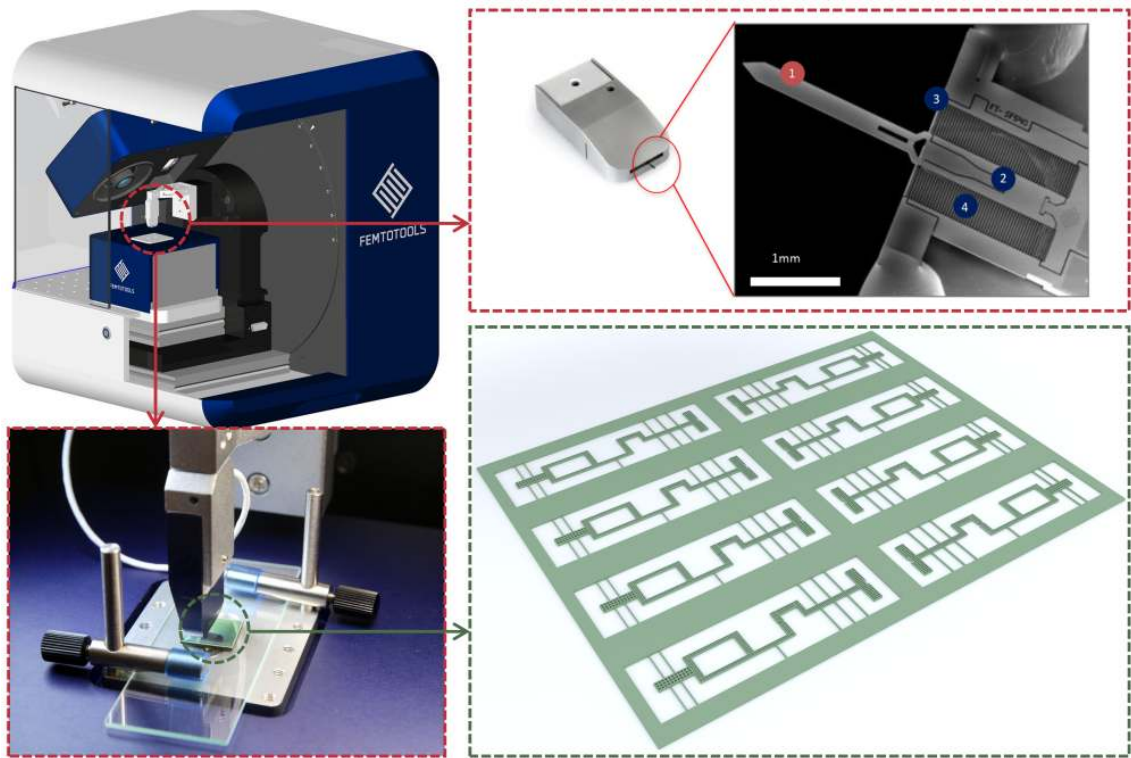


Figure 12.3: Micromechanical testing setup for the automated testing. (a) Schematic diagram of the FemtoTools testing device [Fem, ]. (b) The 3-axis nanopositioning stage with the chip. (c) Close-up of the micro-manipulator tip and co-fabricated MEMS stage-micro-sample. (d) Schematic of the chip housing an array of MEMS testing stage for demonstration of automated testing.

#### 12.3.4 Analytical Modeling

The analytical modeling approach employed in this study is based on the principles of the Euler-Bernoulli beam theory [Wang, 1995]. According to this theory, the bending response of a beam is described using Equation 12.1.

$$\frac{d^2w(x)}{dx^2} + \frac{M(x)}{EI} = 0 \quad (12.1)$$

The deflection of the beam is denoted by  $w$ , while  $x$  represents the coordinate along the length of the beam. The bending moment is denoted by  $M$ , the modulus of elasticity by  $E$ , and the moment of inertia by  $I$ . By solving Equation 12.1, the analytical stiffness of a beam can be calculated.

## 12.4 Results

The calibration process for the mechanical testing along with the analytical procedure are given in Section 12.4.1. Additionally, the fabrication process outcome is detailed in Section 12.4.2. The experimental setup for conducting automated multi-testing is discussed in Section 12.4.3.

### 12.4.1 Calibration of Mechanical Testing

This section presents the calibration process for the in-plane mechanical testing of a sample consisting of six folded micro-beams, utilizing a previously fabricated sample from Ref. [Ali et al., 2023]. The folded micro-beams have lengths of  $347.5 \mu\text{m}$  and  $400 \mu\text{m}$ , and their width and height are  $10.0 \pm 0.5 \mu\text{m}$  and  $7.5 \pm 0.5 \mu\text{m}$ , respectively. The modulus of elasticity is assumed to be 130 GPa for micro-beams oriented along  $\langle 100 \rangle$ -Si. The analytical formulation Equation 12.1 described in Section 12.3.4 is employed to calculate the linear stiffness, taking into account geometric uncertainties with standard deviations of  $\pm 0.5 \mu\text{m}$ . In-plane testing is performed on six similar folded micro-beams using the testing protocol discussed in Section 12.3.3. Figure 12.4 (a) shows the force vs. displacement ( $F-d$ ) responses obtained from the mechanical testing, enhanced with linear fits. The applied force ( $F$ ) ranges up to  $15 \mu\text{N}$  while the folded micro-beams are subjected to displacements ( $d$ ) up to  $1.5 \mu\text{m}$ . The obtained  $F-d$  responses exhibit similar slopes with slight deviations, providing valuable feedback for calibrating the identical micro-probe tip used for testing multiple folded micro-beams within the same sample. The average and associated

standard deviation of the in-plane tests on the calibration micro-beams are plotted in Figure 12.4 (b), along with the analytical stiffness results incorporating the mentioned deviations. Considering the geometric non-linearity in the analysis and the small deviations accounted for in the linear analytical calculations, the calibration results provide reasonable estimations for the testing protocol. The presented testing procedure and calibration process will be utilized for the testing of the MEMS stage–micro-sample, with the fabricated and automated testing results presented in Section 12.4.2 and Section 12.4.3, respectively.

#### 12.4.2 Fabrication Results

Characterization of the co-fabricated MEMS stage and micro-sample is carried out via scanning electron microscope (SEM) imaging after the fabrication, given in Figure 12.5. The bulk geometry of the MEMS stage, except for the springs, is patterned with release holes for the dry release of MEMS stage by etching underneath BOX layer. Moreover, as the MEMS stage derive its stiffness in the bending direction of micro-sample from the springs therefore the release holes are found to not affect the bending response of the micro-sample. Besides, to prevent charging-induced deformation and subsequent potential stiction of the MEMS stage with handle layer of sample, SEM imaging is performed before BOX removal (Figure 12.2 (d)). Figure 12.5 (a) shows the far-field view of the co-fabricated micro-sample with MEMS stage (in false coloring), with location of the micro-sample denoted in dotted red box. Figure 12.5 (b) shows a closeup of the region with micro-sample bridging the gap between frame of the MEMS stage. An overview of the micro-sample, Figure 12.5 (c), imply a smooth etching profile with slight undercut of the Si below the SiN layer. The micro-sample involves a trapezoidal profile, with a length of  $40\ \mu\text{m}$  and bottom surface with of  $3\ \mu\text{m}$ . Due to the substantial difference in dimensions, adjusting Si etching for sub- $\mu\text{m}$  micro-sample width has minimal impact on MEMS stage dimensions. As compared to the conventional methods for the co-fabrication of the MEMS stage–micro-sample [Elhebeary and Saif, 2018], the proposed fabrication approach bypass the complex, expensive, and time intensive through-wafer deep

reactive ion etching (DRIE) approach to release the MEMS stage–micro-sample. On the other hand, due to the inherent nature of the Si wet etching, the cross-section of the micro-sample yields a trapezoidal shape compared to the near-vertical sidewall profile typically encountered in DRIE-based Si etching approach [Elhebeary and Saif, 2018]. The single-side patterning approach utilized in the current process avoids the use of double-side alignment typically required for double-sided lithography using commercial mask aligners. After SiN patterning step, the fabrication method also allows potential control of the micro-sample width through slight over etching of the Si, Figure 12.2 (d), as described above. This process allows for supplementary control of the device layer thickness through epitaxy [Robert et al., 2009]. The fabrication process eliminates the need for the time-consuming and resource-intensive pick and place assembly method typically used to integrate samples onto the MEMS testing stage [Ali et al., 2022]. Furthermore, the pick and place testing approach, which relies on gluing the sample to testing stage using specialized equipment, introduces additional interface material between the micro-sample and the testing stage. This added material can make experimental testing and its interpretation more challenging. On the contrary, the co-fabrication of micro-sample and the MEMS stage overcomes these challenges, making it highly advantageous for automated testing efforts. In Figure 12.5 (d), the optical image illustrates the fabrication outcomes of eight MEMS stage–micro-sample. The samples are labeled as A, B, C, and D representing an array of prepared samples intended for automated testing.

### 12.4.3 Automated Measurements

An array of MEMS stage–micro-sample, with fabrication details provided in Section 12.4.1 and following the testing protocol for in-plane testing of beams as described in Section 12.4.2, is employed for automated testing. Four samples, labeled as A, B, C, and D are subjected to in-plane testing in the direction of loading ( $x$ -direction). The  $F - d$  results obtained from the testing process, along with the complete characterization procedure, are carried out automatically without any user intervention. Appendix movie A.1 provides a detailed video recording of the auto-

mated testing procedure. Figure 12.6 displays the  $F - d$  results obtained from a single automated testing session for samples A to D. The applied force reaches up to  $120 \mu\text{N}$  within a displacement range of  $0.2 \mu\text{m}$ , and linear fits are provided for each data set. The results obtained indicate a reliable agreement with the anticipated slope of the  $F - d$  curves when compared to the elastic range of  $F - d$  relationship reported in Ref. [Elhebeary and Saif, 2018]. This comparison serves as evidence for the reliability of the generated technology in automated testing applications. Additional analytical or finite element modeling can be performed to provide a more comprehensive analysis of the automated testing outcomes. Considering the distinctions from previous designs [Elhebeary et al., 2020, Elhebeary and Saif, 2017a], such as variations in read-out methods (microprobes vs. strain gauges), loading application (compression vs. tensile), anticipated sample cross-sectional shape (trapezoidal vs. rectangular), incorporation of an additional beam for one-directional testing (axial beam), and differences in co-fabrication technology (wet etching vs. two-step DRIE), this study seeks to explore the potential for extending this technology to smaller samples, such as NWs.

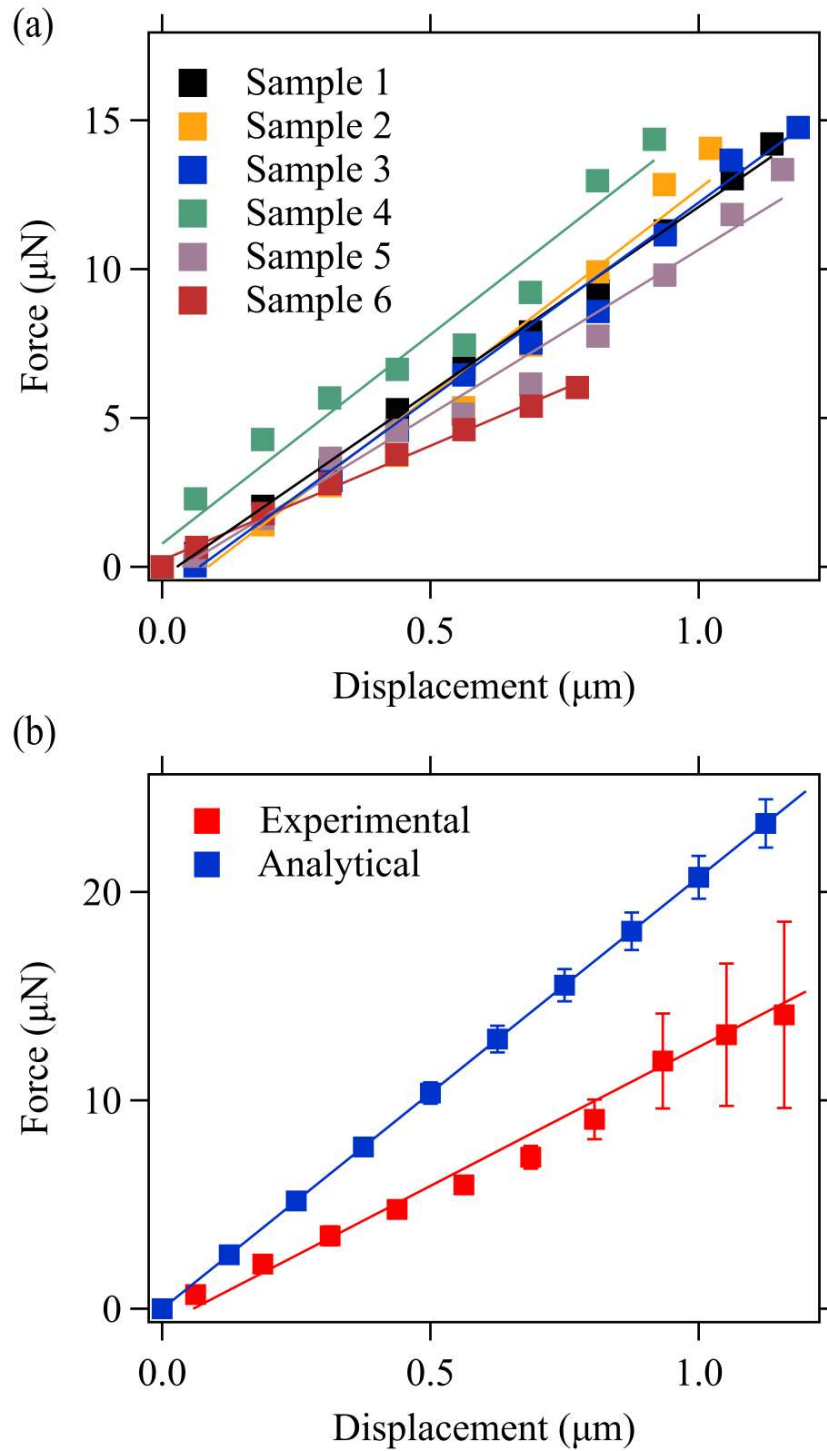


Figure 12.4: (a) Force-displacement ( $F-d$ ) curves obtained for six micro-beam samples using the calibration of testing. (b) Experimental and analytical  $F-d$  responses obtained via testing and modeling, respectively.

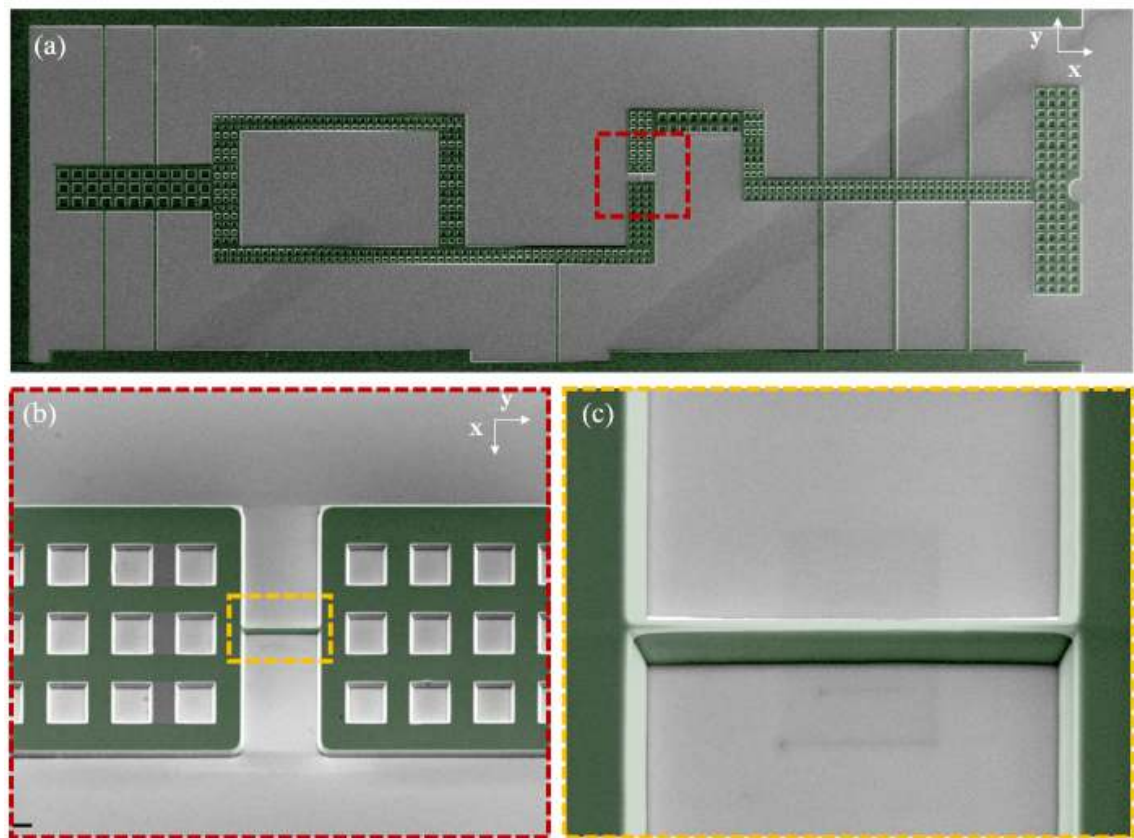


Figure 12.5: SEM micrograph of the co-fabricated MEMS stage–micro-sample, before BOX etch. (a) MEMS stage, scale bar corresponds to 300  $\mu\text{m}$ . (b) Close-up of highlighted red box with scale bar corresponding to 20  $\mu\text{m}$ . (c) Close-up of the micro-sample (highlighted orange box), and scale bar corresponds to 2  $\mu\text{m}$ . (d) Optical image of the fabricated array of MEMS stage on a  $15 \times 15 \text{ mm}^2$  chip, housing eight (8) stages with the scale bar corresponding to 500  $\mu\text{m}$ .



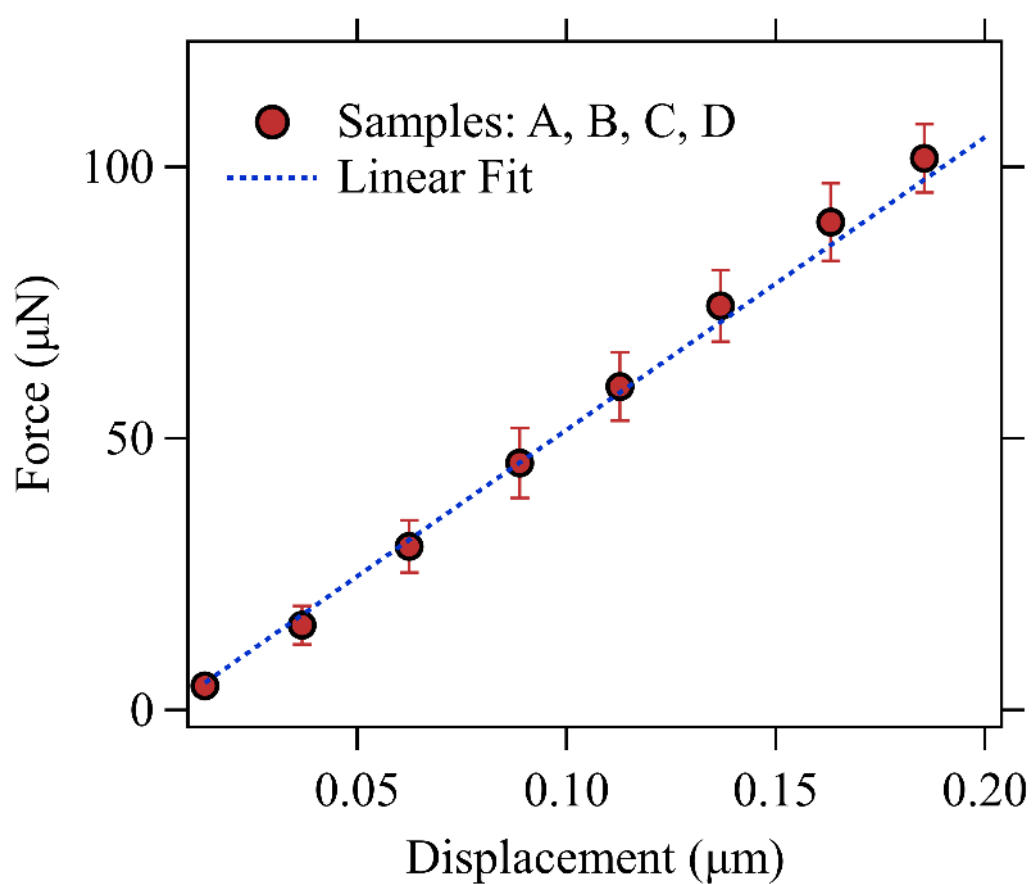


Figure 12.6: Force-displacement ( $F - d$ ) curve obtained using automated testing on samples A, B, C, and D with the standard deviation of measurements.

## Chapter 13

# MACHINE LEARNING INSIGHTS INTO THE ELASTICITY OF BOTTOM-UP SILICON NANOWIRES

### 13.1 Overview

This investigation integrates molecular dynamics simulations and machine learning algorithms to comprehensively explore the size-dependent elastic properties of  $\langle 111 \rangle$ -oriented silicon nanowires. Molecular dynamics simulations encompass various aspects, such as tensile and bending modeling, providing detailed insights into the mechanical behavior of silicon nanowires. Feature selection and algorithm evaluation reveal the non-linear nature of elasticity, utilizing over 1000 simulation results for this analysis. The study introduces the application of machine learning to predict the modulus of elasticity for Si NWs and analyzes trendlines for  $\langle 111 \rangle$ -oriented Si NWs while compared with computational and experimental literature domain. Despite variations, machine learning emerges as a promising method for understanding the elastic properties of silicon nanowires, providing valuable insights for future studies on modeling at the nanoscale.

### 13.2 Introduction

Nanowires (NWs) possess substantial potential as fundamental components in the development of nanoelectromechanical systems (NEMS) [Bachtold et al., 2022], nanoelectronics [Gao et al., 2022, Badawy and Bakkers, 2024], and photonics [Quan et al., 2019, Bronstrup et al., 2010]. They find applications as highly sensitive sensors [Zhang et al., 2023] and in energy-related technologies [Panda et al., 2022, Nehra et al., 2020]. Advances in fabrication techniques and the expanding scope of technological applications have generated increased interest in the comprehensive charac-

terization of NWs [Wang et al., 2016a, Zare Pakzad et al., 2023a, Zare Pakzad et al., 2023b]. The application of multi-scale modeling methods further contributes to this growing interest [Zare Pakzad et al., 2023c]. The reduction in size of NWs results in an increased significance of surface contribution, leading to distinct physical properties compared to their bulk counterparts [Wang et al., 2017, Mead et al., 2023]. In this context, comprehending the impact of scale becomes increasingly complex [Zare Pakzad et al., 2023c, Nasr Esfahani et al., 2022]. Due to their compatibility with semiconductor fabrication processes, Silicon (Si) NWs hold promise for enhancing existing technologies or innovating new methods in areas such as electromechanical/biochemical sensors and energy applications [Bachtold et al., 2022, Nehra et al., 2020, Zare Pakzad et al., 2023c, Shekhar et al., 2024].

The size-dependent mechanical properties of Si NWs poses a challenge for their successful integration into nanoelectromechanical systems (NEMS) devices [Wang et al., 2017, Yang et al., 2022, Nasr Esfahani and Alaca, 2019]. The lack of reliable modeling approaches is evident in a series of conflicting observations, which encompass a wide range of estimations for elastic properties of Si NWs [Yang et al., 2022, Nasr Esfahani and Alaca, 2019]. These methods can be categorized into continuum mechanics, analytical models, atomistic simulations, and first-principle methods, offering comprehensive analyses of the scale effect [Zare Pakzad et al., 2023c, Park et al., 2009, Sofiah et al., 2018, Momeni et al., 2020]. A recent investigation highlights the crucial role that nanomechanical modeling plays in interpreting experimental results for Si NWs [Zare Pakzad et al., 2023c]. The integration of high-throughput computing and advanced machine learning (ML) algorithms has revolutionized the structural design and performance improvement of nanomaterials [Jain et al., 2013, Curtarolo et al., 2013, Deringer et al., 2021, Catal et al., 2024], significantly influencing the discovery of novel materials [Deringer et al., 2019, Wang et al., 2023, Butler et al., 2018]. Recent research underscores the significance of integrating ML techniques into material science and mechanics [Catal et al., 2022, Yang and Guo, 2024, Brugnolotto et al., 2024], enabling more robust and reliable analysis of the findings.

More specifically, despite numerous publications focusing on the bottom-up fabrication of Si NWs and addressing their elastic properties, interpreting size effects remains challenging [Zare Pakzad et al., 2023c, Yang et al., 2022, Nasr Esfahani and Alaca, 2019]. With the potential incorporation of ML algorithms into atomistic methods, the present study seeks to investigate the size effect in the existing bottom-up literature on Si NWs. In this context, considering the broad range of modulus of elasticity reported for Si NWs and the existing contradictions between experimental and computational results, this study addresses the common understanding of 10-nm scale barrier between the two methods. In this respect, ML algorithms are enabled via molecular dynamics (MD) simulations for detailed analysis of size-dependent elastic properties of bottom-up Si NWs. In line with this, MD simulations are used to subject  $\langle 111 \rangle$ -oriented Si NWs to tensile and bending tests. This enables ML algorithms to conduct in-depth examinations of size effects through MD-based modeling of Si NWs.

The present study focuses on the size-dependent elastic properties of bottom-up Si NWs employing ML-driven atomistic simulations. Section 13.3.1 elaborates the details of the atomistic simulations, while Section 13.3.2 provides the specifics of the ML modeling efforts. The results are comprehensively discussed in the subsequent sections: Section 13.4.1 provides a detailed examination of atomistic findings, and Section 13.4.2 explores the ML-driven discoveries. Finally, Section 13.4.3 offers an interpretation of the ML-based atomistic findings, specifically addressing the size effect in bottom-up Si NWs. This work contributes significant insights into the elastic properties of Si NWs, thereby expanding our understanding of their mechanical characteristics at the nanoscale.

### **13.3 Methods and Materials**

#### *13.3.1 Atomistic Simulations*

This section offers a comprehensive overview of the modeling of tensile and bending behaviors in Si NWs with an unreconstructed surface state through MD simula-

tions. The modeling efforts encompass exploration of the two prevalent approaches for simulating tensile behavior: non-periodic and periodic tensile tests, along with three-point bending simulations for Si NWs. Dedicated discussions for each of the two tensile modeling approaches are presented in Sections 13.3.1A and 13.3.1B. In Section 13.3.1C, detailed information is provided concerning the modeling of bending behavior. Each subsection delivers specific computational details, including the preparation of atomic configurations, utilization of interatomic potentials, and other related parameters.

#### *Non-periodic tensile simulation*

In this subsection, the atomistic methodology applied to investigate the tensile behavior of Si NWs utilizing non-periodic B.C.s along the NW is discussed. Tensile tests are conducted on Si NWs featuring unreconstructed surface states, employing the MD method through the LAMMPS code [Thompson et al., 2022]. Figure 13.1 (a) depicts the initial atomic configuration of Si NWs, highlighting the geometric characteristics of the NW, characterized by a square cross-sectional shape. This representation includes the width, serving as an indication of the critical dimension (CD) in Si NWs. Figure 13.1 (b) schematically illustrates the non-periodic tensile modeling approach, where the length ( $L$ ) of the Si NW and the fixed and movable boundaries are denoted as  $L_f$  and  $L_m$ , respectively. The lengths  $L_f$  and  $L_m$  correspond to one-eighth of the NW length ( $L$ ). In this context, the length-to-CD ratio ( $L/CD$ ) is referred to as the aspect ratio (AR). For comprehensive geometric and computational details, Table 13.1 provides a detailed description of input parameters. The CD ranges from 2 nm to 10 nm, while predefined ARs are assigned as 7, 8, 9, 10, 12, 14, 16, 18, and 20. The Si NWs are oriented along the  $\langle 111 \rangle$  crystal orientation ( $[111]-x$   $[\bar{1}\bar{1}0]-y$   $[\bar{1}\bar{1}2]-z$ ) and undergo a tensile test, with Si atom interactions modeled using the Tersoff-T3 (TT3) [Tersoff, 1988] and Stillinger-Weber (SW) [Stillinger and Weber, 1985] potentials. For a thorough understanding of potential expressions and coefficients, readers can refer to the respective references [Tersoff, 1988, Stillinger and Weber, 1985].

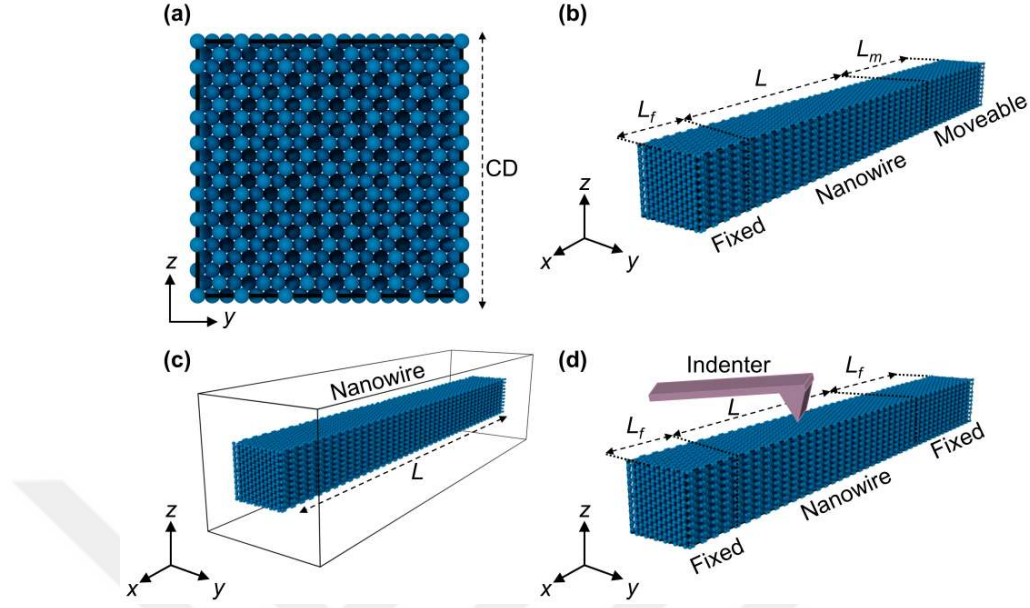


Figure 13.1: (a) Cross-sections of a Si NW with dimensional parameter defined as  $CD$ , representing NW width. (b) Non-periodic tensile simulation of Si NWs exhibited with the associated NW length ( $L$ ) and B.C.s regions are referred as fixed ( $L_f$ ) and movable boundaries ( $L_m$ ). (c) Periodic tensile simulation of Si NWs exhibited with the associated NW length ( $L$ ) and simulation box. (d) Bending simulation with the perspective view of a double-clamped Si NW showing the atomic configuration under 3-point bending simulation using a spherical indenter with associated support regions. The NW length ( $L$ ) and fixed region lengths ( $L_f$ ) are shown here.

Non-periodic boundary conditions are applied in all directions ( $x$ ,  $y$ , and  $z$ ) to model a finite size nanostructure. An energy minimization step is performed using the conjugate gradient method, followed by assigning an initial velocity distribution based on a finite temperature to all atoms. Subsequently, a relaxation process is conducted for 60 ps at a constant temperature, employing a 1 fs time step in the canonical NVT ensemble. Throughout the relaxation, the support and movable regions connected to the NW remain in fixed configurations. The subsequent tensile test involves fixing one end of the NW ( $L_f$ ) while allowing the other end ( $L_m$ ) to move. To mitigate shock wave generation due to rapid loading, a linearly increasing constant velocity is applied along the longitudinal direction ( $x$ ). The velocity starts from zero at the support and gradually increases to its maximum at the movable boundary. A velocity of  $1.0 \text{ \AA/ps}$  is applied at a constant temperature, corresponding

Table 13.1: Summary of input parameters used for modeling the tensile and bending behavior of  $\langle 111 \rangle$ -oriented Si NWs with unreconstructed surface state.

| Definition             | Descriptor | Values                                                                                                                                           |
|------------------------|------------|--------------------------------------------------------------------------------------------------------------------------------------------------|
| Critical Dimension     | CD         | Tensile (2, 3, 4, 5, 6, 7, 8, 9, 10 nm)<br>& Bending (2, 3, 4, 5 nm)                                                                             |
| Length to Width Ratio  | AR         | 7, 8, 9, 10, 12, 14, 16, 18, 20                                                                                                                  |
| Interatomic Potentials | POT        | Tersoff (TT3 [Tersoff, 1988] and TM [Munetoh et al., 2007]) & Stillinger-Weber (SW [Stillinger and Weber, 1985] and m-SW [Ganster et al., 2010]) |
| Temperature            | T          | 10, 300, 600 K                                                                                                                                   |
| Boundary Condition     | BC         | Tensile (Non-periodic) & Tensile (Periodic) & Bending                                                                                            |
| Surface State          | SS         | Unreconstructed and Native Oxide (Refs. [Pakzad et al., 2021, Pakzad et al., 2024, Pakzad et al., 2023b] & Section 13.3.1)                       |

to a strain rate of  $\dot{\epsilon} \approx 1.0 \times 10^9 \text{ s}^{-1}$ . This rate aligns with the strain rate employed in previous MD-based tensile tests on NWs [Kang and Cai, 2007, Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024]. The simulations are conducted at three distinct temperatures: specifically, 10 K, 300 K, and 600 K. The Virial theorem [Cormier et al., 2001] is utilized for stress calculations, as detailed in Equation 13.1. Employing the obtained stress-strain curves, the modulus of elasticity for Si NWs modeled through non-periodic tensile simulations is determined.

$$\pi_{ij} = \frac{1}{2\Omega_0} \left[ \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \frac{1}{r^{\alpha\beta}} \frac{\partial V(r^{\alpha\beta})}{\partial r} (v_i^{\alpha\beta} v_j^{\alpha\beta}) \right] \quad (13.1)$$

### *Periodic tensile simulation*

This section outlines the MD methodology employed to investigate the tensile behavior of Si NWs with unreconstructed surfaces, utilizing periodic B.C.s along the NW. Similar to the Si NWs described in Section 13.3.1A, atomistic simulations are conducted on Si NWs with a  $\langle 111 \rangle$  crystal orientation ( $[111]-x$   $[\bar{1}\bar{1}0]-y$   $[\bar{1}\bar{1}2]-z$ ) using the LAMMPS code [Thompson et al., 2022]. In contrast to the previously discussed Si NWs, periodic B.C.s are applied along the  $x$ -direction, while the  $y$ - and  $z$ -directions are constrained to model an infinitely long NW segment (see Figure 13.1 (c)).

Parameters, including the CD, AR, interatomic potential, and temperature, are consistent with Si NWs studied using the non-periodic tensile method. The MD simulations start with an energy minimization step utilizing the conjugate gradient method, followed by assigning initial velocities based on a Gaussian distribution at the specified temperature. Subsequently, dynamic equilibration at the designated temperature is carried out for 60 ps, utilizing the Nose-Hoover isobaric-isothermal (NPT) ensemble with a time step of 1 fs. Following equilibration, the simulation cell undergoes longitudinal deformation at a strain rate of  $\dot{\epsilon} = 1 \times 10^9 s^{-1}$ , falling within the suitable range for MD-based tensile testing [Kang and Cai, 2007, Pakzad et al., 2023b], as well as for Si NWs discussed in Section 13.3.1A. This ensures consistency in the examination of deformation and properties of Si NWs within the scope of this study. The stress-strain curves obtained for Si NWs are utilized to determine the modulus of elasticity, employing the formulation provided in Equation 13.1.

### *Bending simulation*

Simulations of three-point bending are performed on double-clamped unreconstructed Si NWs using the MD method [Thompson et al., 2022]. The Si NWs feature a square cross-section shown in Figure 13.1 (a) with the representative CD, similar to the Si NWs discussed in Section 13.3.1A and Section 13.3.1B are modeled. For the bending modeling of Si NWs, the AR, interatomic potential, and temperature assignments are consistent and provided in Table 13.1. The length of the fixed regions, denoted



Table 13.2: Surface stress ( $f_{11}$  and  $f_{22}$ ) and surface elastic constants ( $d_{11}$  and  $d_{22}$ ) for unreconstructed Si thin film model with (111) free surface [Pakzad et al., 2024].

| Structure                | Surface Properties(N/m) |          |          |          |
|--------------------------|-------------------------|----------|----------|----------|
|                          | $f_{11}$                | $f_{22}$ | $d_{11}$ | $d_{22}$ |
| Unreconstructed Si (111) | -0.88                   | -1.23    | -18.67   | +8.42    |

as  $L_f$ , corresponds to one-eighth of the NW length ( $L$ ), with a schematic demonstration of the three-point bending shown in Figure 13.1 (d). To simulate the clamped boundary condition, both fixed regions are constrained in all three dimensions ( $x$ ,  $y$ , and  $z$ ). Non-periodic shrink-wrapped boundary conditions are used in the  $y$  and  $z$  directions, while periodicity is applied along the  $x$ -direction. The Si NWs undergo a relaxation process using the conjugate gradient method to reach a local minimum configuration. Subsequently, a relaxation process is performed on all NWs at a finite temperature given in Table 13.1 for 60 ps, utilizing a time step of 1 fs. This is achieved by employing a canonical NVT ensemble with a Nose-Hoover thermostat.

The force over deflection ( $F/w$ ) ratio, representing the ratio of force to deflection, can be determined by analyzing the slope of the initial linear section of the force-deflection response. This ratio is commonly used to estimate the modulus of elasticity through a linear approach. However, it should be noted that in the case of bending response curves for Si NWs, the displacement of the NW upon loading is expected to be larger than half of the cross-sectional size ( $CD/2$ ), leading to a likely non-linear behavior, as observed in previous experimental and MD studies on the bending of Si NWs [Zare Pakzad et al., 2023c, Pakzad et al., 2021]. In this context, the ExtZP nanomechanical model is employed to estimate the modulus of elasticity of unreconstructed Si NWs [Zare Pakzad et al., 2023c]. The surface properties for unreconstructed Si with (111) free surface, including surface stresses ( $f_{11}$  and  $f_{22}$ ) and surface elastic constants ( $d_{11}$  and  $d_{22}$ ), necessary for interpreting the elastic response of Si NWs, are extracted from Ref. [Pakzad et al., 2024] and are provided in Table 13.2.

### 13.3.2 Machine Learning

This section introduces details associated with extracting data from modeling of Si NWs with unreconstructed surface states. This includes information available in the literature for Si NWs with a native oxide surface state [Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024]. Additional insights into the data will be provided in Section 13.3.2A, while explanations regarding feature selection and the implementation of ML models will be addressed in Section 13.3.2B and Section 13.3.2C, respectively.

#### *Data Preparation*

Effective data preparation plays a crucial role in developing a robust ML algorithm, where the quality of data is as essential as its quantity for successful predictions. To construct the dataset required for training the ML algorithms, two primary sources of input are utilized. The modeling efforts outlined in Section 13.3.1 generate tensile and bending responses for Si NWs under different parameter sets, with a specific focus on Si NWs featuring the unreconstructed surface state. Considering two distinct interatomic potentials, three designated testing temperatures, and differing Si NW CDs, coupled with distinct ARs modeled via different testing methods, this study establishes a comprehensive collection of 1188 Si NWs. Additionally, data from previous research conducted by the authors on  $\langle 111 \rangle$ -oriented Si NWs with a native oxide surface state, as documented in relevant literature [Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024], is assimilated into the overall dataset. Si NWs featuring a native oxide surface state exhibit variations in critical dimension, native oxide layer thickness, applied B.C.s, temperature, and interatomic potentials (TM [Munetoh et al., 2007] and m-SW [Ganster et al., 2010]). Notably, two key distinctions arise upon integrating data from Si NWs with these distinct surface conditions. Firstly, the unreconstructed Si NWs maintain their original surface thickness without any native oxide layer, whereas the Si NWs with native oxide exhibit values that account for differing oxide layer thicknesses. Secondly, recognizing the structural deviations resulting from oxygen atom presence in Si NWs with

native oxide surfaces, a consolidation is performed concerning the categorization of Tersoff and SW potentials. Consequently, TT3 and TM, as well as SW and m-SW, are grouped within the same potential family, and comparable values are attributed during dataset preparation. In this context, the Tersoff (TT3 [Tersoff, 1988] and TM [Munetoh et al., 2007]) and Stillinger-Weber (SW [Stillinger and Weber, 1985] and m-SW [Ganster et al., 2010]) represent two distinct families of interatomic potentials within the framework of this study. With the inclusion of the dataset pertaining to Si NWs with native oxide surface states, a total of 53 additional data points are appended to this study's collection. This extension elevates the overall number of data points to 1241, each representing the modulus of elasticity of a unique Si NW.

In this context, every data point within the dataset encompasses six distinct features, as delineated in Table 13.1, along with a single target variable representing the modulus of elasticity of the Si NW. The tabulated features encompass CD, AR, interatomic potential (POT), temperature (T), B.C., and surface state (SS). Each unique combination detailed in Table 13.1 for the unreconstructed surface condition is simulated, and the dataset is further enriched through the incorporation of Si NWs with native oxide surface states from given literature [Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024]. In the context of ML applications, the intrinsic nature of predictors within the dataset might necessitate preprocessing to enhance the overall performance of the ML process. Specifically, variables within a dataset can exhibit non-normal distributions or disparate scales, all of which can adversely impact the efficacy of ML algorithms. Therefore, prior to training, an in-depth analysis of the dataset will be undertaken to comprehend the data distribution and subsequently implement suitable data transformation techniques. Through data transformation, the variables are normalized and scaled to ensure equitable treatment by ML algorithms. In this study, a z-score normalization (standardization) approach is employed to achieve standard scaling and normalization of features, ensuring a mean of zero and a standard deviation of one. The next section will cover the details associated with descriptors and feature selection for ML algorithms.

*Feature Selection*

A detailed feature selection process precedes the creation of the dataset. Within this framework, the six parameters outlined in the previous section, along with their corresponding details as presented in Table 13.1, are identified as essential for this task. In this context, highly correlated features are excluded from this scheme, as they would represent a similar information. Despite the selection of six features for this study, the evaluation of correlation between these features is crucial, considering both linear and non-linear perspectives. To address potential linear correlations, the Pearson's correlation coefficient (PCC) is calculated [Sedgwick, 2012]. To tackle broader correlation issues, the random forest (RF) method is also utilized for feature correlation study [Archer and Kimes, 2008]. Before implementing ML algorithms for data generation, the initial focus revolves around refining the dimensionality of the dataset by emphasizing the most pertinent features. The following section will address the specifics pertaining to ML algorithms.

*Machine Learning Algorithms*

The analysis of the dataset and associated features using ML algorithms including Random Forest (RF), K-Nearest Neighbors (KNN), Linear Regression (LR), Decision Trees (DT), Multi-Layer Perceptron (MLP), and Support Vector Machines (SVM), is assessed for their ability to forecast the target variable. Before model training, the original dataset is divided into training data, facilitating model optimization, and a test dataset, employed to gauge the models' predictive accuracy on unseen data. The evaluation of ML models is grounded in their predictive errors on the test dataset, measured by root mean squared error (RMSE), mean absolute error (MAE), and coefficient of efficiency ( $R^2$ ), as defined by Equation 13.2, Equation 13.3, and Equation 13.4, respectively. In this regard,  $y_i$  and  $\tilde{y}_i$  are true and predicted values, respectively. Here,  $\bar{y}$  is the average of the predicted values, and  $n$  is the total number of samples. All computations are executed using the scikit-learn library within the Python programming language [Pedregosa et al., 2011]. Upon identifying the most effective models, additional optimization techniques, including

hyperparameter tuning, are experimented with to determine optimal configurations. These optimizations are iterated to enhance the training process and mitigate the risk of overfitting given the current training dataset.

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \tilde{y}_i)^2} \quad (13.2)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \tilde{y}_i| \quad (13.3)$$

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \tilde{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (13.4)$$

## 13.4 Results

### 13.4.1 Atomistic Results

MD offers a viable avenue for exploring the elastic properties of Si NWs. Considering the widespread applications of Si NWs in future electronics and NEMS, there exists a pressing need for a precise investigation into elasticity, particularly concerning size effects. In this respect, the integration of ML algorithms with computational approaches holds the potential to streamline this exploration. This section elucidates the results of MD simulations conducted in the scope of this study, incorporating both the outcomes of these simulations and previous data points from prior studies. Within this framework, the modulus of elasticity of Si NWs is derived from stress-strain curves for tensile tests and force-deflection results for bending, serving as the output parameter. This comprehensive analysis encompasses data from 1188 Si NWs modeled in this study, along with an additional 53 data points extracted from the prior literature on Si NWs with native oxide surface state [Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2024]. The combination of these datasets results in a compilation of 1241 data points, each representing the modulus of elasticity for a unique Si NW. Due to the computational demands associated with modeling Si NWs

with a native oxide layer – attributed to the increased number of atoms involved – the primary focus of the modeling efforts is directed towards unreconstructed Si NWs. Specifically, all possible combinations of Si NWs with unreconstructed surface states, accounting for different CDs, ARs, three distinct temperatures, three types of testing methodologies, and two types of interatomic potentials, are simulated. This extensive dataset serves as a valuable resource for ongoing and prospective studies on bottom-up Si NWs, given its unique size and composition. The dataset presented in this section will undergo thorough examination and analysis through the utilization of ML models, as discussed in Section 13.4.2.

#### 13.4.2 Machine Learning Results

The evaluation of ML algorithms involves assessing RF, KNN, LR, DT, MLP, and SVR across various training data percentages, ranging from 30% to 90% with 10% intervals, to evaluate their performance. Given the size of the dataset in this study, careful data splitting is essential, aiming for a balanced distribution in both the training and test datasets to avoid overfitting. The ML models are then evaluated based on their prediction errors on the test dataset. Subsequently, calculations of RMSE, MAE, and  $R^2$  are performed, with their respective standard deviations presented in Figures 13.2 (a), (b), and (c), respectively. When considering RMSE as the most critical performance evaluation parameter in the context of ML algorithms, clear distinctions emerge in the errors obtained. Specifically, four models – RF, KNN, MLP, and DT – report RMSE values below 20%, while LR and SVR, both employing linear kernels in this study, exhibit higher RMSE values. This emphasizes the non-linearity of the problem when examining the elasticity of Si NWs. Furthermore, MAE, a common measure of forecast error in time series analysis, confirms the findings from the RMSE analysis, showing a greater dependence on the training data percentage for smaller data subsets. In this context, the calculation of  $R^2$  provides an additional quantitative assessment of the observation of non-linearity. Linear models exhibit a degree of correlation below 50% within the context of prediction and target values, while the remaining four models (RF, KNN,

MLP, and DT) demonstrate more than a 90% coefficient of efficiency, underscoring their suitability for this task.

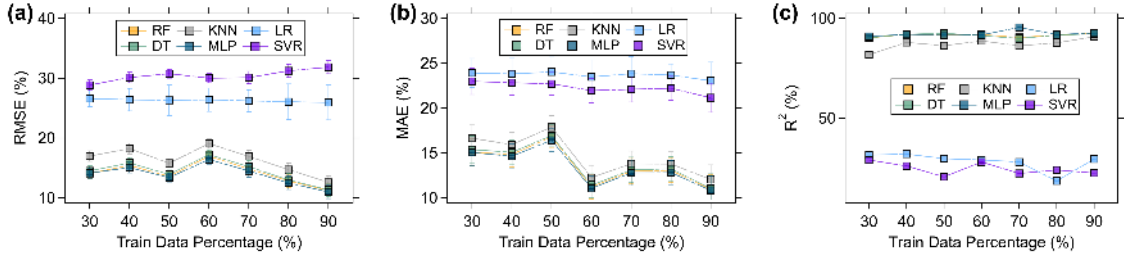


Figure 13.2: The evolution of (a) RMSE, (b) MAE, and (c)  $R^2$  on test dataset with changing training dataset proportions for the RF, KNN, LR, DT, MLP, and SVR algorithms.

Regarding feature importances, Figure 13.3 (a) presents a heatmap illustrating the PCC among the input variables. Notably, the parameters representing dimensionality, specifically CD and AR, exhibit the highest correlation, reaching approximately 0.8. This correlation represents the strongest linear relationship among all the features. However, it is essential to acknowledge the limitations of the PCC method, as it disregards model performance variations and overlooks non-linear relationships among variables. Consequently, reliance on importance calculations based on the RF method is considered to be more reliable. In this context, the RF method, with its ability to provide feature importance, makes it an appealing tool for potential follow-up analyses. The feature importance results obtained from the RF algorithm in this study are depicted in Figure 13.3 (b). Among these features, the BC and SS emerge as the most crucial parameters, showcasing the highest importance within the context of this problem. Conversely, the numerous simulations conducted on geometric properties, including CD and AR, exhibit lower importance when compared to the previously mentioned features. This observation is consistent with earlier research, which emphasizes the significant impact of surface effects on the mechanical properties of Si NWs [Zare Pakzad et al., 2023c, Zare Pakzad et al., 2021, Pakzad et al., 2023b, Pakzad et al., 2021, Pakzad et al., 2023a, Pakzad et al., 2024]. Moreover, the performance of the KNN algorithm is contingent upon

the hyperparameter  $K$  which determines the number of nearest neighbors considered from the training dataset when making predictions for a new data point. This presents an opportunity for further enhancing the KNN model through fine-tuning the  $K$  hyperparameter. In this context, Figure 13.3 (c) illustrates the RMSE across a range of  $K$  hyperparameter values, ranging from 1 to 20. The optimal value of  $K$  is identified as 2, corresponding to the minimum error achieved.

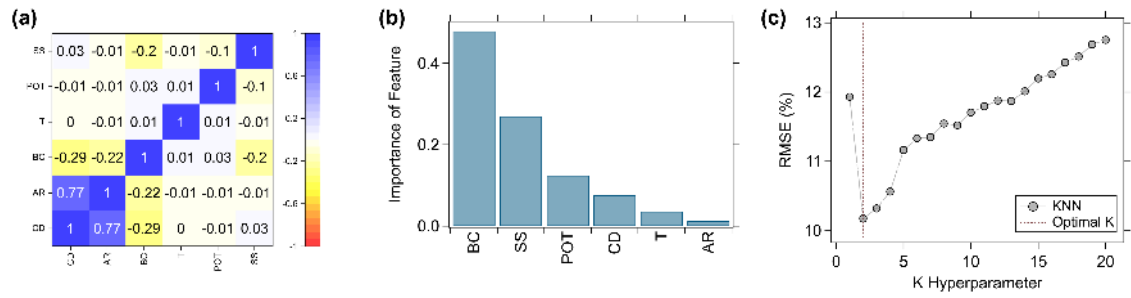


Figure 13.3: (a) The heatmap of PCCs for associated features discussed in Table 13.1, The higher color intensities exhibit the enhanced correlation between the two features while the blue and red colors indicate positive and negative correlation, respectively. (b) The relative feature importance for input variables based on their performance obtained via the RF method. (c) The change in RMSE with increasing  $K$  hyperparameter for KNN algorithm.

As illustrated in Figure 13.4, the performance of six algorithms in predicting the modulus of elasticity of Si NWs, considering the actual modulus of elasticity obtained via MD simulations, is presented. Due to notable performance differences among different models while excluding the linear models (LR and SVR) from consideration within the scope of this study, it becomes imperative to conduct a more detailed examination of these models. To ensure robustness and prevent overfitting, a ten-fold cross-validation approach is employed. Among these algorithms, the non-linear models consistently deliver more dependable results, accounting for deviations resulting from hyperparameter tuning. In contrast, LR and SVR with linear kernels exhibit the least favorable performance. Given this, a more thorough analysis of the KNN model, as one of the best-performing models in the context of size-dependent elastic properties of Si NWs, is followed next, including a comparison with the lit-



erature domain from experimental and computational studies for  $\langle 111 \rangle$ -oriented Si NWs.

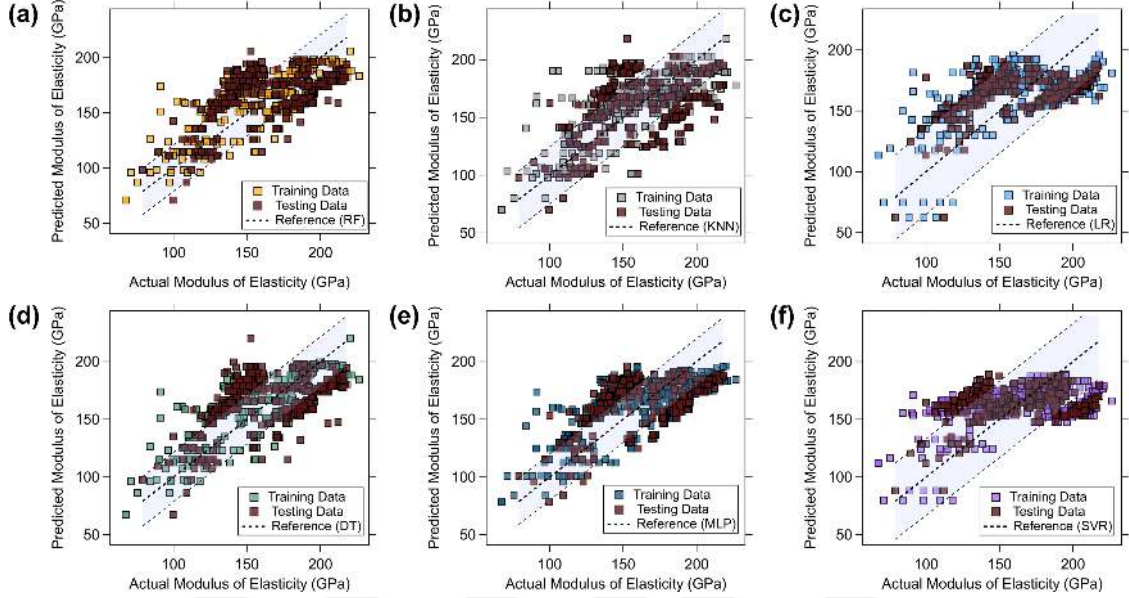


Figure 13.4: Performance of (a) RF, (b) KNN, (c) LR, (d) DT, (e) MLP, and (f) SVR algorithms in predicting modulus of elasticity as a function of actual modulus of elasticity available in the testing set. The line of references, along with their corresponding standard deviations, is also provided for each model.

### 13.4.3 Interpretation of Elastic Properties

Bottom-up fabricated Si NWs with a  $\langle 111 \rangle$  crystalline orientation have been extensively studied, with a wealth of modulus data available in both experimental and computational research [Zhu et al., 2009, Heidelberg et al., 2006, Gordon et al., 2009, San Paulo et al., 2005, Kim et al., 2011, Sohn et al., 2010, Liu and Shen, 2012, Liu et al., 2015, Jing et al., 2009a, Zhuo and Beom, 2019]. This study focuses on MD calculations of elasticity for  $\langle 111 \rangle$ -oriented Si NWs, coupled with ML predictions incorporating different input parameters that connect atomistic predictions to size-dependent elasticity. The ML trendline for the modulus of elasticity of  $\langle 111 \rangle$ -oriented Si NWs considers deviations resulting from different inputs, such as AR, interatomic potential, testing type, and surface state. The temperature is set at 300

K for this analysis to align with experimental works conducted at room temperature.

The trendline, depicted in Figure 13.5 demonstrates ML predictions via the KNN algorithm up to 100 nm while the results are compared with the literature domain on the modulus of elasticity of  $\langle 111 \rangle$ -oriented Si NWs. A red dashed line at 10 nm represents the common scale barrier discussed in the literature [Yang et al., 2022]. Consistent with the findings of Zhu *et al.* [Zhu et al., 2009], the combined ML and atomistic methods reveal an increasing trend in  $E$  for  $\langle 111 \rangle$ -oriented Si NWs, validating the accuracy of ML techniques in capturing the size effect. Notably, the ML predictions align well with experimental and computational trends within the established framework. Identifying outliers is crucial due to significant disparities between predicted and experimental  $E$  for Si NWs, and Refs. [Heidelberg et al., 2006, Sohn et al., 2010] highlight some of these outliers. Enabled by unreconstructed Si NWs and including Si NWs with a native oxide surface state, this study builds upon previous efforts to develop ML-based atomistic analysis of the mechanical behavior of Si NWs. ML algorithms provide a reliable understanding of the size effect on the elastic properties of Si NWs. Despite variations from experimental and atomistic trendlines, ML emerges as another viable method for investigating the size effect in Si NWs.

### 13.5 Conclusion

In conclusion, this study employs a combined approach of MD simulations and ML algorithms to comprehensively investigate the size-dependent elastic properties of  $\langle 111 \rangle$ -oriented Si NWs. MD simulations examine different mechanical aspects, including tensile and bending modeling, offering detailed insights into the behavior of Si NWs. The analysis, featuring over 1000 simulation results, underscores the non-linear nature of elasticity. Utilizing ML, the study successfully predicts the modulus of elasticity for Si NWs and examines trendlines specific to  $\langle 111 \rangle$ -oriented Si NWs. Despite some variations, ML emerges as a promising tool for understanding the elastic properties of Si NWs, presenting valuable implications for future nanomechanical studies. This approach enhances our understanding of the

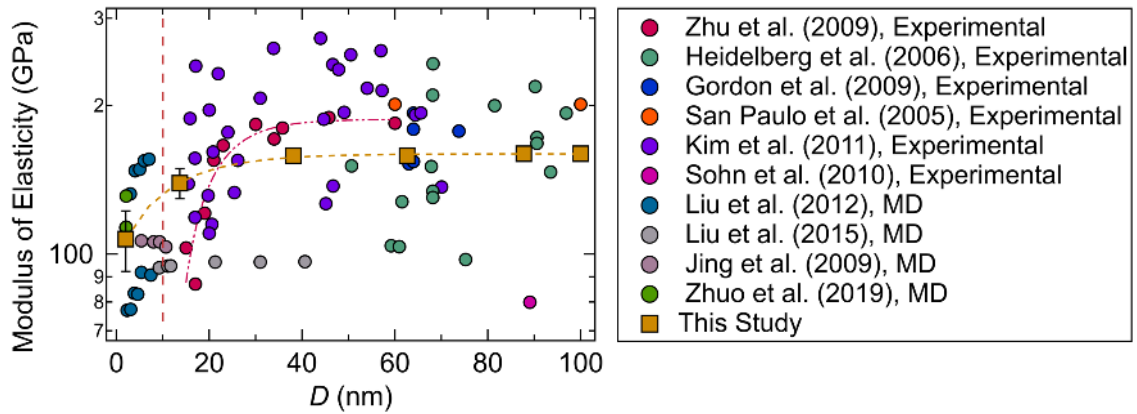


Figure 13.5: The elastic moduli obtained for Si NW sets in the current study via ML-driven atomistic modeling are illustrated for KNN algorithm. The literature domain in this figure extends beyond experimental findings (including MD results from the literature), encompassing a diverse range of moduli of elasticity reported for  $\langle 111 \rangle$ -oriented Si NWs below and beyond the 10-nm scale barrier [Zhu et al., 2009, Heidelberg et al., 2006, Gordon et al., 2009, San Paulo et al., 2005, Kim et al., 2011, Sohn et al., 2010, Liu and Shen, 2012, Liu et al., 2015, Jing et al., 2009a, Zhuo and Beom, 2019].

intricate relationship between structural characteristics and mechanical responses in Si NWs, contributing to the broader field of nanomaterials research.

## Chapter 14

# MOLECULAR DYNAMICS STUDY OF ORIENTATION-DEPENDENT TENSILE PROPERTIES OF SI NANOWIRES WITH NATIVE OXIDE: SURFACE STRESS AND SURFACE ENERGY EFFECTS

### 14.1 Overview

Molecular dynamics (MD) simulations are employed to investigate the influence of native oxide layer on the mechanical properties of Si nanowires (NWs) through analyzing surface stress and surface energy effect. This work studies the tensile response of Si NWs along  $\langle 100 \rangle$  and  $\langle 110 \rangle$  crystal orientations. MD results are compared with the traditional core-shell model on the estimation of the modulus of elasticity of Si NWs with a native oxide layer. Density functional theory (DFT) methods are used to verify MD results on the surface energy calculations. Surface stress and surface elastic constants are studied for native oxide surface using MD simulations and compared with unreconstructed surfaces. In this work, the role of native oxide is addressed to understand the difference between experimental and computational findings on the modulus of elasticity of Si NWs.

### 14.2 Introduction

In the multi-disciplinary world of nanotechnology, materials based on nanometer-sized structures have attracted a great deal of interest in various fields. Nanowires are one of the most important one-dimensional (1-D) nanostructures introducing unique mechanical, electrical, and optical properties with their highly anisotropic geometry as well as finite size effects. There is a strong size dependency in the

mechanical properties of NWs [Nasr Esfahani and Alaca, 2019]. However, due to lack of detailed investigation of surface and interface effects on mechanical properties of Si NWs, analyzing the surface related constants effect on elastic behavior of Si NWs needs further examinations of crystal orientations as well as native oxide effects. In this study, we examine native oxide effect on the mechanical behavior of Si NWs by performing tensile tests using MD simulations while the native oxide has proven to have an amorphous crystal structure [Steinruck et al., 2014]. Surface effect is studied by surface energy estimations of unreconstructed (100) and (110) Si surfaces using both MD and DFT methods. Furthermore, surface energy, surface stress and surface elasticity parameters are calculated for unreconstructed Si surfaces and native oxide surface using MD simulations.

### **14.3 Simulation Methods**

#### *14.3.1 Nanowire Tensile Simulation using MD*

In MD simulations, the Tersoff Munetoh potential [Munetoh et al., 2007] is used to describe interatomic potentials for Si-Si and Si-O interactions. The Tersoff potential is an empirical function composed of two-body terms depending on the local environments. This work studies the mechanical behavior of Si NWs with two different surface configurations including unreconstructed surface and native oxide. NWs with native oxide will be indicated as aSiO<sub>2</sub>-Si NWs in the remainder. The initial atomic configurations of NWs along  $\langle 100 \rangle$  and  $\langle 110 \rangle$  crystal orientations are shown in Figure 14.1. The NW width ( $w$ ) and oxide layer thickness ( $t$ ) are selected as 5 nm and 0.5 nm, respectively. NW length ( $L$ ) of 100 nm is considered for both crystal orientations having 25 nm on each side of the NW length denoted as support and movable regions ( $L_0$ ) as shown in Figure 14.1 (e) and Figure 14.1 (f). The LAMMPS code is used for MD calculations considering non-periodic boundary conditions along all directions. NWs are first quasi-statically relaxed to a local minimum configuration through the conjugate gradient method. Then, all NWs are relaxed at a temperature of 1.0 K for 120 ps with a time step of 1 fs using a

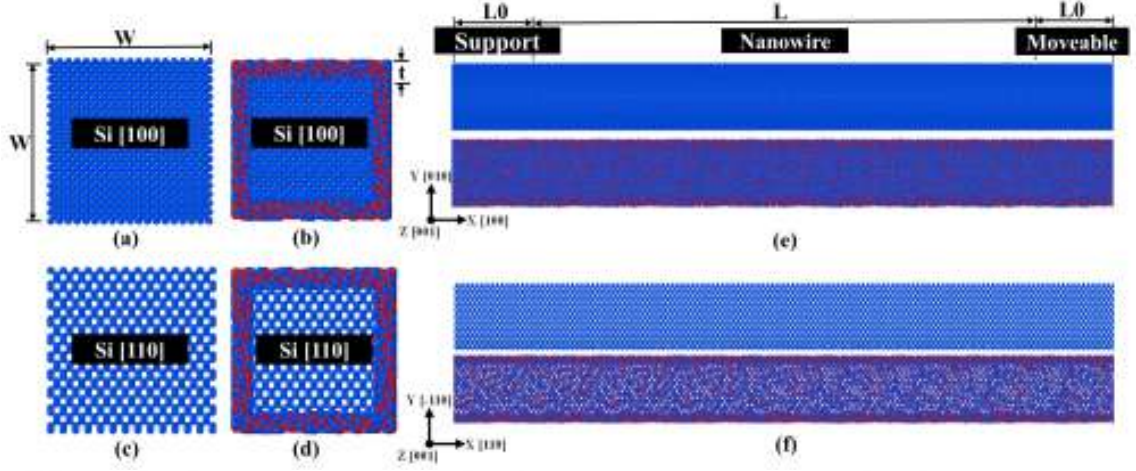


Figure 14.1: The initial configuration of NWs. The models in this figure are nanowire of width ( $W$ ) of 5 nm and oxide thickness ( $t$ ) of 0.5 nm for (a) unreconstructed Si  $\langle 100 \rangle$ , (b) aSiO<sub>2</sub>-Si  $\langle 100 \rangle$ , (c) unreconstructed Si  $\langle 110 \rangle$ , (d) aSiO<sub>2</sub>-Si  $\langle 110 \rangle$  and, geometry of a NW length of  $L$  and Si orientation of NW of (e)  $\langle 100 \rangle$  and (f)  $\langle 110 \rangle$ . Si atoms are colored with blue and oxygens are in red.

canonical NVT ensemble (Nose-Hoover thermostat). To mitigate the shock wave from the high loading rate, constant velocities that vary linearly from zero at the fixed end to a maximum of 1.0 Å/ps at the free end of the NW as well as a constant velocity value of 1.0 Å/ps for the moveable region are applied to the atoms along the  $x$ -directions as shown in Figure 14.1 (e) and Figure 14.1 (f).

### 14.3.2 Modulus of elasticity using core-shell

The core-shell model is often used for studying the surface effect on modulus of elasticity of NWs [Miller and Shenoy, 2000]. This model describes the NW as a combination of core and surface regions with distinct moduli of elasticity for the core ( $E_0$ ) and the surface ( $E_s$ ). For a NW with diameter of  $D$  and a finite surface layer thickness of  $r_s$  under tensile loading, the effective modulus of elasticity,  $E_{eff}$ , of the NW is given by Equation 14.1 [Chen et al., 2006a].

$$E_{eff} = E_0 \left[ 1 + 4 \left( \frac{E_s}{E_0} - 1 \right) \left( \frac{r_s}{D} - \frac{r_s^2}{D^2} \right) \right] \quad (14.1)$$

Modulus of elasticity for the core and shell parts of aSiO<sub>2</sub>-Si NWs is estimated by performing tensile simulation on bulk structure of Si with  $\langle 100 \rangle$  and  $\langle 110 \rangle$  crystal orientations and bulk structure of aSiO<sub>2</sub> using the Tersoff-Munetoh potential by applying periodic boundary conditions along all directions. Core-shell model is applied using the modulus of elasticity of the bulk Si as  $E_0$  and modulus of elasticity of shell oxide as  $E_s$  and the results are used for estimation of the effective modulus of elasticity for the Si NW with native oxide ( $E_{eff}$ ).

### 14.3.3 Surface Energy using MD

Surface energy,  $\gamma$  is the energy variation per unit area due to the surface creation and it is defined as the difference in the energy of the system with and without free surface [Izumi et al., 2004]. MD simulations were performed using the Tersoff-Munetoh potential to estimate the surface energies of Si and aSiO<sub>2</sub> models. The unrelaxed and relaxed surface energies are denoted as  $\gamma_u$  and  $\gamma_r$ , respectively and are determined using Equation 14.2 and Equation 14.3, respectively.

$$\gamma_u = (E_{u,slab} - N \times E_{bulk})/2 \times A \quad (14.2)$$

$$\gamma_r = ((E_{u,slab} - N \times E_{bulk})/A) - \gamma_u \quad (14.3)$$

Here,  $A$  and  $N$  represent the surface area of the slab and number of atoms, respectively and  $E_u$ ,  $E_r$ , and  $E_{bulk}$  are the energies of the unrelaxed slab, the relaxed slab, and the bulk, respectively [Ungerer et al., 2019]. To calculate the surface energy of unreconstructed (100) and (110) Si surfaces, a film model with periodic boundary conditions applied in  $x$  and  $y$  directions but not in the  $z$  direction is used which provides an infinite size film model with limited thickness ( $L_z$ ) as shown in Figure 14.2 (a) and Figure 14.2 (b), respectively. In order to define the free surfaces, thin film models are built with crystal orientations of  $(x, y, z) = ([100], [010], [001])$  and  $(x, y, z) = ([-110], [001], [110])$  for unreconstructed (100) and (110) Si surfaces,

respectively. The simulation boxes are set as 8 times of the lattice constant of Si while for calculation of bulk energy values, same atomic systems with all periodic B.C.s are used. The evaluation area ( $A$ ) is made up of two surfaces that face each other, where the film must be enough thick to prevent interface of these two free surfaces. The models associated with Si (100) and Si (110) have 4224 and 8448 atoms with an overall size of  $4.35 \text{ nm} \times 4.35 \text{ nm} \times 4.35 \text{ nm}$  and  $6.15 \text{ nm} \times 4.35 \text{ nm} \times 6.15 \text{ nm}$ , respectively. The surface area for the (100) and (110) models are evaluated as  $37.8 \text{ nm}^2$  and  $53.5 \text{ nm}^2$ , respectively. The surface energy associated with the amorphous  $\text{SiO}_2$  structure, as native oxide in Si NWs, is studied by defining a film  $\text{aSiO}_2$  structure as shown in Figure 14.2 (c) while for bulk energy calculation similar to Si models, periodic B.C.s were applied in all directions. The  $\text{aSiO}_2$  film model consists of 11616 atoms (3872 Si and 7744 O atoms) with an overall size of  $5.7 \text{ nm} \times 5.7 \text{ nm} \times 5.8 \text{ nm}$ . The area for the free surface of  $\text{aSiO}_2$  model is evaluated as  $65 \text{ nm}^2$ . Considering the amorphous nature of native oxide, 20  $\text{aSiO}_2$  were built with similar dimensions as discussed before keeping the stoichiometric ratio between Si and O atoms (1:2) while having different distribution of the atoms on the surfaces. For proper statistical treatment, the average values of 20 simulations were reported here.

After the creation of surfaces, the systems are well-relaxed by the conjugated gradient method and the differences between bulk and film energies are used for surface energy calculations.

#### 14.3.4 Surface Energy using DFT

For the verification of orientation dependent surface energy values DFT approach is used. The Vienna Ab Initio Simulation Package (VASP) was used to simulate the Si surfaces with (100) and (110) orientations. The project augmented wave (PAW) potential was employed to describe the interaction between the valence and the core electrons. The Perdew, Burke, and Ernzerhof (PBE) functional within the generalized gradient approximation (GGA) was applied in all calculations. Plane waves were included to a cutoff of 400 eV. The Methfessel-Paxton scheme order 1



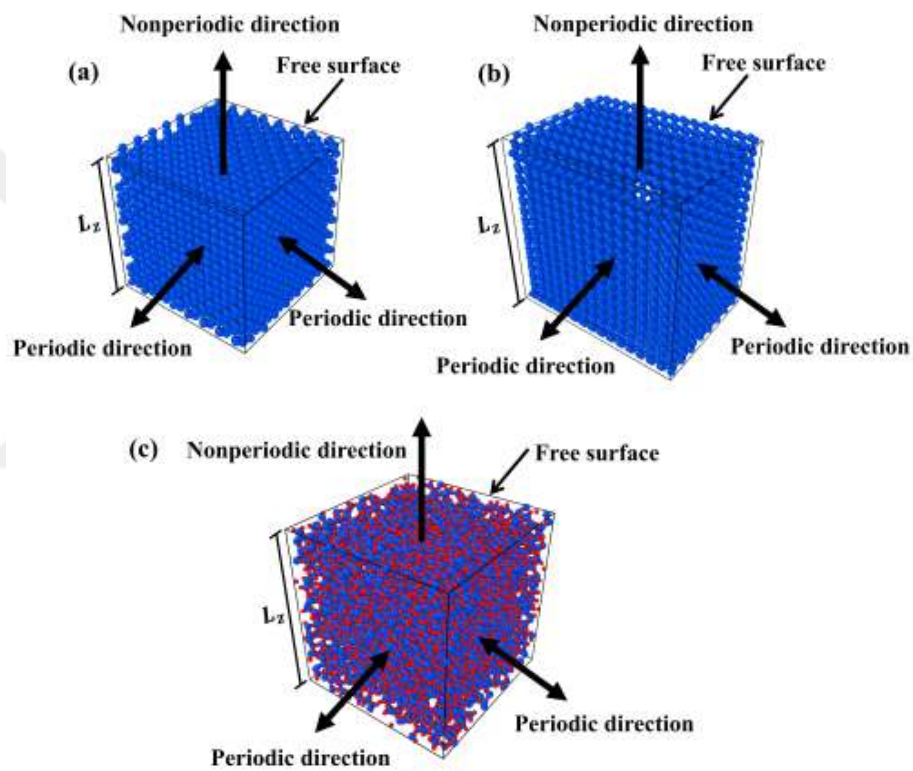


Figure 14.2: Surface models with non-periodic boundary conditions in  $z$ -directions for (a) Si (100), (b) Si (110) and (c) aSiO<sub>2</sub> used for the calculation of surface-related parameters (Blue atoms correspond to Si and red ones represent oxygen atoms).

was used with a smearing of 0.05 eV to determine the particle occupancies during the geometry optimization. The electronic and ionic optimization criteria were  $10^{-5}$  eV and  $10^{-2}$  eV. $\text{\AA}^{-1}$ , respectively and the conjugate gradient technique was adopted for the geometry optimizations. Si has an Fd3m structure, and the bulk Si structure was calculated within a diamond cubic cell using a  $17 \times 17 \times 17$  Monkhorst-Pack k-point mesh. Our calculated Si lattice constant was 5.431  $\text{\AA}$  and the Si (100) and (110) surfaces were investigated by simulating the periodic  $p(3 \times 3)$  supercells. Vacuum of 15  $\text{\AA}$ , in the  $z$  direction was added to avoid the interaction between the neighboring cells. Four atomic layers were considered for the slabs, and the surface area of the supercells were 260.3  $\text{\AA}^2$  and 190.1  $\text{\AA}^2$  for the (100) and (110) surfaces, respectively. The relaxed and unrelaxed surface energies were calculated using Equation 14.2 and Equation 14.3. A  $7 \times 7 \times 1$  Monkhorst-Pack k-point grid was used in all surfaces to sample the Brillouin zone.

#### 14.3.5 Surface Elastic Constants using MD

Surface elastic constants ( $d_{ijkl}$ ) as an important surface parameter can be calculated using the method recommended by Ref. [Izumi et al., 2004], where  $d_{ijkl}$  is defined as second-order derivative of surface energy with respect to the strain under plane-stress condition, which represents the variation in elastic constants due to the surface creation. Elastic constants for bulk ( $C_{ij}^{bulk}$ ) and film ( $C_{ij}^{film}$ ) models could be calculated using MD simulations while for the bulk model, the elastic constants should be defined under plane-stress condition ( $C_{ij}^{bulk,plane}$ ) using the definitions in Equation 14.4, Equation 14.5 and Equation 14.6.

$$C_{11}^{bulk,plane} = C_{11} - \frac{C_{13}^2}{C_{33}} \quad (14.4)$$

$$C_{22}^{bulk,plane} = C_{22} - \frac{C_{12}^2}{C_{33}} \quad (14.5)$$

$$C_{12}^{bulk,plane} = C_{12} - \frac{C_{12}C_{13}}{C_{33}} \quad (14.6)$$

The relationship between the plane-stress elastic constants of the bulk and film models with the surface elastic constants is represented in Equation 14.7.

$$C_{ijkl}^{film,plane} = C_{ijkl}^{bulk,plane} - \frac{2}{L_z} d_{ijkl} \quad (14.7)$$

This method is applied to nano-scale thin films in quasistatic states with no temperature effect, which are shown in Figure 14.2 (a) and Figure 14.2 (b) denoted as unreconstructed Si surfaces and in Figure 14.2 (c) denoted as native oxide surface. The Tersoff-Munetoh potential is used for all MD calculations and to obtain elastic constants, small strains in different directions are applied to the simulation box and the variation of the energy is measured.

#### 14.3.6 Surface Stress using MD

Surface stress is defined as the generated stress due to the surface creation being equal to the variation in the total surface energy per unit area with respect to the strain. By assuming the film thickness of  $L_z$ , the surface stress components denoted as  $f_{ij}$  are formulated as shown in Equation 14.8 where  $\eta$  represents the averaged strain due to the relaxation.

$$f_{ij}(\eta) = f_{ij}^{film}(\eta) - f_{ij}^{bulk}(\eta) \quad (14.8)$$

Bulk surface stress must be estimated separately by the bulk model and surface stress for the film model can be defined by using the stress tensor definition as shown in Equation 14.9.

$$f_{ij}^{film}(\eta) = \sigma_{ij}^{film}(\eta) \frac{L_z}{2} \quad (14.9)$$

This method is applied to thin films of unreconstructed Si with (100) and (110) surfaces, shown in Figure 14.2 (a) and Figure 14.2 (b), respectively, and aSiO<sub>2</sub> model represented in Figure 14.2 (c) where  $f_{11}$  and  $f_{22}$  are calculated using Equation 14.9. The Tersoff-Munetoh potential was used for interatomic potential.

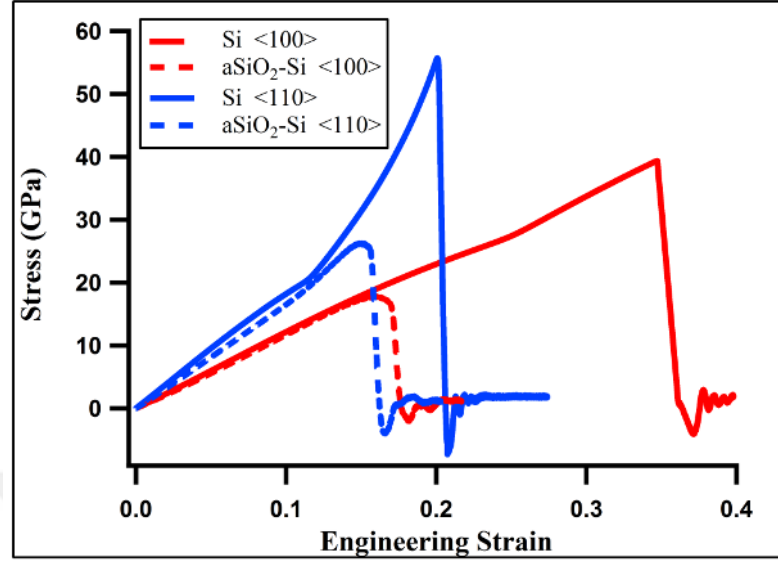


Figure 14.3: Stress-strain curves for tensile of unreconstructed Si and Si NWs with native oxide along  $\langle 100 \rangle$  and  $\langle 110 \rangle$  crystal orientations.

## 14.4 Results

### 14.4.1 Modulus of Elasticity

The stress-strain curves for unreconstructed Si NWs and aSiO<sub>2</sub>-Si NWs are shown in Figure 14.3. The stress-strain relation is essentially linear in elastic regime for all NWs and the modulus of elasticity can be directly evaluated in such elastic region. The modulus of elasticity estimation for  $\langle 100 \rangle$  Si NWs exhibits a change from 115.6 GPa to 82.7 GPa for unreconstructed NW and NW with native oxide, respectively. Similar examination for  $\langle 110 \rangle$  Si NWs, shows the modulus drop from 189.8 GPa to 130.5 GPa for unreconstructed NW and NW with native oxide, respectively.

Such decrease in modulus of elasticity is due to the presence of native oxide layer. Those results for Si NWs with native oxide are much closer to the experimental observations [Nasr Esfahani and Alaca, 2019] compared to unreconstructed Si NWs mostly modeled previously. Estimation of the modulus of elasticity for bulk silicon with  $\langle 100 \rangle$  and  $\langle 100 \rangle$  crystal orientations reveals moduli values of 87.4 GPa

Table 14.1: Effective Modulus of Elasticity Estimations for Si NWs with Native Oxide Using Tensile MD simulation and Core-Shell Model.

| Nanowire                      | $E_{eff}$ : MD Simulation (GPa) | $E_{eff}$ : Core-Shell Model (GPa) |
|-------------------------------|---------------------------------|------------------------------------|
| aSiO <sub>2</sub> -Si < 100 > | 82.7                            | 77.5                               |
| aSiO <sub>2</sub> -Si < 110 > | 130.5                           | 106.6                              |

and 133.1 GPa, respectively, while for the bulk structure of aSiO<sub>2</sub>, the modulus of elasticity value is predicted as 59.4 GPa. Using core-shell model and considering of the modulus of elasticity of the bulk Si as  $E_0$  and modulus of elasticity of bulk aSiO<sub>2</sub> as  $E_s$ , the effective modulus of elasticity for aSiO<sub>2</sub>-Si NWs are calculated as summarized in Table 14.1 and compared with MD simulations.

#### 14.4.2 Surface Energy Constants

After studying the elastic behavior, the surface features for unreconstructed surfaces and native oxide are investigated. The predicted surface energies of unreconstructed Si surfaces and aSiO<sub>2</sub> structures are summarized in Table 14.2. The unrelaxed surface energies for unreconstructed (100)-Si using MD, and DFT method results in 2.29 J/m<sup>2</sup>, and 2.20 J/m<sup>2</sup>, respectively where the relaxed energies are reduced to 2.21 J/m<sup>2</sup> and 2.15 J/m<sup>2</sup>, respectively. For unreconstructed (110)-Si surface the unrelaxed surface energies are estimated as 1.57 and 1.76 J/m<sup>2</sup> and the relaxed surface energies are calculated as 1.45 and 1.73 J/m<sup>2</sup>. Calculated surface energies for unreconstructed Si surfaces are in good agreement with previous MD and DFT based estimations for unreconstructed (100) and (110) Si surfaces [Izumi et al., 2004, Xu and Kim, 2019]. Results exhibit the surface energy of  $2.19 \pm 0.2$  J/m<sup>2</sup> for a SiO<sub>2</sub>, which is also close to the range of surface energy calculations of crystalline SiO<sub>2</sub> structures [Pishkenari and Rezaei, 2017]. Surface energy constants calculated for unreconstructed surfaces using both MD and DFT methods verifies the lower surface energy in (110)-Si surface compared to (100)-Si.

Table 14.2: Surface Energy, Surface Stress and Surface Elastic Constants for Atomic Structures using MD. The value inside the parentheses shows the DFT estimation.

| Surface Properties             | Structures  |             |                   |
|--------------------------------|-------------|-------------|-------------------|
|                                | Si (100)    | Si (110)    | aSiO <sub>2</sub> |
| $\gamma_r$ (J/m <sup>2</sup> ) | 2.21 (2.15) | 1.45 (1.73) | 2.19 $\pm$ 0.2    |
| $d_{11}$ N/m                   | -8.77       | +3.4        | -22.1 $\pm$ 1.3   |
| $d_{22}$ N/m                   | -8.77       | -15.1       | -22.1 $\pm$ 1.3   |
| $f_{11}$ N/m                   | -0.88       | -1.57       | -1.11 $\pm$ 0.10  |
| $f_{22}$ N/m                   | -0.88       | -0.95       | -0.91 $\pm$ 0.09  |

#### 14.4.3 Surface Elastic Constants

Using the film models with limited thicknesses as shown in Figure 14.2 for unreconstructed Si and aSiO<sub>2</sub> surfaces, the elastic constants are obtained for film structures. Also, it is obvious that the bulk models are with periodic definition in every direction without any dependence on the thickness. To calculate surface elastic constants, Equation 14.7 is used with the associated film thickness of  $L_z$ , where for free surface of (100)-Si the surface elastic constants are evaluated as  $d_{11} = d_{22} = -8.77$  N/m while for (110)-Si surface, surface elastic constants are estimated as  $d_{11} = +3.4$  N/m and  $d_{22} = -15.1$  N/m, respectively. The findings are in close agreement with the Tersoff-T3 and SW potentials reported in previous studies [Miller and Shenoy, 2000, Izumi et al., 2004, Pishkenari and Rezaei, 2017]. For the native oxide model, the calculations show the surface elastic constants of  $d_{11} = d_{22} = -22.1 \pm 1.3$  N/m. The results are summarized in Table 14.2.

#### 14.4.4 Surface Stress Constants

As shown in Table 14.2, for unreconstructed (100) Si surface, compressive in plane stresses of  $f_{11} = f_{22} = -0.88$  N/m are obtained using Tersoff-Munetoh potential while for unreconstructed (110) Si, the surface stresses of  $f_{11} = -1.57$  N/m and  $f_{22} = -0.95$  N/m are computed. The calculated surface stresses of unreconstructed Si surfaces

are in close agreement with the values obtained using the Tersoff-T3 by authors in [Izumi et al., 2004]. For aSiO<sub>2</sub> structure, the averaged values for the surface stress were estimated as  $f_{11} = +1.11 \pm 0.10$  N/m and  $f_{22} = +0.91 \pm 0.09$  N/m while the results are averaged over 20 repetitions of calculations on native oxide surfaces.

The decrease in modulus of elasticity for aSiO<sub>2</sub>-Si NWs exhibit the crucial impact of native oxide in understanding of the elastic properties of Si NWs where the role of free surfaces combined with the presence of the amorphous oxide layer around the Si crystal. The predicted surface stress and surface elastic constants in this study reveals the need for detailed investigations on the surface effect in the mechanical behavior of Si NWs. Differences observed in calculated constants for unreconstructed Si and aSiO<sub>2</sub> surfaces suggest the importance of correct selection of such parameters for potential usage in other studies.

### **14.5 Conclusion**

The modulus of elasticity due to the presence of native oxide for Si NWs is calculated using MD simulations. Results are compared with the effective modulus of elasticity estimated through a core-shell model. Lack of reliability of the core-shell model, as an analytical calculation, is demonstrated, where the surface parameters necessitate to be implemented into analytical models. Those surface parameters including the surface energy, surface elasticity and surface stress have been calculated for Si and aSiO<sub>2</sub> surfaces. This work provides a guideline for the analysis of the size and orientation-dependent mechanical properties of Si NWs.

## Chapter 15

## CONCLUSION AND REMARKS

This thesis explores the multifaceted fundamentals of silicon nanowire (Si NW) mechanical behavior through fabrication, characterization, and modeling efforts. Key contributions include:

**Fabrication and Characterization:** Si NWs obtained through top-down fabrication are tested *in-situ* in a three-point bending configuration, providing well-defined boundary conditions and ample space for accommodating bending deflections during testing. Additionally, new fabrication methodology of Si NWs and a small-scale testing MEMS platform are presented within the context of this thesis.

**Modeling:** Newly developed multiscale models that incorporate surface effects through different formulations, combining molecular dynamics (MD) simulations and continuum mechanics are presented. The interpretation of the scale effect is accomplished through an integrated approach utilizing MD simulations and the modified core-shell model. The role of native oxide on the mechanical properties of Si NWs is discussed in detail, with the formation of residual stresses due to native oxide formation presented through detailed characterization and atomistic modeling.

**Integration of Machine Learning:** Machine learning (ML) techniques, facilitated by extensive MD simulations, broaden the applicability of the methodology established in this research. Through ML analysis, insights into the orientation-dependent elasticity of Si NWs are revealed, alongside a comprehensive examination of surface states. Additionally, MD-based ML findings contribute to the understanding of the size-dependent elastic properties for both top-down and bottom-up fabricated Si NWs.

**Uncertainty Analysis:** A comprehensive analysis of uncertainties arising from the interplay between *processing, structure, and property* in Si NWs is performed,



addressing enduring issues related to the interpretation of the scale effect in Si NWs.

The findings of this thesis include:

**Bridge the Gap Between Computational and Experimental Studies:** Overcoming challenges in both realms, the thesis resolves inconsistencies observed among reported trends concerning the relationship between mechanical behavior and scale in Si NWs.

**Identify Size-Dependent Mechanical Properties:** Through an integrated approach utilizing MD simulations and the modified core-shell model, the research sheds light on the size-dependent mechanical properties of Si NWs, crucial for their prospective integration as fundamental mechanical components.

**Revealing Theoretical Strength Limits:** An insight emerges regarding the theoretical strength limit achieved by Si NWs below 20 nm within the context of this study. Contrary to previous literature reporting strength values ranging from a few MPa to 20 GPa for Si NWs of similar dimensions, this research presents a robust finding that challenges existing state of literature, shedding light on the mechanical behavior of ultra-small Si NWs.

**Linking Modulus of Elasticity to Critical Dimension:** A pivotal insight uncovered in this thesis is the correlation between the evolution of the modulus of elasticity and Si NW critical dimension. By parameterizing surface inhomogeneity, a stiffening trend is quantified with increasing critical dimension. Moreover, experimental trendlines are rigorously validated through independent analytical and machine learning methods, leveraging atomistic simulations for enhanced accuracy and reliability.

**Enable Practical Applications:** The methodology established in this thesis, integrating theoretical modeling, multi-scale simulations, advanced fabrication, and multi-modal characterization techniques, enables practical applications in the development of highly precise sensor platforms through ultimate miniaturization, aligning with the trend of electronics miniaturization driven by Moore's law.

**Addressing the Effect of Native Oxide:** A thorough investigation into the impact of the native oxide on the mechanical characteristics of Si NWs reveals the

fundamental significance of surface effect at nanoscale regime. Through detailed characterization and atomistic modeling, the formation of residual stresses due to native oxide formation is elucidated, enriching our understanding of the intricate interplay between surface states and mechanical behavior in NWs.

**Enhancing Confidence in Estimations:** Through meticulous error analysis of systematic and random error sources, this thesis achieves confidence levels surpassing 95% for fracture strength and 85% for modulus of elasticity estimations of Si NWs. These enhanced confidence levels strengthen the validity and reliability of the derived mechanical properties, providing a solid foundation for further research and practical applications.

Outlined below are the prospective paths and methodologies to be explored in future research endeavors:

**Exploration of Other Materials:** The methodology established in this study can be extended to explore the mechanical characteristics of other low-dimensional materials such as SiC, ZnO, core-shell and alloy nanowires, as well as 2D materials including MoS<sub>2</sub> and WS<sub>2</sub>. Further investigation into these materials could yield valuable insights into their mechanical behavior and applications.

**Advanced Modeling Techniques:** Future research could focus on refining and expanding the modeling techniques used in this study. This may involve incorporating additional factors or utilizing existing models to provide a more comprehensive understanding of mechanical behavior in nanomaterials.

**Experimental Validation:** Further experimental validation of the findings presented in this thesis could enhance confidence in the results. This may involve conducting additional experiments using different methodologies (vibration or compression testing) or materials to validate the observed trends and behaviors.

**Application in Sensor Technology:** Continued research into the practical applications in sensor technology could focus on developing NEMS based on Si NWs for different types of sensors. This could involve optimizing fabrication techniques and exploring novel sensor designs leveraging the unique properties of Si NWs.

**Other Structural and Future Studies:** Studies tracking the evolution of Si

NWs properties over time or temperature domains could provide insights into their stability and reliability. By monitoring changes in mechanical properties under different environmental conditions, researchers can gain a deeper understanding of the factors influencing NW behavior.

In conclusion, while this thesis has made significant strides in understanding the mechanical behavior of Si NWs, there are numerous opportunities for further exploration and advancement. By addressing these future research directions, scholars can continue to push the boundaries of knowledge in this field and unlock the full potential of nanomaterials in various applications.

## BIBLIOGRAPHY

- [Fem, ] The schematic diagram of the femtotoools testing device is sourced from the provided website. [www.femtotoools.com](http://www.femtotoools.com). Accessed: 2023-07-18.
- [Acuna et al., 2021] Acuna, A., Jimenez, J. M., Deneke, N., Rothenberger, S. M., Libring, S., Solorio, L., Rayz, V. L., Davis, C. S., and Calve, S. (2021). Design and validation of a modular micro-robotic system for the mechanical characterization of soft tissues. *Acta biomaterialia*, 134:466–476.
- [Agrawal et al., 2008] Agrawal, R., Peng, B., Gdoutos, E. E., and Espinosa, H. D. (2008). Elasticity size effects in zno nanowires- a combined experimental-computational approach. *Nano letters*, 8(11):3668–3674.
- [Ahoulou et al., 2021] Ahoulou, S., Perret, E., and Nedelec, J.-M. (2021). Functionalization and characterization of silicon nanowires for sensing applications: A review. *Nanomaterials*, 11(4):999.
- [Akbari-Saatlu et al., 2020] Akbari-Saatlu, M., Procek, M., Mattsson, C., Thungström, G., Nilsson, H.-E., Xiong, W., Xu, B., Li, Y., and Radamson, H. H. (2020). Silicon nanowires for gas sensing: A review. *Nanomaterials*, 10(11):2215.
- [Al-Bayati et al., 1991] Al-Bayati, A. H., Orrman-Rossiter, K. G., Van Den Berg, J., and Armour, D. (1991). Composition and structure of the native si oxide by high depth resolution medium energy ion scattering. *Surface science*, 241(1-2):91–102.
- [Alaca and Karimzadehkhoei, 2023] Alaca, B. E. and Karimzadehkhoei, M. (2023). Piezoresistive nanowire-based electromechanical sensors. In *Reference Module in Biomedical Sciences*. Elsevier.

- [Alan et al., 2006a] Alan, T., Hines, M. A., and Zehnder, A. T. (2006a). Effect of surface morphology on the fracture strength of silicon nanobeams. *Applied Physics Letters*, 89(9):091901.
- [Alan et al., 2006b] Alan, T., Zehnder, A. T., Sengupta, D., and Hines, M. A. (2006b). Methyl monolayers improve the fracture strength and durability of silicon nanobeams. *Applied physics letters*, 89(23):231905.
- [Alerhand et al., 1988] Alerhand, O., Vanderbilt, D., Meade, R. D., and Joannopoulos, J. (1988). Spontaneous formation of stress domains on crystal surfaces. *Physical review letters*, 61(17):1973.
- [Ali et al., 2023] Ali, B., Karimzadehkhoei, M., Esfahani, M. N., Leblebici, Y., and Alaca, B. E. (2023). Stencil lithography for bridging mems and nems. *Micro and Nano Engineering*, 19:100206.
- [Ali et al., 2022] Ali, U. E., Yang, H., Khayrudinov, V., Modi, G., Cheng, Z., Agarwal, R., Lipsanen, H., and Bhaskaran, H. (2022). A universal pick-and-place assembly for nanowires. *Small*, 18(38):2201968.
- [Allain et al., 2012] Allain, P., Bosseboeuf, A., Parrain, F., Maaroufi, S., Coste, P., and Walther, A. (2012). Large range mems motion detection using integrated piezo-resistive silicon nanowire. In *2012 IEEE 25th International Conference on micro electro mechanical systems (MEMS)*, pages 1320–1323. IEEE.
- [Ambhorkar et al., 2018] Ambhorkar, P., Wang, Z., Ko, H., Lee, S., Koo, K.-i., Kim, K., and Cho, D.-i. D. (2018). Nanowire-based biosensors: from growth to applications. *Micromachines*, 9(12):679.
- [Ando and Namazu, 2023] Ando, H. and Namazu, T. (2023). Influence of vacuum annealing on mechanical characteristics of focused ion beam fabricated silicon nanowires. *Journal of Vacuum Science & Technology B*, 41(6).

- [Archer and Kimes, 2008] Archer, K. J. and Kimes, R. V. (2008). Empirical characterization of random forest variable importance measures. *Computational statistics & data analysis*, 52(4):2249–2260.
- [Arjmand et al., 2022] Arjmand, T., Legallais, M., Nguyen, T. T. T., Serre, P., Vallejo-Perez, M., Morisot, F., Salem, B., and Ternon, C. (2022). Functional devices from bottom-up silicon nanowires: A review. *Nanomaterials*, 12(7):1043.
- [Arkan et al., 2011] Arkan, E. F., Sacchetto, D., Yildiz, I., Leblebici, Y., and Alaca, B. E. (2011). Monolithic integration of si nanowires with metallic electrodes: Nems resonator and switch applications. *Journal of Micromechanics and Microengineering*, 21(12):125018.
- [B Spejo et al., 2023] B Spejo, L., Arrieta-Concha, J. L., Puydinger dos Santos, M. V., D Barros, A., Diniz, J. A., and A Minamisawa, R. (2023). In situ electron-beam-induced mechanical loading and fracture of suspended strained silicon nanowires. *Journal of Vacuum Science & Technology B*, 41(2).
- [Bachtold et al., 2022] Bachtold, A., Moser, J., and Dykman, M. (2022). Mesoscopic physics of nanomechanical systems. *Reviews of Modern Physics*, 94(4):045005.
- [Badawy and Bakkers, 2024] Badawy, G. and Bakkers, E. P. (2024). Electronic transport and quantum phenomena in nanowires. *Chemical Reviews*.
- [Barlian et al., 2009] Barlian, A. A., Park, W.-T., Mallon, J. R., Rastegar, A. J., and Pruitt, B. L. (2009). Semiconductor piezoresistance for microsystems. *Proceedings of the IEEE*, 97(3):513–552.
- [Barrios et al., 2023] Barrios, A., Kunka, C., Nogan, J., Hattar, K., and Boyce, B. L. (2023). Automated high-throughput fatigue testing of freestanding thin films. *Small Methods*, page 2201591.

- [Bartók et al., 2018] Bartók, A. P., Kermode, J., Bernstein, N., and Csányi, G. (2018). Machine learning a general-purpose interatomic potential for silicon. *Physical Review X*, 8(4):041048.
- [Bauchau and Craig, 2009] Bauchau, O. A. and Craig, J. I. (2009). Euler-bernoulli beam theory. *Structural analysis*, pages 173–221.
- [Baumer et al., 2004] Baumer, A., Stutzmann, M., Brandt, M., Au, F., and Lee, S. (2004). Paramagnetic defects of silicon nanowires. *Applied physics letters*, 85(6):943–945.
- [Beccari et al., 2022] Beccari, A., Visani, D., Fedorov, S., Bereyhi, M., Boureau, V., Engelsens, N., and Kippenberg, T. (2022). Strained crystalline nanomechanical resonators with quality factors above 10 billion. *Nature Physics*, pages 1–6.
- [Belytschko et al., 2002] Belytschko, T., Xiao, S., Schatz, G., and Ruoff, R. (2002). Atomistic simulations of nanotube fracture. *Physical Review B*, 65(23):235430.
- [Bernal et al., 2014] Bernal, R. A., Filleter, T., Connell, J. G., Sohn, K., Huang, J., Lauhon, L. J., and Espinosa, H. D. (2014). In situ electron microscopy four-point electromechanical characterization of freestanding metallic and semiconducting nanowires. *small*, 10(4):725–733.
- [Bhowmick et al., 2019] Bhowmick, S., Espinosa, H., Jungjohann, K., Pardo, T., and Pierron, O. (2019). Advanced microelectromechanical systems-based nanomechanical testing: beyond stress and strain measurements. *Mrs Bulletin*, 44(6):487–493.
- [Boodhoo et al., 2015] Boodhoo, L., Crudgington, L., Chong, H. M., Tsuchiya, Y., Moktadir, Z., Hasegawa, T., and Mizuta, H. (2015). Fabrication and characterisation of suspended narrow silicon nanowire channels for low-power nano-electromechanical (nem) switch applications. *Microelectronic Engineering*, 145:66–70.

- [Brand et al., 2019] Brand, U., Xu, M., Doering, L., Langfahl-Klabes, J., Behle, H., Bütetisch, S., Ahbe, T., Peiner, E., Völlmeke, S., Frank, T., et al. (2019). Long slender piezo-resistive silicon microprobes for fast measurements of roughness and mechanical properties inside micro-holes with diameters below 100  $\mu\text{m}$ . *Sensors*, 19(6):1410.
- [Bronstrup et al., 2010] Bronstrup, G., Jahr, N., Leiterer, C., Csáki, A., Fritzsche, W., and Christiansen, S. (2010). Optical properties of individual silicon nanowires for photonic devices. *ACS nano*, 4(12):7113–7122.
- [Brugnotto et al., 2024] Brugnotto, E., Aleksandrov, P., Sousa, M., and Georgiev, V. (2024). Machine learning inspired nanowire classification method based on nanowire array scanning electron microscope images. *Open Research Europe*, 4:43.
- [Buehler et al., 2007] Buehler, M. J., Tang, H., Van Duin, A. C., and Goddard III, W. A. (2007). Threshold crack speed controls dynamical fracture of silicon single crystals. *Physical Review Letters*, 99(16):165502.
- [Butler et al., 2018] Butler, K. T., Davies, D. W., Cartwright, H., Isayev, O., and Walsh, A. (2018). Machine learning for molecular and materials science. *Nature*, 559(7715):547–555.
- [Buttard et al., 2011] Buttard, D., Gentile, P., and Renevier, H. (2011). Grazing incidence x-ray diffraction investigation of strains in silicon nanowires obtained by gold catalytic growth. *Surface Science*, 605(5-6):570–576.
- [Cakirlar et al., 2022] Cakirlar, C., Galderisi, G., Beyer, C., Simon, M., Mikolajick, T., and Trommer, J. (2022). Challenges in electron beam lithography of silicon nanostructures. In *2022 IEEE 22nd International Conference on Nanotechnology (NANO)*, pages 207–210. IEEE.



- [Calahorra et al., 2015] Calahorra, Y., Shtempluck, O., Kotchetkov, V., and Yaish, Y. (2015). Young’s modulus, residual stress, and crystal orientation of doubly clamped silicon nanowire beams. *Nano letters*, 15(5):2945–2950.
- [Catal et al., 2024] Catal, A., Bedir, E., Yilmaz, R., Swider, M., Lee, C., El-Atwani, O., Maier, H., Ozdemir, H., and Canadinc, D. (2024). Machine learning assisted design of novel refractory high entropy alloys with enhanced mechanical properties. *Computational Materials Science*, 231:112612.
- [Catal et al., 2022] Catal, A. A., Bedir, E., Yilmaz, R., and Canadinc, D. (2022). Design of a nitihf shape memory alloy with an austenite finish temperature beyond 400 c utilizing artificial intelligence. *Journal of Alloys and Compounds*, 904:164135.
- [Chen et al., 2006a] Chen, C. Q., Shi, Y., Zhang, Y. S., Zhu, J., and Yan, Y. J. (2006a). Size dependence of young’s modulus in zno nanowires. *Physical review letters*, 96(7):075505.
- [Chen et al., 2010] Chen, J., Conache, G., Pistol, M.-E., Gray, S. M., Borgstrom, M. T., Xu, H., Xu, H., Samuelson, L., and Håkanson, U. (2010). Probing strain in bent semiconductor nanowires with raman spectroscopy. *Nano letters*, 10(4):1280–1286.
- [Chen and MacDonald, 2004] Chen, J. and MacDonald, N. (2004). Measuring the nonlinearity of silicon piezoresistance by tensile loading of a submicron diameter fiber using a microinstrument. *Review of scientific instruments*, 75(1):276–278.
- [Chen et al., 2018] Chen, J., Shi, J., Wang, Y., Sun, J., Han, J., Sun, K., and Fang, L. (2018). Nanoindentation and deformation behaviors of silicon covered with amorphous sio 2: a molecular dynamic study. *RSC advances*, 8(23):12597–12607.
- [Chen et al., 2024] Chen, L., Zhang, S., Duan, Y., Song, X., Chang, M., Feng, W., and Chen, Y. (2024). Silicon-containing nanomedicine and biomaterials: mate-

rials chemistry, multi-dimensional design, and biomedical application. *Chemical Society Reviews*.

[Chen et al., 2006b] Chen, T., Chiu, M.-S., and Weng, C.-N. (2006b). Derivation of the generalized young-laplace equation of curved interfaces in nanoscaled solids. *Journal of Applied Physics*, 100(7):074308.

[Chen et al., 2017] Chen, Y., An, X., and Liao, X. (2017). Mechanical behaviors of nanowires. *Applied Physics Reviews*, 4(3):031104.

[Cheng et al., 2015] Cheng, G., Miao, C., Qin, Q., Li, J., Xu, F., Haftbaradaran, H., Dickey, E. C., Gao, H., and Zhu, Y. (2015). Large anelasticity and associated energy dissipation in single-crystalline nanowires. *Nature nanotechnology*, 10(8):687–691.

[Cheng et al., 2019] Cheng, G., Zhang, Y., Chang, T.-H., Liu, Q., Chen, L., Lu, W. D., Zhu, T., and Zhu, Y. (2019). In situ nano-thermomechanical experiment reveals brittle to ductile transition in silicon nanowires. *Nano Letters*, 19(8):5327–5334.

[Chhapadia et al., 2011] Chhapadia, P., Mohammadi, P., and Sharma, P. (2011). Curvature-dependent surface energy and implications for nanostructures. *Journal of the Mechanics and Physics of Solids*, 59(10):2103–2115.

[Chiu and Chen, 2011] Chiu, M.-S. and Chen, T. (2011). Effects of high-order surface stress on static bending behavior of nanowires. *Physica E: Low-dimensional Systems and Nanostructures*, 44(3):714–718.

[Cook, 2006] Cook, R. (2006). Strength and sharp contact fracture of silicon. *Journal of Materials Science*, 41:841–872.

[Cormier et al., 2001] Cormier, J., Rickman, J., and Delph, T. (2001). Stress calculation in atomistic simulations of perfect and imperfect solids. *Journal of Applied Physics*, 89(1):99–104.

- [Cui et al., 2023] Cui, J., Sun, Y., Chen, H., Yang, Y., Chen, G., Ke, P., Nishimura, K., Yang, Y., Tang, C., and Jiang, N. (2023). Atomic insights of self-healing in silicon nanowires. *Advanced Functional Materials*, 33(6):2210053.
- [Cui et al., 2003] Cui, Y., Zhong, Z., Wang, D., Wang, W. U., and Lieber, C. M. (2003). High performance silicon nanowire field effect transistors. *Nano letters*, 3(2):149–152.
- [Cullinan et al., 2012] Cullinan, M. A., Panas, R. M., DiBiasio, C. M., and Culpepper, M. L. (2012). Scaling electromechanical sensors down to the nanoscale. *Sensors and Actuators A: Physical*, 187:162–173.
- [Curtarolo et al., 2013] Curtarolo, S., Hart, G. L., Nardelli, M. B., Mingo, N., Sanvito, S., and Levy, O. (2013). The high-throughput highway to computational materials design. *Nature materials*, 12(3):191–201.
- [Dasgupta et al., 2014] Dasgupta, N. P., Sun, J., Liu, C., Brittman, S., Andrews, S. C., Lim, J., Gao, H., Yan, R., and Yang, P. (2014). 25th anniversary article: semiconductor nanowires—synthesis, characterization, and applications. *Advanced materials*, 26(14):2137–2184.
- [Dávila et al., 2009] Dávila, L. P., Leppert, V. J., and Bringa, E. M. (2009). The mechanical behavior and nanostructure of silica nanowires via simulations. *Scripta Materialia*, 60(10):843–846.
- [De Marchi et al., 2014] De Marchi, M., Zhang, J., Frache, S., Sacchetto, D., Gailardon, P.-E., Leblebici, Y., and De Micheli, G. (2014). Configurable logic gates using polarity-controlled silicon nanowire gate-all-around fets. *IEEE Electron Device Letters*, 35(8):880–882.
- [De Wolf, 1996] De Wolf, I. (1996). Micro-raman spectroscopy to study local mechanical stress in silicon integrated circuits. *Semiconductor science and technology*, 11(2):139.

- [Deal and Grove, 1965] Deal, B. E. and Grove, A. (1965). General relationship for the thermal oxidation of silicon. *Journal of applied physics*, 36(12):3770–3778.
- [del Moral et al., 2021] del Moral, A., Amat, E., Bausells, J., and Perez-Murano, F. (2021). Benefits of using arrays of vertical nanowire fets in integrated circuits to mitigate variability. *Semiconductor Science and Technology*, 36(12):125017.
- [Delph, 2008] Delph, T. (2008). Near-surface stresses in silicon (0 0 1). *Surface science*, 602(1):259–267.
- [DelRio et al., 2015] DelRio, F. W., Cook, R. F., and Boyce, B. L. (2015). Fracture strength of micro-and nano-scale silicon components. *Applied Physics Reviews*, 2(2):021303.
- [DelRio et al., 2022] DelRio, F. W., Grutzik, S. J., Mook, W. M., Dickens, S. M., Kotula, P. G., Hintsala, E. D., Stauffer, D. D., and Boyce, B. L. (2022). Eliciting stable nanoscale fracture in single-crystal silicon. *Materials Research Letters*, 10(11):728–735.
- [DelRio et al., 2016] DelRio, F. W., White, R. M., Krylyuk, S., Davydov, A. V., Friedman, L. H., and Cook, R. F. (2016). Near-theoretical fracture strengths in native and oxidized silicon nanowires. *Nanotechnology*, 27(31):31LT02.
- [Deringer et al., 2021] Deringer, V. L., Bartók, A. P., Bernstein, N., Wilkins, D. M., Ceriotti, M., and Csányi, G. (2021). Gaussian process regression for materials and molecules. *Chemical Reviews*, 121(16):10073–10141.
- [Deringer et al., 2018] Deringer, V. L., Bernstein, N., Bartók, A. P., Cliffe, M. J., Kerber, R. N., Marbella, L. E., Grey, C. P., Elliott, S. R., and Csányi, G. (2018). Realistic atomistic structure of amorphous silicon from machine-learning-driven molecular dynamics. *The journal of physical chemistry letters*, 9(11):2879–2885.

- [Deringer et al., 2019] Deringer, V. L., Caro, M. A., and Csányi, G. (2019). Machine learning interatomic potentials as emerging tools for materials science. *Advanced Materials*, 31(46):1902765.
- [Diao et al., 2004] Diao, J., Gall, K., and Dunn, M. L. (2004). Atomistic simulation of the structure and elastic properties of gold nanowires. *Journal of the Mechanics and Physics of Solids*, 52(9):1935–1962.
- [Dickel et al., 2021] Dickel, D., Nitol, M., and Barrett, C. (2021). Lammmps implementation of rapid artificial neural network derived interatomic potentials. *Computational Materials Science*, 196:110481.
- [Dolabella et al., 2020] Dolabella, S., Frison, R., Chahine, G. A., Richter, C., Schulli, T. U., Tasdemir, Z., Alaca, B. E., Leblebici, Y., Dommann, A., and Neels, A. (2020). Real-and q-space travelling: multi-dimensional distribution maps of crystal-lattice strain ( $\epsilon_{044}$ ) and tilt of suspended monolithic silicon nanowire structures. *Journal of applied crystallography*, 53(1):58–68.
- [Dupre et al., 2012] Dupre, L., Buttard, D., Leclere, C., Renevier, H., and Gentile, P. (2012). Gold contamination in vls-grown si nanowires: multiwavelength anomalous diffraction investigations. *Chemistry of Materials*, 24(23):4511–4516.
- [Ekinci and Roukes, 2005] Ekinci, K. and Roukes, M. (2005). Nanoelectromechanical systems. *Review of scientific instruments*, 76(6):061101.
- [El Nabi et al., 2015] El Nabi, F. A., Godet, J., Brochard, S., and Pizzagalli, L. (2015). Onset of ductility and brittleness in silicon nanowires mediated by dislocation nucleation. *Modelling and Simulation in Materials Science and Engineering*, 23(2):025010.
- [Elhebeary et al., 2020] Elhebeary, M., Harzer, T., Dehm, G., and A. Saif, M. T. (2020). Time-dependent plasticity in silicon microbeams mediated by dislocation

- nucleation. *Proceedings of the National Academy of Sciences*, 117(29):16864–16871.
- [Elhebeary and Saif, 2017a] Elhebeary, M. and Saif, M. (2017a). Design, simulation, and testing of a novel bending stage for mechanical characterization of materials. *Experimental Mechanics*, 57:89–96.
- [Elhebeary and Saif, 2017b] Elhebeary, M. and Saif, M. T. A. (2017b). Lessons learned from nanoscale specimens tested by mems-based apparatus. *Journal of Physics D: Applied Physics*, 50(24):243001.
- [Elhebeary and Saif, 2017c] Elhebeary, M. and Saif, M. T. A. (2017c). Thermo-mechanical characterization of materials at micro/nanoscale under bending. In *2017 IEEE 30th International Conference on Micro Electro Mechanical Systems (MEMS)*, pages 736–739. IEEE.
- [Elhebeary and Saif, 2018] Elhebeary, M. and Saif, M. T. A. (2018). A novel mems stage for in-situ thermomechanical testing of single crystal silicon microbeams under bending. *Extreme Mechanics Letters*, 23:1–8.
- [Emon et al., 2021] Emon, B., Li, Z., Joy, M. S. H., Doha, U., Kosari, F., and Saif, M. T. A. (2021). A novel method for sensor-based quantification of single/multicellular force dynamics and stiffening in 3d matrices. *Science Advances*, 7(15):eabf2629.
- [Erhard et al., 2023] Erhard, L. C., Rohrer, J., Albe, K., and Deringer, V. L. (2023). Modelling atomic and nanoscale structure in the silicon-oxygen system through active machine learning. *arXiv preprint arXiv:2309.03587*.
- [Esfahani, 2022] Esfahani, M. N. (2022). Comparing empirical interatomic potentials to modeling silicon surface stress. *Solid State Communications*, 344:114656.

- [Esfahani and Alaca, 2018] Esfahani, M. N. and Alaca, B. E. (2018). Surface Stress Effect on Silicon Nanowire Mechanical Behavior: Size and Orientation Dependence. *Mechanics of Materials*, 127:112–123.
- [Esfahani et al., 2018] Esfahani, M. N., Kilinc, Y., Karakan, M. Ç., Orhan, E., Hanay, M. S., Leblebici, Y., and Alaca, B. E. (2018). Piezoresistive silicon nanowire resonators as embedded building blocks in thick soi. *Journal of Micromechanics and Microengineering*, 28(4):045006.
- [Esfahani et al., 2017a] Esfahani, M. N., Leblebici, Y., and Alaca, B. E. (2017a). A monolithic approach to downscaling silicon piezoresistive sensors. *Journal of Microelectromechanical Systems*, 26(3):624–631.
- [Esfahani et al., 2017b] Esfahani, M. N., Yilmaz, M., Wollschläger, N., Rangelow, I. W., Leblebici, Y., and Alaca, B. E. (2017b). Monolithic technology for silicon nanowires in high-topography architectures. *Microelectronic Engineering*, 183:42–47.
- [Espinosa et al., 2013] Espinosa, H. D., Bernal, R. A., and Filleter, T. (2013). In-situ tem electromechanical testing of nanowires and nanotubes. *Nano and Cell Mechanics: Fundamentals and Frontiers*, pages 191–226.
- [Espinosa et al., 2012] Espinosa, H. D., Bernal, R. A., and Minary-Jolandan, M. (2012). A review of mechanical and electromechanical properties of piezoelectric nanowires. *Advanced Materials*, 24(34):4656–4675.
- [Fain et al., 2018] Fain, B., Souchon, F., Berthelot, A., Anciant, R., Robert, P., and Jourdan, G. (2018). Dynamic control of an accelerometer bandwidth through tunable damping factor and effective moment of inertia. In *2018 IEEE Micro Electro Mechanical Systems (MEMS)*, pages 948–951. IEEE.
- [Fan et al., 2017] Fan, D., Sigg, H., Spolenak, R., and Ekinici, Y. (2017). Strain and

thermal conductivity in ultrathin suspended silicon nanowires. *Physical Review B*, 96(11):115307.

[Fedorov et al., 2019] Fedorov, S. A., Engelsen, N. J., Ghadimi, A. H., Bereyhi, M. J., Schilling, R., Wilson, D. J., and Kippenberg, T. J. (2019). Generalized dissipation dilution in strained mechanical resonators. *Physical Review B*, 99(5):054107.

[Fiorillo et al., 2018] Fiorillo, A., Critello, C., and Pullano, S. (2018). Theory, technology and applications of piezoresistive sensors: A review. *Sensors and Actuators A: Physical*, 281:156–175.

[Fleetwood, 2023] Fleetwood, D. M. (2023). Low-frequency noise in nanowires. *Nanoscale*, 15(29):12175–12192.

[Fujii et al., 2013] Fujii, T., Namazu, T., Sudoh, K., Sakakihara, S., and Inoue, S. (2013). Focused ion beam induced surface damage effect on the mechanical properties of silicon nanowires. *Journal of engineering materials and technology*, 135(4).

[Fukata and Jevasuwan, 2024] Fukata, N. and Jevasuwan, W. (2024). Formation and characterization of group iv semiconductor nanowires. *Nanotechnology*, 35(12):122001.

[Fukata et al., 2017] Fukata, N., Subramani, T., Jevasuwan, W., Dutta, M., and Bando, Y. (2017). Functionalization of silicon nanostructures for energy-related applications. *Small*, 13(45):1701713.

[Furmanchuk et al., 2012] Furmanchuk, A., Isayev, O., Dinadayalane, T. C., Leszczynska, D., and Leszczynski, J. (2012). Mechanical properties of silicon nanowires. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, 2(6):817–828.



- [Gadea et al., 2018] Gadea, G., Pacios, M., Morata, Á., and Tarancón, A. (2018). Silicon-based nanostructures for integrated thermoelectric generators. *Journal of Physics D: Applied Physics*, 51(42):423001.
- [Gadola et al., 2021] Gadola, M., Buffoli, A., Sansa, M., Berthelot, A., Robert, P., and Langfelder, G. (2021). 1.3 mm 2 nav-grade nems-based gyroscope. *Journal of Microelectromechanical Systems*, 30(4):513–520.
- [Ganster et al., 2010] Ganster, P., Treglia, G., and Saul, A. (2010). Atomistic modeling of strain and diffusion at the si/sio<sub>2</sub> interface. *Physical Review B*, 81(4):045315.
- [Gao et al., 2022] Gao, S., Hong, S., Park, S., Jung, H. Y., Liang, W., Lee, Y., Ahn, C. W., Byun, J. Y., Seo, J., Hahm, M. G., et al. (2022). Catalyst-free synthesis of sub-5 nm silicon nanowire arrays with massive lattice contraction and wide bandgap. *Nature communications*, 13(1):3467.
- [Geiger et al., 2015] Geiger, R., Zabel, T., and Sigg, H. (2015). Group iv direct band gap photonics: methods, challenges, and opportunities. *Frontiers in Materials*, 2:52.
- [Gerberich et al., 2017] Gerberich, W., Tadmor, E. B., Kysar, J., Zimmerman, J. A., Minor, A. M., Szlufarska, I., Amodeo, J., Devincre, B., Hintsala, E., and Ballarini, R. (2017). Case studies in future trends of computational and experimental nanomechanics. *Journal of Vacuum Science & Technology A*, 35(6).
- [Ghosh, 2023] Ghosh, R. (2023). Recent progress in piezotronic sensors based on one-dimensional zinc oxide nanostructures and its regularly ordered arrays: From design to application. *Nano Energy*, 113:108606.
- [Godet et al., 2015] Godet, J., El Nabi, F. A., Brochard, S., and Pizzagalli, L. (2015). Surface effects on the mechanical behavior of silicon nanowires: Con-

sequence on the brittle to ductile transition at low scale and low temperature. *physica status solidi (a)*, 212(8):1643–1648.

[Godet et al., 2009] Godet, J., Hirel, P., Brochard, S., and Pizzagalli, L. (2009). Evidence of two plastic regimes controlled by dislocation nucleation in silicon nanostructures. *Journal of Applied Physics*, 105(2).

[Goktas et al., 2018] Goktas, N. I., Wilson, P., Ghukasyan, A., Wagner, D., McNamee, S., and LaPierre, R. (2018). Nanowires for energy: A review. *Applied Physics Reviews*, 5(4):041305.

[Gordon et al., 2009] Gordon, M. J., Baron, T., Dhalluin, F., Gentile, P., and Ferret, P. (2009). Size effects in mechanical deformation and fracture of cantilevered silicon nanowires. *Nano letters*, 9(2):525–529.

[Gu et al., 2023] Gu, J., Shen, Y., Tian, S., Xue, Z., and Meng, X. (2023). Recent advances in nanowire-based wearable physical sensors. *Biosensors*, 13(12):1025.

[Guénolé et al., 2011] Guénolé, J., Godet, J., and Brochard, S. (2011). Deformation of silicon nanowires studied by molecular dynamics simulations. *Modelling and Simulation in Materials Science and Engineering*, 19(7):074003.

[Guerfi and Larrieu, 2016] Guerfi, Y. and Larrieu, G. (2016). Vertical silicon nanowire field effect transistors with nanoscale gate-all-around. *Nanoscale research letters*, 11(1):1–7.

[Guo et al., 2011] Guo, H., Chen, K., Oh, Y., Wang, K., Dejoie, C., Syed Asif, S., Warren, O., Shan, Z., Wu, J., and Minor, A. (2011). Mechanics and dynamics of the strain-induced m1–m2 structural phase transition in individual vo2 nanowires. *Nano letters*, 11(8):3207–3213.

[Gurtin and Ian Murdoch, 1975] Gurtin, M. E. and Ian Murdoch, A. (1975). A continuum theory of elastic material surfaces. *Archive for rational mechanics and analysis*, 57(4):291–323.

- [Han et al., 2020] Han, T., Stone-Weiss, N., Huang, J., Goel, A., and Kumar, A. (2020). Machine learning as a tool to design glasses with controlled dissolution for healthcare applications. *Acta biomaterialia*, 107:286–298.
- [Han et al., 2007] Han, X., Zheng, K., Zhang, Y., Zhang, X., Zhang, Z., and Wang, Z. L. (2007). Low-temperature in situ large-strain plasticity of silicon nanowires. *Advanced Materials*, 19(16):2112–2118.
- [Han et al., 2013] Han, X.-L., Larrieu, G., and Krzeminski, C. (2013). Modelling and engineering of stress based controlled oxidation effects for silicon nanostructure patterning. *Nanotechnology*, 24(49):495301.
- [Han et al., 2023] Han, Y., Wang, L., Cao, K., Zhou, J., Zhu, Y., Hou, Y., and Lu, Y. (2023). In situ tem characterization and modulation for phase engineering of nanomaterials. *Chemical Reviews*, 123(24):14119–14184.
- [Harris et al., 2004] Harris, S. J., O’neill, A. E., Yang, W., Gustafson, P., Boileau, J., Weber, W., Majumdar, B., and Ghosh, S. (2004). Measurement of the state of stress in silicon with micro-raman spectroscopy. *Journal of Applied Physics*, 96(12):7195–7201.
- [Hashemi et al., 2009] Hashemi, P., Gomez, L., and Hoyt, J. L. (2009). Gate-all-around n-mosfets with uniaxial tensile strain-induced performance enhancement scalable to sub-10-nm nanowire diameter. *IEEE electron device letters*, 30(4):401–403.
- [He and Lilley, 2008] He, J. and Lilley, C. M. (2008). Surface effect on the elastic behavior of static bending nanowires. *Nano letters*, 8(7):1798–1802.
- [He et al., 2005] He, R., Gao, D., Fan, R., Hochbaum, A. I., Carraro, C., Maboudian, R., and Yang, P. (2005). Si nanowire bridges in microtrenches: Integration of growth into device fabrication. *Advanced Materials*, 17(17):2098–2102.

- [He and Galli, 2012] He, Y. and Galli, G. (2012). Microscopic origin of the reduced thermal conductivity of silicon nanowires. *Physical review letters*, 108(21):215901.
- [Heidelberg et al., 2006] Heidelberg, A., Ngo, L. T., Wu, B., Phillips, M. A., Sharma, S., Kamins, T. I., Sader, J. E., and Boland, J. J. (2006). A generalized description of the elastic properties of nanowires. *Nano letters*, 6(6):1101–1106.
- [Hielscher and Schaeben, 2008] Hielscher, R. and Schaeben, H. (2008). A novel pole figure inversion method: specification of the mtex algorithm. *Journal of Applied Crystallography*, 41(6):1024–1037.
- [Hoffmann et al., 2006] Hoffmann, S., Utke, I., Moser, B., Michler, J., Christiansen, S. H., Schmidt, V., Senz, S., Werner, P., Gösele, U., and Ballif, C. (2006). Measurement of the bending strength of vapor- liquid- solid grown silicon nanowires. *Nano letters*, 6(4):622–625.
- [Hofmann et al., 2020] Hofmann, M., Weidenfeller, L., Supreeti, S., Mechold, S., Holz, M., Reuter, C., Sinzinger, S., Manske, E., and Rangelow, I. W. (2020). Mix-and-match lithography and cryogenic etching for nil template fabrication. *Microelectronic Engineering*, 224:111234.
- [Hsin et al., 2008] Hsin, C.-L., Mai, W., Gu, Y., Gao, Y., Huang, C.-T., Liu, Y., Chen, L.-J., and Wang, Z.-L. (2008). Elastic properties and buckling of silicon nanowires. *Advanced Materials*, 20(20):3919–3923.
- [Hsu et al., 2023] Hsu, C.-Y., Rheima, A. M., sabri Abbas, Z., Faryad, M. U., Kadhim, M. M., Altimari, U. S., Dawood, A. H., Abed, Z. T., Radhi, R. S., Jaber, A. S., et al. (2023). Nanowires properties and applications: a review study. *South African Journal of Chemical Engineering*.
- [Huang et al., 2023] Huang, J., Zhang, Y., Fan, A., Li, Y., Wang, H., Ma, W., and Zhang, X. (2023). Remarkable thermal conductivity reduction of silicon nanowires during the bending process. *ACS Applied Materials & Interfaces*.

- [Huang et al., 2011] Huang, P.-H., Fang, T.-H., and Chou, C.-S. (2011). The coupled effects of size, shape, and location of vacancy clusters on the structural deformation and mechanical strength of defective nanowires. *Current Applied Physics*, 11(3):878–887.
- [Huang et al., 2009] Huang, S., Zhang, S., Belytschko, T., Terdalkar, S. S., and Zhu, T. (2009). Mechanics of nanocrack: fracture, dislocation emission, and amorphization. *Journal of the Mechanics and Physics of Solids*, 57(5):840–850.
- [Hudson et al., 2013] Hudson, S. D., Zhurov, V., Grbić, V., Grbić, M., and Hutter, J. L. (2013). Measurement of the elastic modulus of spider mite silk fibers using atomic force microscopy. *Journal of Applied Physics*, 113(15):154307.
- [Hung and Hong, 2009] Hung, P. and Hong, N. (2009). Simulation study of polymorphism and diffusion anomaly for  $\text{SiO}_2$  and  $\text{GeO}_2$  liquid. *The European Physical Journal B*, 71(1):105–110.
- [Hwang et al., 2023] Hwang, S., Lee, W., Carr, W. N., and Yoon, Y.-K. (2023). Metal assisted chemical etching toward scallop-free sidewall through silicon vias: A review. *IEEE Transactions on Components, Packaging and Manufacturing Technology*.
- [Iakab et al., 2019] Iakab, S. A., Rafols, P., García-Altares, M., Yanes, O., and Correig, X. (2019). Silicon-based laser desorption ionization mass spectrometry for the analysis of biomolecules: a progress report. *Advanced Functional Materials*, 29(45):1903609.
- [Ilinov and Kuronen, 2014] Ilinov, A. and Kuronen, A. (2014). Atomistic modeling of bending properties of oxidized silicon nanowires. *Journal of Applied Physics*, 115(10):104305.
- [Inc., 2022] Inc., T. M. (2022). Matlab version: 9.13.0 (r2022b).

- [Izumi et al., 2004] Izumi, S., Hara, S., Kumagai, T., and Sakai, S. (2004). A method for calculating surface stress and surface elastic constants by molecular dynamics: application to the surface of crystal and amorphous silicon. *Thin Solid Films*, 467(1-2):253–260.
- [Jain et al., 2013] Jain, A., Ong, S. P., Hautier, G., Chen, W., Richards, W. D., Dacek, S., Cholia, S., Gunter, D., Skinner, D., Ceder, G., et al. (2013). Commentary: The materials project: A materials genome approach to accelerating materials innovation. *APL materials*, 1(1).
- [Jarzabek et al., 2014] Jarzabek, D., Kaufmann, A., Schiff, H., Rymuza, Z., and Jung, T. (2014). Elastic modulus and fracture strength evaluation on the nanoscale by scanning force microscope experiments. *Nanotechnology*, 25(21):215701.
- [Jayaram, 2022] Jayaram, V. (2022). Small-scale mechanical testing. *Annual Review of Materials Research*, 52:473–523.
- [Jeng et al., 2005] Jeng, Y.-R., Tsai, P.-C., and Fang, T.-H. (2005). Effects of temperature, strain rate, and vacancies on tensile and fatigue behaviors of silicon-based nanotubes. *Physical Review B*, 71(8):085411.
- [Jia et al., 2019] Jia, C., Lin, Z., Huang, Y., and Duan, X. (2019). Nanowire electronics: from nanoscale to macroscale. *Chemical reviews*, 119(15):9074–9135.
- [Jin et al., 2023] Jin, H., Zhang, E., and Espinosa, H. D. (2023). Recent advances and applications of machine learning in experimental solid mechanics: A review. *arXiv preprint arXiv:2303.07647*.
- [Jing and Meng, 2010a] Jing, Y. and Meng, Q. (2010a). Molecular dynamics simulations of the mechanical properties of crystalline/amorphous silicon core/shell nanowires. *Physica B: Condensed Matter*, 405(10):2413–2417.

- [Jing and Meng, 2010b] Jing, Y. and Meng, Q. (2010b). Molecular dynamics simulations of the mechanical properties of crystalline/amorphous silicon core/shell nanowires. *Physica B: Condensed Matter*, 405(10):2413–2417.
- [Jing et al., 2009a] Jing, Y., Meng, Q., and Gao, Y. (2009a). Molecular dynamics simulation on the buckling behavior of silicon nanowires under uniaxial compression. *Computational Materials Science*, 45(2):321–326.
- [Jing et al., 2009b] Jing, Y., Meng, Q., and Zhao, W. (2009b). Molecular dynamics simulations of the tensile and melting behaviours of silicon nanowires. *Physica E: Low-dimensional Systems and Nanostructures*, 41(4):685–689.
- [Johansson et al., 1988] Johansson, S., Schweitz, J.-Å., Tenerz, L., and Tirén, J. (1988). Fracture testing of silicon microelements insitu in a scanning electron microscope. *Journal of applied physics*, 63(10):4799–4803.
- [Johnson et al., 1999] Johnson, G. C., Jones, P. T., and Howe, R. T. (1999). Materials characterization for mems: a comparison of uniaxial and bending tests. In *Micromachining and Microfabrication Process Technology V*, volume 3874, pages 94–101. SPIE.
- [Jung and Shin, 2017] Jung, H.-E. and Shin, M. (2017). Effects of si/sio<sub>2</sub> interface stress on the performance of ultra-thin-body field effect transistors: a first-principles study. *Nanotechnology*, 29(2):025201.
- [Justo et al., 2007] Justo, J. F., Menezes, R. D., and Assali, L. V. C. (2007). Stability and plasticity of silicon nanowires: The role of wire perimeter. *Physical Review B*, 75(4):045303.
- [Kaestner and Rangelow, 2020] Kaestner, M. and Rangelow, I. W. (2020). Scanning probe lithography on calixarene towards single-digit nanometer fabrication. *International Journal of Extreme Manufacturing*, 2(3):032005.

- [Kakiuchi et al., 2007] Kakiuchi, H., Ohmi, H., Harada, M., Watanabe, H., and Yasutake, K. (2007). Highly efficient oxidation of silicon at low temperatures using atmospheric pressure plasma. *Applied Physics Letters*, 90(9):091909.
- [Kang and Cai, 2007] Kang, K. and Cai, W. (2007). Brittle and ductile fracture of semiconductor nanowires—molecular dynamics simulations. *Philosophical Magazine*, 87(14-15):2169–2189.
- [Kang and Cai, 2010] Kang, K. and Cai, W. (2010). Size and temperature effects on the fracture mechanisms of silicon nanowires: Molecular dynamics simulations. *International Journal of Plasticity*, 26(9):1387–1401.
- [Karimzadehkhoei et al., 2023] Karimzadehkhoei, M., Ali, B., Jedari Ghourichaei, M., and Alaca, B. E. (2023). Silicon nanowires driving miniaturization of microelectromechanical systems physical sensors: A review. *Advanced Engineering Materials*, 25(12):2300007.
- [Katakam and Yedla, 2022] Katakam, K. C. and Yedla, N. (2022). Tensile and creep behavior of nickel nanowires containing volume defects: Insight into the deformation mechanisms and microstructural evolution using molecular dynamics simulations. *Materials Chemistry and Physics*, 277:125560.
- [Kawamoto et al., 2013] Kawamoto, N., Tang, D.-M., Wei, X., Wang, X., Mitome, M., Bando, Y., and Golberg, D. (2013). Transmission electron microscope as an ultimate tool for nanomaterial property studies. *Microscopy*, 62(1):157–175.
- [Khalilov et al., 2017] Khalilov, U., Bogaerts, A., and Neyts, E. C. (2017). Toward the understanding of selective si nano-oxidation by atomic scale simulations. *Accounts of Chemical Research*, 50(4):796–804.
- [Khalilov et al., 2011] Khalilov, U., Neyts, E., Pourtois, G., and Van Duin, A. C. (2011). Can we control the thickness of ultrathin silica layers by hyperthermal



- silicon oxidation at room temperature? *The Journal of Physical Chemistry C*, 115(50):24839–24848.
- [Khalilov et al., 2013a] Khalilov, U., Pourtois, G., Bogaerts, A., Van Duin, A. C., and Neyts, E. C. (2013a). Reactive molecular dynamics simulations on sio 2-coated ultra-small si-nanowires. *Nanoscale*, 5(2):719–725.
- [Khalilov et al., 2013b] Khalilov, U., Pourtois, G., Huygh, S., Van Duin, A., Neyts, E., and Bogaerts, A. (2013b). New mechanism for oxidation of native silicon oxide. *The Journal of Physical Chemistry C*, 117(19):9819–9825.
- [Khalilov et al., 2012a] Khalilov, U., Pourtois, G., Van Duin, A., and Neyts, E. (2012a). Hyperthermal oxidation of si (100)  $2 \times 1$  surfaces: effect of growth temperature. *The Journal of Physical Chemistry C*, 116(15):8649–8656.
- [Khalilov et al., 2012b] Khalilov, U., Pourtois, G., Van Duin, A., and Neyts, E. (2012b). On the c-si— a-sio<sub>2</sub> interface in hyperthermal si oxidation at room temperature. *The Journal of Physical Chemistry C*, 116(41):21856–21863.
- [Kilinc et al., 2020] Kilinc, Y., Karakan, M. Ç., Leblebici, Y., Hanay, M. S., and Alaca, B. E. (2020). Observation of coupled mechanical resonance modes within suspended 3d nanowire arrays. *Nanoscale*, 12(43):22042–22048.
- [Kim et al., 2006] Kim, J., Park, S., Park, J., and Lee, J. (2006). Molecular dynamics simulation of elastic properties of silicon nanocantilevers. *Nanoscale and Microscale Thermophysical Engineering*, 10(1):55–65.
- [Kim et al., 2019] Kim, T., Jang, S., Chang, B., Sung, J., Lee, S., Ko, H., Koo, K.-i., and Dong-il, D. C. (2019). A new simple fabrication method for silicon nanowire-based accelerometers. In *2019 20th International Conference on Solid-State Sensors, Actuators and Microsystems & Eurosensors XXXIII (TRANSDUCERS & EUROSENSORS XXXIII)*, pages 1949–1952. IEEE.

- [Kim et al., 2011] Kim, Y.-J., Son, K., Choi, I.-C., Choi, I.-S., Park, W. I., and Jang, J.-i. (2011). Exploring nanomechanical behavior of silicon nanowires: Afn bending versus nanoindentation. *Advanced Functional Materials*, 21(2):279–286.
- [Kizuka et al., 2005] Kizuka, T., Takatani, Y., Asaka, K., and Yoshizaki, R. (2005). Measurements of the atomistic mechanics of single crystalline silicon wires of nanometer width. *Physical Review B*, 72(3):035333.
- [Kon et al., 2007] Kon, S., Oldham, K., and Horowitz, R. (2007). Piezoresistive and piezoelectric mems strain sensors for vibration detection. In *Sensors and Smart Structures Technologies for Civil, Mechanical, and Aerospace Systems 2007*, volume 6529, pages 898–908. SPIE.
- [Kulik et al., 2022] Kulik, H. J., Hammerschmidt, T., Schmidt, J., Botti, S., Marques, M. A., Boley, M., Scheffler, M., Todorović, M., Rinke, P., Oses, C., et al. (2022). Roadmap on machine learning in electronic structure. *Electronic Structure*, 4(2):023004.
- [Kuo et al., 2014] Kuo, J.-K., Huang, P.-H., Wu, W.-T., and Lu, C.-M. (2014). Mechanical and fracture behaviors of defective silicon nanowires: combined effects of vacancy clusters, temperature, wire size, and shape. *Applied Physics A*, 114:1247–1256.
- [Kushima et al., 2012] Kushima, A., Huang, J. Y., and Li, J. (2012). Quantitative fracture strength and plasticity measurements of lithiated silicon nanowires by in situ tem tensile experiments. *ACS nano*, 6(11):9425–9432.
- [Lao et al., 2013] Lao, J., Naghdi Tam, M., Pinisetty, D., and Gupta, N. (2013). Molecular dynamics simulation of fcc metallic nanowires: a review. *Jom*, 65:175–184.
- [Lapouge et al., 2017] Lapouge, P., Onimus, F., Coulombier, M., Raskin, J.-P., Par-

- doen, T., and Bréchet, Y. (2017). Creep behavior of submicron copper films under irradiation. *Acta Materialia*, 131:77–87.
- [Le and Nguyen, 2014] Le, M.-Q. and Nguyen, D.-T. (2014). Atomistic simulations of pristine and defective hexagonal bn and sic sheets under uniaxial tension. *Materials Science and Engineering: A*, 615:481–488.
- [Le and Nguyen, 2015] Le, M.-Q. and Nguyen, D.-T. (2015). The role of defects in the tensile properties of silicene. *Applied Physics A*, 118(4):1437–1445.
- [Lee and Rudd, 2007] Lee, B. and Rudd, R. E. (2007). First-principles study of the young’s modulus of si [001] nanowires. *Physical review B*, 75(4):041305.
- [Li et al., 2020] Li, F., Huang, Y., Wang, S., and Zhang, S. (2020). Critical review: Growth mechanisms of the self-assembling of silicon wires. *Journal of Vacuum Science & Technology A*, 38(1).
- [Li and Sun, 2012] Li, H. and Sun, F. (2012). Recent advances in mechanical properties of nanowires. *Nanowires-Recent Advances*.
- [Li et al., 2022] Li, J., Lei, X., Ding, J., Gao, Z., Wang, H., and Shi, Y. (2022). Surface effect on size dependent young’s modulus of nanowires: Exponentially decreased surface elasticity model. *Materials Letters*, 307:131001.
- [Li et al., 2023] Li, Q., Tan, X., and Yang, Y. (2023). Sub-5 nm gate length selenium nanowire transistors: Implications for nanoelectronics. *ACS Applied Nano Materials*, 6(5):4067–4077.
- [Li et al., 2019] Li, R., Chen, H., Zhu, H., Wang, M., Chen, C., and Yuan, T. (2019). Effect of aging treatment on the microstructure and mechanical properties of al-3.02 mg-0.2 sc-0.1 zr alloy printed by selective laser melting. *Materials & Design*, 168:107668.

- [Li and Gao, 2013] Li, S. and Gao, X.-L. (2013). *Handbook of micromechanics and nanomechanics*. CRC Press.
- [Li et al., 2005] Li, X., Kasai, T., Nakao, S., Ando, T., Shikida, M., Sato, K., and Tanaka, H. (2005). Anisotropy in fracture of single crystal silicon film characterized under uniaxial tensile condition. *Sensors and Actuators A: Physical*, 117(1):143–150.
- [Li et al., 2003] Li, X., Ono, T., Wang, Y., and Esashi, M. (2003). Ultrathin single-crystalline-silicon cantilever resonators: Fabrication technology and significant specimen size effect on young’s modulus. *Applied Physics Letters*, 83(15):3081–3083.
- [Li et al., 2021] Li, X., Yang, X., Zhang, Z., Wang, T., Sun, Y., Liu, Z., Li, X., Shi, Y., and Xu, J. (2021). Impact of process fluctuations on reconfigurable silicon nanowire transistor. *IEEE Transactions on Electron Devices*, 68(2):885–891.
- [Li et al., 2014] Li, X.-F., Zhang, H., and Lee, K. Y. (2014). Dependence of young’s modulus of nanowires on surface effect. *International Journal of Mechanical Sciences*, 81:120–125.
- [Li et al., 2006] Li, Y., Qian, F., Xiang, J., and Lieber, C. M. (2006). Nanowire electronic and optoelectronic devices. *Materials today*, 9(10):18–27.
- [Liang et al., 2023] Liang, Y., Qian, W., Hu, R., Gan, X., Shi, S., Li, Y., Wang, J., Liu, Z., He, D., Shi, Y., et al. (2023). High-fidelity moulding growth and cross-section shaping of ultrathin monocrystalline silicon nanowires. *Applied Surface Science*, page 157635.
- [Liou and Pretzer, 1998] Liou, H.-C. and Pretzer, J. (1998). Effect of curing temperature on the mechanical properties of hydrogen silsesquioxane thin films. *Thin solid films*, 335(1-2):186–191.

- [Liu and Li, 2022] Liu, M. and Li, X. (2022). Mechanical properties measurement of materials and devices at micro-and nano-scale by optical methods: A review. *Optics and Lasers in Engineering*, 150:106853.
- [Liu and Shen, 2012] Liu, Q. and Shen, S. (2012). On the large-strain plasticity of silicon nanowires: Effects of axial orientation and surface. *International journal of plasticity*, 38:146–158.
- [Liu et al., 2015] Liu, Q., Wang, L., and Shen, S. (2015). Effects of geometry and shape on the mechanical behaviors of silicon nanowires. *Computers, Materials and Continua*, 46(2):105–123.
- [Liu et al., 2022] Liu, X., Chen, Z., Wang, T., Jiang, X., Qu, X., Duan, W., Xi, F., He, Z., and Wu, J. (2022). Tissue imprinting on 2d nanoflakes-capped silicon nanowires for lipidomic mass spectrometry imaging and cancer diagnosis. *ACS nano*, 16(4):6916–6928.
- [Lorenzoni et al., 2016] Lorenzoni, M., Llobet, J., Gramazio, F., Sansa, M., Fraxedas, J., and Perez-Murano, F. (2016). Evaluating the compressive stress generated during fabrication of si doubly clamped nanobeams with afm. *Journal of Vacuum Science & Technology B, Nanotechnology and Microelectronics: Materials, Processing, Measurement, and Phenomena*, 34(6):06KK02.
- [Lou et al., 2012] Lou, L., Zhang, S., Park, W.-T., Tsai, J., Kwong, D.-L., and Lee, C. (2012). Optimization of nems pressure sensors with a multilayered diaphragm using silicon nanowires as piezoresistive sensing elements. *Journal of Micromechanics and Microengineering*, 22(5):055012.
- [Lu and Lieber, 2010] Lu, W. and Lieber, C. M. (2010). Nanoelectronics from the bottom up. *Nanoscience And Technology: A Collection of Reviews from Nature Journals*, pages 137–146.

- [Ma et al., 2003] Ma, D., Lee, C., Au, F., Tong, S., and Lee, S. (2003). Small-diameter silicon nanowire surfaces. *Science*, 299(5614):1874–1877.
- [Maita et al., 2023] Maita, F., Maiolo, L., Lucarini, I., Del Rio De Vicente, J. I., Sciortino, A., Ledda, M., Mussi, V., Lisi, A., and Convertino, A. (2023). Revealing low amplitude signals of neuroendocrine cells through disordered silicon nanowires-based microelectrode array. *Advanced Science*, page 2301925.
- [Maras et al., 2016] Maras, E., Trushin, O., Stukowski, A., Ala-Nissila, T., and Jonsson, H. (2016). Global transition path search for dislocation formation in ge on si (001). *Computer Physics Communications*, 205:13–21.
- [Marola et al., 2021] Marola, S., Bosia, S., Veltro, A., Fiore, G., Manfredi, D., Lombardi, M., Amato, G., Baricco, M., and Battezzati, L. (2021). Residual stresses in additively manufactured als10mg: Raman spectroscopy and x-ray diffraction analysis. *Materials & Design*, 202:109550.
- [Massa et al., 2020] Massa, E., Sasso, C. P., and Mana, G. (2020). The measurement of the silicon lattice parameter and the count of atoms to realise the kilogram. *MAPAN*, 35(4):511–519.
- [Matteini et al., 2015] Matteini, F., Dubrovskii, V. G., Rüffer, D., Tütüncüoğlu, G., Fontana, Y., and Morral, A. F. I. (2015). Tailoring the diameter and density of self-catalyzed gaas nanowires on silicon. *Nanotechnology*, 26(10):105603.
- [McDowell et al., 2011] McDowell, M. T., Lee, S. W., Ryu, I., Wu, H., Nix, W. D., Choi, J. W., and Cui, Y. (2011). Novel size and surface oxide effects in silicon nanowires as lithium battery anodes. *Nano Letters*, 11(9):4018–4025.
- [McIntyre and i Morral, 2020] McIntyre, P. and i Morral, A. F. (2020). Semiconductor nanowires: to grow or not to grow? *Materials Today Nano*, 9:100058.

- [Mead et al., 2023] Mead, J. L., Wang, S., Zimmermann, S., Fatikow, S., and Huang, H. (2023). Resolving the adhesive behavior of 1d materials: A review of experimental approaches. *Engineering*.
- [Meade et al., 1992] Meade, C., Hemley, R. J., and Mao, H. (1992). High-pressure x-ray diffraction of sio 2 glass. *Physical Review Letters*, 69(9):1387.
- [Meier, 2005] Meier, R. J. (2005). On art and science in curve-fitting vibrational spectra. *Vibrational spectroscopy*, 2(39):266–269.
- [Melis et al., 2015] Melis, C., Colombo, L., and Mana, G. (2015). Lattice strain at c-si surfaces: a density functional theory calculation. *Metrologia*, 52(2):214.
- [Melis et al., 2016] Melis, C., Giordano, S., Colombo, L., and Mana, G. (2016). Density functional theory calculations of the stress of oxidised (1 1 0) silicon surfaces. *Metrologia*, 53(6):1339.
- [Meng and Li, 2020] Meng, J. and Li, Z. (2020). Schottky-contacted nanowire sensors. *Advanced Materials*, 32(28):2000130.
- [Miani et al., 2021] Miani, T., Verdot, T., Berthelot, A., Maspero, F., Koumela, A., Robert, P., Langfelder, G., Arcamone, J., and Sansa, M. (2021). Resonant accelerometers based on nanomechanical piezoresistive transduction. In *2021 IEEE 34th International Conference on Micro Electro Mechanical Systems (MEMS)*, pages 192–195. IEEE.
- [Miani et al., 2022] Miani, T., Verdot, T., Berthelot, A., Maspero, F., Koumela, A., Robert, P., Langfelder, G., Arcamone, J., and Sansa, M. (2022). Nanoresonator-based accelerometer with large bandwidth and improved bias stability. In *2022 IEEE International Symposium on Inertial Sensors and Systems (INERTIAL)*, pages 1–4. IEEE.
- [Miller and Shenoy, 2000] Miller, R. E. and Shenoy, V. B. (2000). Size-dependent elastic properties of nanosized structural elements. *Nanotechnology*, 11(3):139.

- [Mills et al., 2017] Mills, S., Sader, J. E., and Boland, J. J. (2017). Material characterisation of nanowires with intrinsic stress. *Nanotechnology*, 28(35):355706.
- [Minamisawa et al., 2012] Minamisawa, R. A., Süess, M. J., Spolenak, R., Faist, J., David, C., Gobrecht, J., Bourdelle, K. K., and Sigg, H. (2012). Top-down fabricated silicon nanowires under tensile elastic strain up to 4.5%. *Nature communications*, 3(1):1–6.
- [Minor et al., 2005] Minor, A., Lilleodden, E., Jin, M., Stach, E., Chrzan, D., and Morris, J. (2005). Room temperature dislocation plasticity in silicon. *Philosophical Magazine*, 85(2-3):323–330.
- [Miyamoto, 1994] Miyamoto, Y. (1994). Comparative study of si (100) surface stresses with dimerized group-iv adatoms. *Physical Review B*, 49(3):1947.
- [Moffat, 1988] Moffat, R. J. (1988). Describing the uncertainties in experimental results. *Experimental thermal and fluid science*, 1(1):3–17.
- [Momeni et al., 2020] Momeni, K., Ji, Y., Wang, Y., Paul, S., Neshani, S., Yilmaz, D. E., Shin, Y. K., Zhang, D., Jiang, J.-W., Park, H. S., et al. (2020). Multiscale computational understanding and growth of 2d materials: a review. *npj Computational Materials*, 6(1):22.
- [Morita et al., 1990] Morita, M., Ohmi, T., Hasegawa, E., Kawakami, M., and Ohwada, M. (1990). Growth of native oxide on a silicon surface. *Journal of Applied Physics*, 68(3):1272–1281.
- [Müller and Saúl, 2004] Müller, P. and Saúl, A. (2004). Elastic effects on surface physics. *Surface Science Reports*, 54(5-8):157–258.
- [Munetoh et al., 2007] Munetoh, S., Motooka, T., Moriguchi, K., and Shintani, A. (2007). Interatomic potential for si-o systems using tersoff parameterization. *Computational Materials Science*, 39(2):334–339.



- [Namazu, 2023] Namazu, T. (2023). Mechanical property measurement of micro/nanoscale materials for mems: A review. *IEEJ Transactions on Electrical and Electronic Engineering*, 18(3):308–324.
- [Namazu et al., 2000] Namazu, T., Isono, Y., and Tanaka, T. (2000). Evaluation of size effect on mechanical properties of single crystal silicon by nanoscale bending test using afm. *Journal of Microelectromechanical systems*, 9(4):450–459.
- [Namdari et al., 2016] Namdari, P., Daraee, H., and Eatemadi, A. (2016). Recent advances in silicon nanowire biosensors: synthesis methods, properties, and applications. *Nanoscale research letters*, 11:1–16.
- [Nasr Esfahani and Alaca, 2019] Nasr Esfahani, M. and Alaca, B. E. (2019). A review on size-dependent mechanical properties of nanowires. *Advanced Engineering Materials*, 21(8):1900192.
- [Nasr Esfahani and Jabbari, 2020] Nasr Esfahani, M. and Jabbari, M. (2020). Influence of the surface stress on the size-dependent elastic behavior of silicon nanowires. *Journal of Applied Physics*, 127(19).
- [Nasr Esfahani et al., 2022] Nasr Esfahani, M., Zare Pakzad, S., Li, T., Li, X., Tasdemir, Z., Wollschlager, N., Leblebici, Y., and Alaca, B. E. (2022). Effect of native oxide on stress in silicon nanowires: Implications for nanoelectromechanical systems. *ACS Applied Nano Materials*.
- [Nehra et al., 2020] Nehra, M., Dilbaghi, N., Marrazza, G., Kaushik, A., Abolhasani, R., Mishra, Y. K., Kim, K. H., and Kumar, S. (2020). 1d semiconductor nanowires for energy conversion, harvesting and storage applications. *Nano Energy*, 76:104991.
- [Newsome et al., 2012] Newsome, D. A., Sengupta, D., Foroutan, H., Russo, M. F., and Van Duin, A. C. (2012). Oxidation of silicon carbide by o<sub>2</sub> and h<sub>2</sub>o: a reaxff

reactive molecular dynamics study, part i. *The Journal of Physical Chemistry C*, 116(30):16111–16121.

[Neyts et al., 2011] Neyts, E., Khalilov, U., Pourtois, G., and Van Duin, A. (2011). Hyperthermal oxygen interacting with silicon surfaces: adsorption, implantation, and damage creation. *The Journal of Physical Chemistry C*, 115(11):4818–4823.

[Ngo et al., 2006] Ngo, L. T., Alméjija, D., Sader, J. E., Daly, B., Petkov, N., Holmes, J. D., Erts, D., and Boland, J. J. (2006). Ultimate-strength germanium nanowires. *Nano letters*, 6(12):2964–2968.

[Ni et al., 2006] Ni, H., Li, X., and Gao, H. (2006). Elastic modulus of amorphous SiO<sub>2</sub> nanowires. *Applied Physics Letters*, 88(4):1–3.

[Nugent and Prawer, 1998] Nugent, K. and Prawer, S. (1998). Confocal raman strain mapping of isolated single cvd diamond crystals. *Diamond and related materials*, 7(2-5):215–221.

[Ohta et al., 2007] Ohta, H., Watanabe, T., and Ohdomari, I. (2007). Strain distribution around sio<sub>2</sub>/si interface in si nanowires: A molecular dynamics study. *Japanese journal of applied physics*, 46(5S):3277.

[Ollier et al., 2012] Ollier, E., Dupré, C., Arndt, G., Arcamone, J., Vizioz, C., Duraffourg, L., Sage, E., Koumela, A., Hentz, S., Cibrario, G., et al. (2012). Ultra-scaled high-frequency single-crystal si nems resonators and their front-end co-integration with cmos for high sensitivity applications. In *2012 IEEE 25th International Conference on Micro Electro Mechanical Systems (MEMS)*, pages 1368–1371. IEEE.

[Östlund et al., 2009] Östlund, F., Rzepiejewska-Malyska, K., Leifer, K., Hale, L. M., Tang, Y., Ballarini, R., Gerberich, W. W., and Michler, J. (2009). Brittle-to-ductile transition in uniaxial compression of silicon pillars at room temperature. *Advanced Functional Materials*, 19(15):2439–2444.

- [Pakzad et al., 2021] Pakzad, S. Z., Esfahani, M. N., and Alaca, B. E. (2021). Molecular dynamics study of orientation-dependent tensile properties of si nanowires with native oxide: Surface stress and surface energy effects. In *2021 IEEE 21st International Conference on Nanotechnology (NANO)*, pages 370–373. IEEE.
- [Pakzad et al., 2023a] Pakzad, S. Z., Esfahani, M. N., and Alaca, B. E. (2023a). Investigation of the bending behavior in silicon nanowires: A nanomechanical modeling perspective. *arXiv preprint arXiv:2308.13610*.
- [Pakzad et al., 2023b] Pakzad, S. Z., Esfahani, M. N., and Alaca, B. E. (2023b). The role of native oxide on the mechanical behavior of silicon nanowires. *Materials Today Communications*, 34:105002.
- [Pakzad et al., 2024] Pakzad, S. Z., Esfahani, M. N., and Alaca, B. E. (2024). Mechanical properties of silicon nanowires with native oxide surface state. *Materials Today Communications*, page 108321.
- [Panda et al., 2022] Panda, S., Hajra, S., Mistewicz, K., In-na, P., Sahu, M., Rajitha, P. M., and Kim, H. J. (2022). Piezoelectric energy harvesting systems for biomedical applications. *Nano Energy*, page 107514.
- [Pantano et al., 2012] Pantano, M. F., Espinosa, H. D., and Pagnotta, L. (2012). Mechanical characterization of materials at small length scales. *Journal of Mechanical Science and technology*, 26:545–561.
- [Pantano and Kuljanishvili, 2020] Pantano, M. F. and Kuljanishvili, I. (2020). Advances in mechanical characterization of 1d and 2d nanomaterials: progress and prospects. *Nano express*, 1(2):022001.
- [Park, 2008] Park, H. S. (2008). Surface stress effects on the resonant properties of silicon nanowires. *Journal of Applied Physics*, 103(12):123504.
- [Park et al., 2009] Park, H. S., Cai, W., Espinosa, H. D., and Huang, H. (2009). Mechanics of crystalline nanowires. *MRS bulletin*, 34(3):178–183.

- [Park et al., 2010] Park, K. T., Kim, H. C., and Chun, K. (2010). Fabrication of single crystal silicon nanowire bridge. In *2010 First International Conference on Sensor Device Technologies and Applications*, pages 246–248. IEEE.
- [Park et al., 2005] Park, S., Kim, J., Park, J., Lee, J., Choi, Y., and Kwon, O. (2005). Molecular dynamics study on size-dependent elastic properties of silicon nanocantilevers. *Thin solid films*, 492(1-2):285–289.
- [Park et al., 2015] Park, S., Rho, H., Song, J., Lee, S.-K., Kim, G.-S., and Lee, C. (2015). Spatially-resolved and polarized raman scattering from a single si nanowire. *Journal of Raman Spectroscopy*, 46(6):524–530.
- [Passi et al., 2012] Passi, V., Bhaskar, U., Pardoen, T., Sodervall, U., Nilsson, B., Petersson, G., Hagberg, M., and Raskin, J.-P. (2012). High-throughput on-chip large deformation of silicon nanoribbons and nanowires. *Journal of microelectromechanical systems*, 21(4):822–829.
- [Payne et al., 1989] Payne, M., Roberts, N., Needs, R., Needels, M., and Joannopoulos, J. (1989). Total energy and stress of metal and semiconductor surfaces. *Surface Science*, 211:1–20.
- [Pedregosa et al., 2011] Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R., Dubourg, V., et al. (2011). Scikit-learn: Machine learning in python. *the Journal of machine Learning research*, 12:2825–2830.
- [Pennelli et al., 2012] Pennelli, G., Totaro, M., and Nannini, A. (2012). Correlation between surface stress and apparent young’s modulus of top-down silicon nanowires. *ACS nano*, 6(12):10727–10734.
- [Petersen, 1982] Petersen, K. E. (1982). Silicon as a mechanical material. *Proceedings of the IEEE*, 70(5):420–457.

- [Philipp and Taft, 1982] Philipp, H. R. and Taft, E. (1982). An optical characterization of native oxides and thin thermal oxides on silicon. *Journal of Applied Physics*, 53(7):5224–5229.
- [Piscanec et al., 2003] Piscanec, S., Cantoro, M., Ferrari, A., Zapien, J., Lifshitz, Y., Lee, S., Hofmann, S., and Robertson, J. (2003). Raman spectroscopy of silicon nanowires. *Physical Review B*, 68(24):241312.
- [Pishkenari and Rezaei, 2017] Pishkenari, H. N. and Rezaei, S. (2017). Characterization of silicon surface elastic constants based on different interatomic potentials. *Thin Solid Films*, 626:104–109.
- [Plimpton, 1995] Plimpton, S. (1995). Fast parallel algorithms for short-range molecular dynamics. *Journal of computational physics*, 117(1):1–19.
- [Poborchii et al., 2007] Poborchii, V., Tada, T., and Kanayama, T. (2007). Study of stress in a shallow-trench-isolated si structure using polarized confocal near-uv raman microscopy of its cross section. *Applied Physics Letters*, 91(24):241902.
- [Poborchii et al., 2013] Poborchii, V., Tada, T., Morita, Y., and Kanayama, T. (2013). Ultraviolet raman spectra of single uncoated and sio<sub>2</sub>-coated silicon-on-insulator nanowires: Phonon boundary scattering, wave-vector relaxation and stress. *Applied Physics Letters*, 103(15):153104.
- [Poindexter et al., 1981] Poindexter, E. H., Caplan, P. J., Deal, B. E., and Razouk, R. R. (1981). Interface states and electron spin resonance centers in thermally oxidized (111) and (100) silicon wafers. *Journal of Applied Physics*, 52(2):879–884.
- [Prüßing et al., 2022] Prüßing, J. K., Böckendorf, T., Kipke, F., Xu, J., Puranto, P., Lundsgaard Hansen, J., Bougeard, D., Peiner, E., and Bracht, H. (2022). Retarded boron and phosphorus diffusion in silicon nanopillars due to stress induced vacancy injection. *Journal of Applied Physics*, 131(7):075702.

- [Purcek et al., 2012] Purcek, G., Saray, O., Nagimov, M., Nazarov, A., Safarov, I., Danilenko, V., Valiakhmetov, O., and Mulyukov, R. (2012). Microstructure and mechanical behavior of ufg copper processed by ecap following different processing regimes. *Philosophical Magazine*, 92(6):690–704.
- [Qu, 2016] Qu, H. (2016). Cmos mems fabrication technologies and devices. *Micro-machines*, 7(1):14.
- [Quagliotti et al., 2013] Quagliotti, D., Mana, G., Massa, E., Sasso, C., and Kuettgens, U. (2013). A finite element analysis of surface-stress effects on measurement of the si lattice parameter. *Metrologia*, 50(3):243.
- [Quan et al., 2019] Quan, L. N., Kang, J., Ning, C.-Z., and Yang, P. (2019). Nanowires for photonics. *Chemical reviews*, 119(15):9153–9169.
- [Raman et al., 2023] Raman, S., Sindhuja, M., et al. (2023). Advances in silicon nanowire applications in energy generation, storage, sensing, and electronics: A review. *Nanotechnology*, 34(18):182001.
- [Ramprasad et al., 2017] Ramprasad, R., Batra, R., Pilia, G., Mannodi-Kanakkithodi, A., and Kim, C. (2017). Machine learning in materials informatics: recent applications and prospects. *npj Computational Materials*, 3(1):54.
- [Robert et al., 2009] Robert, P., Nguyen, V., Hentz, S., Duraffourg, L., Jourdan, G., Arcamone, J., and Harrison, S. (2009). M&nems: A new approach for ultra-low cost 3d inertial sensor. In *SENSORS, 2009 IEEE*, pages 963–966. IEEE.
- [Rojo et al., 2013] Rojo, M. M., Calero, O. C., Lopeandia, A., Rodriguez-Viejo, J., and Martin-Gonzalez, M. (2013). Review on measurement techniques of transport properties of nanowires. *Nanoscale*, 5(23):11526–11544.
- [Sacchetto et al., 2009] Sacchetto, D., Ben-Jamaa, M. H., De Micheli, G., and Leblebici, Y. (2009). Fabrication and characterization of vertically stacked gate-

- all-around si nanowire fet arrays. In *2009 Proceedings of the European Solid State Device Research Conference*, pages 245–248. IEEE.
- [Sadeghian et al., 2009] Sadeghian, H., Yang, C., Goosen, J., Van Der Drift, E., Bossche, A., French, P., and Van Keulen, F. (2009). Characterizing size-dependent effective elastic modulus of silicon nanocantilevers using electrostatic pull-in instability. *Applied Physics Letters*, 94(22):221903.
- [Sadeghian et al., 2010] Sadeghian, H., Yang, C.-K., Goosen, J. F., Bossche, A., Stauffer, U., French, P. J., and van Keulen, F. (2010). Effects of size and defects on the elasticity of silicon nanocantilevers. *Journal of Micromechanics and Microengineering*, 20(6):064012.
- [Sage et al., 2018] Sage, E., Sansa, M., Fostner, S., Defoort, M., Gély, M., Naik, A. K., Morel, R., Duraffourg, L., Roukes, M. L., Alava, T., et al. (2018). Single-particle mass spectrometry with arrays of frequency-addressed nanomechanical resonators. *Nature communications*, 9(1):1–8.
- [Samykano, 2021] Samykano, M. (2021). Progress in one-dimensional nanostructures. *Materials Characterization*, 179:111373.
- [San Paulo et al., 2005] San Paulo, A., Bokor, J., Howe, R., He, R., Yang, P., Gao, D., Carraro, C., and Maboudian, R. (2005). Mechanical elasticity of single and double clamped silicon nanobeams fabricated by the vapor-liquid-solid method. *Applied Physics Letters*, 87(5):053111.
- [Sander and Ibach, 1991] Sander, D. and Ibach, H. (1991). Experimental determination of adsorbate-induced surface stress: Oxygen on si (111) and si (100). *Physical Review B*, 43(5):4263.
- [Sang et al., 2016] Sang, S., Wang, Y., Feng, Q., Wei, Y., Ji, J., and Zhang, W. (2016). Progress of new label-free techniques for biosensors: a review. *Critical reviews in biotechnology*, 36(3):465–481.

- [Sannicolo et al., 2016] Sannicolo, T., Lagrange, M., Cabos, A., Celle, C., Simonato, J.-P., and Bellet, D. (2016). Metallic nanowire-based transparent electrodes for next generation flexible devices: a review. *Small*, 12(44):6052–6075.
- [Sato et al., 1998] Sato, K., Yoshioka, T., Ando, T., Shikida, M., and Kawabata, T. (1998). Tensile testing of silicon film having different crystallographic orientations carried out on a silicon chip. *Sensors and Actuators A: Physical*, 70(1-2):148–152.
- [Schaible, 1999] Schaible, M. (1999). Empirical molecular dynamics modeling of silicon and silicon dioxide: a review. *Critical reviews in solid state and materials sciences*, 24(4):265–323.
- [Scholze, 1991] Scholze, H. (1991). *Glass: nature, structure, and properties*. Springer Science & Business Media.
- [Schweitz and Ericson, 1999] Schweitz, J.-Å. and Ericson, F. (1999). Evaluation of mechanical materials properties by means of surface micromachined structures. *Sensors and Actuators A: Physical*, 74(1-3):126–133.
- [Sedgwick, 2012] Sedgwick, P. (2012). Pearson’s correlation coefficient. *Bmj*, 345.
- [Seike et al., 2007] Seike, A., Tange, T., Sugiura, Y., Tsuchida, I., Ohta, H., Watanabe, T., Kosemura, D., Ogura, A., and Ohdomari, I. (2007). Strain-induced transconductance enhancement by pattern dependent oxidation in silicon nanowire field-effect transistors. *Applied Physics Letters*, 91(20):202117.
- [Sessi et al., 2020] Sessi, V., Simon, M., Mulaosmanovic, H., Pohl, D., Loeffler, M., Mauersberger, T., Fengler, F. P., Mittmann, T., Richter, C., Slesazeck, S., et al. (2020). A silicon nanowire ferroelectric field-effect transistor. *Advanced Electronic Materials*, 6(4):1901244.
- [Shaw et al., 1993] Shaw, K. A., Zhang, Z. L., and MacDonald, N. C. (1993). Scream i: A single mask, single-crystal silicon process for microelectromechanical struc-



- tures. In [1993] *Proceedings IEEE Micro Electro Mechanical Systems*, pages 155–160. IEEE.
- [Shaw et al., 1994] Shaw, K. A., Zhang, Z. L., and MacDonald, N. C. (1994). Scream i: a single mask, single-crystal silicon, reactive ion etching process for microelectromechanical structures. *Sensors and Actuators A: Physical*, 40(1):63–70.
- [Shchipalov, 2000] Shchipalov, Y. K. (2000). Surface energy of crystalline and vitreous silica. *Glass and ceramics*, 57(11):374–377.
- [Shekhar et al., 2024] Shekhar, S., Bogaerts, W., Chrostowski, L., Bowers, J. E., Hochberg, M., Soref, R., and Shastri, B. J. (2024). Roadmapping the next generation of silicon photonics. *Nature Communications*, 15(1):751.
- [Shir et al., 2006] Shir, D., Liu, B., Mohammad, A., Lew, K., and Mohnney, S. (2006). Oxidation of silicon nanowires. *Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures Processing, Measurement, and Phenomena*, 24(3):1333–1336.
- [Silva et al., 2006] Silva, E. C., Tong, L., Yip, S., and Van Vliet, K. J. (2006). Size effects on the stiffness of silica nanowires. *Small*, 2(2):239–243.
- [Singh et al., 2023] Singh, A. P., Mishra, V. K., and Akhter, S. (2023). A perspective view of silicon based classical to non-classical mos transistors and their extension in machine learning. *Silicon*, pages 1–22.
- [Sofiah et al., 2018] Sofiah, A., Samykano, M., Kadirgama, K., Mohan, R., and Lah, N. (2018). Metallic nanowires: mechanical properties—theory and experiment. *Applied Materials Today*, 11:320–337.
- [Sohail and Afzaal, 2019] Sohail, I. and Afzaal, M. (2019). A review on mems based micro displacement amplification mechanisms [j]. *Sensors and Actuators: A. Physical*, page 300.

- [Sohn et al., 2010] Sohn, Y.-S., Park, J., Yoon, G., Song, J., Jee, S.-W., Lee, J.-H., Na, S., Kwon, T., and Eom, K. (2010). Mechanical properties of silicon nanowires. *Nanoscale research letters*, 5:211–216.
- [Solanki and Um, 2018] Solanki, A. and Um, H. (2018). Top-down etching of si nanowires. In *Semiconductors and Semimetals*, volume 98, pages 71–149. Elsevier.
- [Song and Huang, 2009] Song, F. and Huang, G. (2009). Modeling of surface stress effects on bending behavior of nanowires: Incremental deformation theory. *Physics letters A*, 373(43):3969–3973.
- [Song et al., 2011] Song, F., Huang, G., Park, H., and Liu, X. (2011). A continuum model for the mechanical behavior of nanowires including surface and surface-induced initial stresses. *International Journal of Solids and Structures*, 48(14-15):2154–2163.
- [Song et al., 2012] Song, T., Lee, S.-T., and Sun, B. (2012). Silicon nanowires for photovoltaic applications: The progress and challenge. *Nano Energy*, 1(5):654–673.
- [Spejo et al., 2020] Spejo, L., Arrieta-Concha, J., Puydinger dos Santos, M., Barros, A., Bourdelle, K., Diniz, J., and Minamisawa, R. (2020). Non-linear raman shift-stress behavior in top-down fabricated highly strained silicon nanowires. *Journal of Applied Physics*, 128(4):045704.
- [Sreejith et al., 2023] Sreejith, S., Ajayan, J., Uma Reddy, N., and Manikandan, M. (2023). Recent advances and prospects in silicon nanowire sensors: A critical review. *Silicon*, pages 1–27.
- [Stan et al., 2007] Stan, G., Ciobanu, C., Parthangal, P. M., and Cook, R. F. (2007). Diameter-dependent radial and tangential elastic moduli of zno nanowires. *Nano Letters*, 7(12):3691–3697.

- [Stan et al., 2012a] Stan, G., Krylyuk, S., Davydov, A., Levin, I., and Cook, R. F. (2012a). Ultimate bending strength of si nanowires. *Nano letters*, 12(5):2599–2604.
- [Stan et al., 2008] Stan, G., Krylyuk, S., Davydov, A., Vaudin, M., Bendersky, L. A., and Cook, R. F. (2008). Surface effects on the elastic modulus of te nanowires. *Applied Physics Letters*, 92(24):241908.
- [Stan et al., 2012b] Stan, G., Krylyuk, S., Davydov, A. V., and Cook, R. F. (2012b). Bending manipulation and measurements of fracture strength of silicon and oxidized silicon nanowires by atomic force microscopy. *Journal of Materials Research*, 27(3):562–570.
- [Stassi et al., 2021] Stassi, S., Cooperstein, I., Tortello, M., Pirri, C. F., Magdassi, S., and Ricciardi, C. (2021). Reaching silicon-based nems performances with 3d printed nanomechanical resonators. *Nature Communications*, 12(1):1–9.
- [Steighner et al., 2011] Steighner, M., Snedeker, L., Boyce, B., Gall, K., Miller, D., and Muhlstein, C. (2011). Dependence on diameter and growth direction of apparent strain to failure of si nanowires. *Journal of Applied Physics*, 109(3):033503.
- [Steigmann and Ogden, 1997] Steigmann, D. and Ogden, R. (1997). Plane deformations of elastic solids with intrinsic boundary elasticity. *Proceedings of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences*, 453(1959):853–877.
- [Steinruck et al., 2014] Steinruck, H.-G., Schiener, A., Schindler, T., Will, J., Magerl, A., Konovalov, O., Li Destri, G., Seeck, O. H., Mezger, M., Haddad, J., et al. (2014). Nanoscale structure of si/sio<sub>2</sub>/organics interfaces. *ACS nano*, 8(12):12676–12681.
- [Stillinger and Weber, 1985] Stillinger, F. H. and Weber, T. A. (1985). Computer

simulation of local order in condensed phases of silicon. *Physical review B*, 31(8):5262.

[Stokes et al., 2023] Stokes, K., Clark, K., Odetade, D., Hardy, M., and Goldberg Oppenheimer, P. (2023). Advances in lithographic techniques for precision nanostructure fabrication in biomedical applications. *Discover Nano*, 18(1):1–43.

[Suess et al., 2014] Suess, M., Minamisawa, R., Geiger, R., Bourdelle, K., Sigg, H., and Spolenak, R. (2014). Power-dependent raman analysis of highly strained si nanobridges. *Nano letters*, 14(3):1249–1254.

[Sundararajan et al., 2002] Sundararajan, S., Bhushan, B., Namazu, T., and Isono, Y. (2002). Mechanical property measurements of nanoscale structures using an atomic force microscope. *Ultramicroscopy*, 91(1-4):111–118.

[Tabib-Azar et al., 2005] Tabib-Azar, M., Nassirou, M., Wang, R., Sharma, S., Kamins, T., Islam, M. S., and Williams, R. S. (2005). Mechanical properties of self-welded silicon nanobridges. *Applied Physics Letters*, 87(11):113102.

[Takeuchi et al., 2009] Takeuchi, T., Tatsumura, K., Shimura, T., and Ohdomari, I. (2009). X-ray diffraction study of strain distribution in oxidized si nanowires. *Journal of Applied Physics*, 106(7):073506.

[Tang et al., 2012] Tang, D.-M., Ren, C.-L., Wang, M.-S., Wei, X., Kawamoto, N., Liu, C., Bando, Y., Mitome, M., Fukata, N., and Golberg, D. (2012). Mechanical properties of si nanowires as revealed by in situ transmission electron microscopy and molecular dynamics simulations. *Nano letters*, 12(4):1898–1904.

[Tao et al., 2015] Tao, Y., Navaretti, P., Hauert, R., Grob, U., Poggio, M., and Degen, C. L. (2015). Permanent reduction of dissipation in nanomechanical si resonators by chemical surface protection. *Nanotechnology*, 26(46):465501.

- [Tasdemir et al., 2018] Tasdemir, Z., Peric, O., Sacchetto, D., Fantner, G. E., Leblebici, Y., and Alaca, B. E. (2018). Monolithic fabrication of silicon nanowires bridging thick silicon structures. *IEEE Transactions on Nanotechnology*, 17(6):1299–1302.
- [Tasdemir et al., 2016] Tasdemir, Z., Wollschläger, N., Österle, W., Leblebici, Y., and Alaca, B. E. (2016). A deep etching mechanism for trench-bridging silicon nanowires. *Nanotechnology*, 27(9):095303.
- [Templeman et al., 2020] Templeman, J. O., Sheil, B. B., and Sun, T. (2020). Multi-axis force sensors: A state-of-the-art review. *Sensors and Actuators A: Physical*, 304:111772.
- [Tersoff, 1988] Tersoff, J. (1988). New empirical approach for the structure and energy of covalent systems. *Physical review B*, 37(12):6991.
- [Thompson et al., 2022] Thompson, A. P., Aktulga, H. M., Berger, R., Bolintineanu, D. S., Brown, W. M., Crozier, P. S., in't Veld, P. J., Kohlmeyer, A., Moore, S. G., Nguyen, T. D., et al. (2022). Lammmps-a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. *Computer Physics Communications*, 271:108171.
- [Tintelott et al., 2021] Tintelott, M., Pachauri, V., Ingebrandt, S., and Vu, X. T. (2021). Process variability in top-down fabrication of silicon nanowire-based biosensor arrays. *Sensors*, 21(15):5153.
- [Tiwari et al., 2022] Tiwari, P., Noelia, V. T., Heinz, S., and Kirsten Emilie, M. (2022). Iii-v infrared emitters on si: fabrication concepts, device architectures and down-scaling with a focus on template-assisted selective epitaxy. *Semiconductor Science and Technology*, 38:5.
- [Toda et al., 2010] Toda, S., Oishi, T., Yoshioka, T., and Okuno, T. (2010). Optical

properties of silicon nanowires fabricated by electroless silver deposition. *Japanese Journal of Applied Physics*, 49(9R):095002.

[Tran et al., 2018] Tran, D. P., Pham, T. T. T., Wolfrum, B., Offenhäusser, A., and Thierry, B. (2018). Cmos-compatible silicon nanowire field-effect transistor biosensor: Technology development toward commercialization. *Materials*, 11(5):785.

[Tran et al., 2023] Tran, V. A., Vo, G. N., Vo, T.-T. T., Doan, V. D., Vo, V., and Le, V. T. (2023). Recent applications and prospects of nanowire-based biosensors. *Processes*, 11(6):1739.

[Tsuchiya et al., 2016] Tsuchiya, T., Hemmi, T., Suzuki, J.-y., Hirai, Y., and Tabata, O. (2016). Tensile fracture of integrated single-crystal silicon nanowire using mems electrostatic testing device. *Procedia Structural Integrity*, 2:1405–1412.

[Tsuchiya et al., 2018] Tsuchiya, T., Hemmi, T., Suzuki, J.-y., Hirai, Y., and Tabata, O. (2018). Tensile strength of silicon nanowires batch-fabricated into electrostatic mems testing device. *Applied Sciences*, 8(6):880.

[Tsuchiya et al., 2001] Tsuchiya, T., Shikida, M., and Sato, K. (2001). Tensile testing system for sub-micrometer thick films. In *Transducers' 01 Eurosensors XV: The 11th International Conference on Solid-State Sensors and Actuators June 10–14, 2001 Munich, Germany*, pages 1350–1353. Springer.

[Uematsu et al., 2004] Uematsu, M., Kageshima, H., Shiraishi, K., Nagase, M., Horiguchi, S., and Takahashi, Y. (2004). Two-dimensional simulation of pattern-dependent oxidation of silicon nanostructures on silicon-on-insulator substrates. *Solid-State Electronics*, 48(6):1073–1078.

[Ungerer et al., 2019] Ungerer, M. J., Santos-Carballal, D., Cadi-Essadek, A., van Sittert, C. G., and De Leeuw, N. H. (2019). Interaction of h<sub>2</sub>o with the platinum pt

- (001),(011), and (111) surfaces: a density functional theory study with long-range dispersion corrections. *The Journal of Physical Chemistry C*, 123(45):27465–27476.
- [Ureña et al., 2013] Ureña, F., Olsen, S. H., and Raskin, J.-P. (2013). Raman measurements of uniaxial strain in silicon nanostructures. *Journal of Applied Physics*, 114(14):144507.
- [Urena et al., 2012] Urena, F., Olsen, S. H., Šiller, L., Bhaskar, U., Pardoen, T., and Raskin, J.-P. (2012). Strain in silicon nanowire beams. *Journal of Applied Physics*, 112(11):114506.
- [Van Duin et al., 2003] Van Duin, A. C., Strachan, A., Stewman, S., Zhang, Q., Xu, X., and Goddard, W. A. (2003). Reaxffsio reactive force field for silicon and silicon oxide systems. *The Journal of Physical Chemistry A*, 107(19):3803–3811.
- [Vashishta et al., 1990] Vashishta, P., Kalia, R. K., Rino, J. P., and Ebbsjö, I. (1990). Interaction potential for sio 2: A molecular-dynamics study of structural correlations. *Physical Review B*, 41(17):12197.
- [Verma et al., 2021] Verma, G., Mondal, K., and Gupta, A. (2021). Si-based mems resonant sensor: A review from microfabrication perspective. *Microelectronics Journal*, 118:105210.
- [Vogl et al., 2021] Vogl, L. M., Schweizer, P., Richter, G., and Spiecker, E. (2021). Effect of size and shape on the elastic modulus of metal nanowires. *MRS Advances*, 6:665–673.
- [Wagesreither et al., 2014] Wagesreither, S., Bertagnolli, E., Kawase, S., Isono, Y., and Lugstein, A. (2014). Electrostatic actuated strain engineering in monolithically integrated vls grown silicon nanowires. *Nanotechnology*, 25(45):455705.
- [Wagner and Ellis, 1964] Wagner, a. R. and Ellis, s. W. (1964). Vapor-liquid-solid mechanism of single crystal growth. *Applied physics letters*, 4(5):89–90.

- [Waldrop, 2016] Waldrop, M. M. (2016). The chips are down for moore’s law. *Nature News*, 530(7589):144.
- [Wang, 1995] Wang, C. M. (1995). Timoshenko beam-bending solutions in terms of euler-bernoulli solutions. *Journal of engineering mechanics*, 121(6):763–765.
- [Wang et al., 2019] Wang, D.-S., Mukhtar, A., Wu, K.-M., Gu, L., and Cao, X. (2019). Multi-segmented nanowires: a high tech bright future. *Materials*, 12(23):3908.
- [Wang et al., 2016a] Wang, F., Dong, A., and Buhro, W. E. (2016a). Solution–liquid–solid synthesis, properties, and applications of one-dimensional colloidal semiconductor nanorods and nanowires. *Chemical reviews*, 116(18):10888–10933.
- [Wang and Feng, 2007] Wang, G.-F. and Feng, X.-Q. (2007). Effects of surface elasticity and residual surface tension on the natural frequency of microbeams. *Applied physics letters*, 90(23):231904.
- [Wang et al., 2021] Wang, J.-J., Fu, C., Cheng, H.-Y., Tong, X.-W., Zhang, Z.-X., Wu, D., Chen, L.-M., Liang, F.-X., and Luo, L.-B. (2021). Leaky mode resonance-induced sensitive ultraviolet photodetector composed of graphene/small diameter silicon nanowire array heterojunctions. *ACS nano*, 15(10):16729–16737.
- [Wang et al., 2017] Wang, S., Shan, Z., and Huang, H. (2017). The mechanical properties of nanowires. *Advanced Science*, 4(4):1600332.
- [Wang et al., 2023] Wang, Y., Adam, M. L., Zhao, Y., Zheng, W., Gao, L., Yin, Z., and Zhao, H. (2023). Machine learning-enhanced flexible mechanical sensing. *Nano-Micro Letters*, 15(1):55.
- [Wang et al., 2016b] Wang, Z., Lee, S., Koo, K.-i., and Kim, K. (2016b). Nanowire-based sensors for biological and medical applications. *IEEE transactions on nanobioscience*, 15(3):186–199.



- [Watanabe et al., 1999] Watanabe, T., Fujiwara, H., Noguchi, H., Hoshino, T., and Ohdomari, I. (1999). Novel Interatomic Potential Energy Function for Si, O Mixed Systems. *Japanese Journal of Applied Physics, Part 1: Regular Papers and Short Notes and Review Papers*, 38(4 PART 2):366–369.
- [Watanabe and Ohdomari, 1999] Watanabe, T. and Ohdomari, I. (1999). Modeling of SiO<sub>2</sub>/Si(100) interface structure by using extended -Stillinger-Weber potential. *Thin Solid Films*, 343-344(1-2):370–373.
- [Watanabe et al., 2004] Watanabe, T., Tatsumura, K., and Ohdomari, I. (2004). SiO<sub>2</sub>/Si interface structure and its formation studied by large-scale molecular dynamics simulation. *Applied Surface Science*, 237(1-4):125–133.
- [Weber et al., 2014] Weber, W., Heinzig, A., Trommer, J., Martin, D., Grube, M., and Mikolajick, T. (2014). Reconfigurable nanowire electronics—a review. *Solid-State Electronics*, 102:12–24.
- [Wilson et al., 1996] Wilson, C., Ormeggi, A., and Narbutovskih, M. (1996). Fracture testing of silicon microcantilever beams. *Journal of Applied Physics*, 79(5):2386–2393.
- [Wollschläger et al., 2016] Wollschläger, N., Tasdemir, Z., Häusler, I., Leblebici, Y., Österle, W., and Alaca, B. E. (2016). Determination of the elastic behavior of silicon nanowires within a scanning electron microscope. *Journal of Nanomaterials*, 2016:36.
- [Wortman and Evans, 1965] Wortman, J. J. and Evans, R. A. (1965). Young’s modulus, shear modulus, and poisson’s ratio in silicon and germanium. *Journal of Applied Physics*, 36(1):153–156.
- [Xiao et al., 2022] Xiao, Y., Shang, J., Kou, L., and Li, C. (2022). Surface deformation-dependent mechanical properties of bending nanowires: an ab initio core-shell model. *Applied Mathematics and Mechanics*, 43(2):219–232.

- [Xie et al., 2023] Xie, S., Zhu, H., Zhang, X., and Wang, H. (2023). A brief review on the recent development of phonon engineering and manipulation at nanoscales. *International Journal of Extreme Manufacturing*.
- [Xu et al., 2022] Xu, B., Zhang, P., Zhu, J., Liu, Z., Eichler, A., Zheng, X.-Q., Lee, J., Dash, A., More, S., Wu, S., et al. (2022). Nanomechanical resonators: toward atomic scale. *Acs Nano*, 16(10):15545–15585.
- [Xu et al., 2010] Xu, F., Qin, Q., Mishra, A., Gu, Y., and Zhu, Y. (2010). Mechanical properties of ZnO Nanowires under different loading modes. *Nano Research*, 3(4):271–280.
- [Xu, 2020] Xu, W. (2020). *Molecular Dynamics Simulations of the Size-dependent Brittle-to-ductile Transition of Silicon Nanowires*. PhD thesis, University of Cincinnati.
- [Xu and Kim, 2019] Xu, W. and Kim, W. K. (2019). Molecular dynamics simulation of the uniaxial tensile test of silicon nanowires using the meam potential. *Mechanics of Materials*, 137:103140.
- [Xu and Kim, 2020] Xu, W. and Kim, W. K. (2020). Role of boundary conditions and thermostats in the uniaxial tensile loading of silicon nanowires. *Computational Materials Science*, 178:109636.
- [Xu et al., 2016] Xu, X.-J., Wang, Y.-C., Wang, B., and Zhang, K. (2016). A modified size-dependent core-shell model and its application in the wave propagation of square cellular networks. *Physica E: Low-dimensional Systems and Nanostructures*, 80:53–61.
- [Yaish et al., 2015] Yaish, Y., Calahorra, Y., Shtempluck, O., and Kotchetkov, V. (2015). Three-point bending analysis of doubly clamped silicon nanowire beams; young’s modulus, initial stress, and crystal orientation. *Journal of Applied Physics*, 117(16):164311.

- [Yang and Chandran, 2023] Yang, C. and Chandran, K. R. (2023). A critical review of silicon nanowire electrodes and their energy storage capacities in li-ion cells. *RSC advances*, 13(6):3947–3957.
- [Yang et al., 2022] Yang, C., Van Der Drift, E., and French, P. (2022). Review of scaling effects on physical properties and practicalities of cantilever sensors. *Journal of Micromechanics and Microengineering*, 32(10):103002.
- [Yang et al., 2002] Yang, J., Ono, T., and Esashi, M. (2002). Energy dissipation in submicrometer thick single-crystal silicon cantilevers. *Journal of Microelectromechanical systems*, 11(6):775–783.
- [Yang et al., 2021] Yang, L., Huh, D., Ning, R., Rapp, V., Zeng, Y., Liu, Y., Ju, S., Tao, Y., Jiang, Y., Beak, J., et al. (2021). High thermoelectric figure of merit of porous si nanowires from 300 to 700 k. *Nature communications*, 12(1):3926.
- [Yang and Guo, 2024] Yang, N. and Guo, J. (2024). Performance potential of transistors based on tellurium nanowire arrays: A quantum transport study. *Solid-State Electronics*, 213:108859.
- [Yang et al., 2006] Yang, Y.-T., Callegari, C., Feng, X., Ekinici, K. L., and Roukes, M. L. (2006). Zeptogram-scale nanomechanical mass sensing. *Nano letters*, 6(4):583–586.
- [Yang et al., 2009] Yang, Z., Lu, Z., and Zhao, Y.-P. (2009). Shape effects on the yield stress and deformation of silicon nanowires: A molecular dynamics simulation. *Journal of Applied Physics*, 106(2).
- [Yao et al., 2012] Yao, H., Yun, G., Bai, N., and Li, J. (2012). Surface elasticity effect on the size-dependent elastic property of nanowires. *Journal of Applied Physics*, 111(8):083506.

- [Ye et al., 2019] Ye, P., Ernst, T., and Khare, M. V. (2019). The last silicon transistor: Nanosheet devices could be the final evolutionary step for moore’s law. *IEEE spectrum*, 56(8):30–35.
- [Yi et al., 2000] Yi, T., Li, L., and Kim, C.-J. (2000). Microscale material testing of single crystalline silicon: process effects on surface morphology and tensile strength. *Sensors and Actuators A: Physical*, 83(1-3):172–178.
- [Yilmaz et al., 2017] Yilmaz, M., Kilinc, Y., Nadar, G., Tasdemir, Z., Wollschlager, N., Oesterle, W., Leblebici, Y., and Alaca, B. E. (2017). Top-down technique for scaling to nano in silicon mems. *Journal of Vacuum Science & Technology B, Nanotechnology and Microelectronics: Materials, Processing, Measurement, and Phenomena*, 35(2):022001.
- [Yokogawa et al., 2017] Yokogawa, R., Hashimoto, S., Asada, S., Tomita, M., Watanabe, T., and Ogura, A. (2017). Evaluation of controlled strain in silicon nanowire by uv raman spectroscopy. *Japanese Journal of Applied Physics*, 56(6S1):06GG10.
- [Yuan and Huang, 2012] Yuan, F. and Huang, L. (2012). Molecular dynamics simulation of amorphous silica under uniaxial tension: From bulk to nanowire. *Journal of Non-Crystalline Solids*, 358(24):3481–3487.
- [Yuan and Huang, 2013] Yuan, F. and Huang, L. (2013). Size-dependent elasticity of amorphous silica nanowire: A molecular dynamics study. *Applied Physics Letters*, 103(20):201905.
- [Zafar et al., 2018] Zafar, S., D’Emic, C., Jagtiani, A., Kratschmer, E., Miao, X., Zhu, Y., Mo, R., Sosa, N., Hamann, H., Shahidi, G., et al. (2018). Silicon nanowire field effect transistor sensors with minimal sensor-to-sensor variations and enhanced sensing characteristics. *Acs Nano*, 12(7):6577–6587.

- [Zare Pakzad et al., 2023a] Zare Pakzad, S., Akinci, S., Karimzadehkhoei, M., and Alaca, B. E. (2023a). Simplified top-down fabrication of sub-micron silicon nanowires. *Semiconductor Science and Technology*, 38(12):125005.
- [Zare Pakzad et al., 2023b] Zare Pakzad, S., Ali, B., Coban, S. B., Karimzadehkhoei, M., and Alaca, B. E. (2023b). Innovative mems stage for automated micromechanical testing. In *2023 International Conference on Manipulation, Automation and Robotics at Small Scales (MARSS)*, pages 1–6. IEEE.
- [Zare Pakzad et al., 2021] Zare Pakzad, S., Nasr Esfahani, M., Tasdemir, Z., Wollschlaeger, N., Li, X., Li, T., Yilmaz, M., Leblebici, Y., and Alaca, B. E. (2021). A new characterization approach to study the mechanical behavior of silicon nanowires. *MRS Advances*, pages 1–6.
- [Zare Pakzad et al., 2023c] Zare Pakzad, S., Nasr Esfahani, M., Tasdemir, Z., Wollschläger, N., Li, T., Li, X., Yilmaz, M., Leblebici, Y., and Alaca, B. E. (2023c). Nanomechanical modeling of the bending response of silicon nanowires. *ACS Applied Nano Materials*, 6(17):15465–15478.
- [Zhan and Gu, 2012] Zhan, H. and Gu, Y. (2012). Modified beam theories for bending properties of nanowires considering surface/intrinsic effects and axial extension effect. *Journal of applied physics*, 111(8):084305.
- [Zhang et al., 2021] Zhang, A., Lee, J.-H., and Lieber, C. M. (2021). Nanowire-enabled bioelectronics. *Nano Today*, 38:101135.
- [Zhang et al., 2010a] Zhang, D., Breguet, J.-M., Clavel, R., Sivakov, V., Christiansen, S., and Michler, J. (2010a). In situ electron microscopy mechanical testing of silicon nanowires using electrostatically actuated tensile stages. *Journal of Microelectromechanical Systems*, 19(3):663–674.

- [Zhang et al., 2022a] Zhang, D., Ren, Y., Barbot, A., Seichepine, F., Lo, B., Ma, Z.-C., and Yang, G.-Z. (2022a). Fabrication and optical manipulation of micro-robots for biomedical applications. *Matter*, 5(10):3135–3160.
- [Zhang et al., 2010b] Zhang, G.-J., Zhang, L., Huang, M. J., Luo, Z. H. H., Tay, G. K. I., Lim, E.-J. A., Kang, T. G., and Chen, Y. (2010b). Silicon nanowire biosensor for highly sensitive and rapid detection of dengue virus. *Sensors and Actuators B: Chemical*, 146(1):138–144.
- [Zhang et al., 2020] Zhang, H., Kikuchi, N., Ohshima, N., Kajisa, T., Sakata, T., Izumi, T., and Sone, H. (2020). Design and fabrication of silicon nanowire-based biosensors with integration of critical factors: toward ultrasensitive specific detection of biomolecules. *ACS Applied Materials & Interfaces*, 12(46):51808–51819.
- [Zhang et al., 2023] Zhang, H., Qiu, Y., Osawa, F., Itabashi, M., Ohshima, N., Kajisa, T., Sakata, T., Izumi, T., and Sone, H. (2023). Estimation of the depletion layer thickness in silicon nanowire-based biosensors from attomolar-level biomolecular detection. *ACS Applied Materials & Interfaces*, 15(16):19892–19903.
- [Zhang et al., 2016] Zhang, H., Tersoff, J., Xu, S., Chen, H., Zhang, Q., Zhang, K., Yang, Y., Lee, C.-S., Tu, K.-N., Li, J., et al. (2016). Approaching the ideal elastic strain limit in silicon nanowires. *Science advances*, 2(8):e1501382.
- [Zhang et al., 2004] Zhang, W., Zhang, W., Turner, K., and Hartwell, P. G. (2004). Scream’03: A single mask process for high-q single crystal silicon mems. In *ASME International Mechanical Engineering Congress and Exposition*, volume 47144, pages 211–215.
- [Zhang et al., 2022b] Zhang, Y., Cai, J., Mi, C., Wang, F., and Akbarzadeh, A. (2022b). Effect of surface residual stress and surface layer stiffness on mechanical properties of nanowires. *Acta Mechanica*, 233(1):233–257.

- [Zheng et al., 2009] Zheng, K., Han, X., Wang, L., Zhang, Y., Yue, Y., Qin, Y., Zhang, X., and Zhang, Z. (2009). Atomic mechanisms governing the elastic limit and the incipient plasticity of bending si nanowires. *Nano letters*, 9(6):2471–2476.
- [Zhou et al., 2003] Zhou, X., Hu, J., Li, C., Ma, D., Lee, C., and Lee, S. (2003). Silicon nanowires as chemical sensors. *Chemical Physics Letters*, 369(1-2):220–224.
- [Zhu et al., 2019] Zhu, J., Liu, X., Shi, Q., He, T., Sun, Z., Guo, X., Liu, W., Sulaiman, O. B., Dong, B., and Lee, C. (2019). Development trends and perspectives of future sensors and mems/nems. *Micromachines*, 11(1):7.
- [Zhu et al., 2020] Zhu, J., Liu, X., Shi, Q., He, T., Sun, Z., Guo, X., Liu, W., Sulaiman, O. B., Dong, B., and Lee, C. (2020). Development trends and perspectives of future sensors and mems/nems. *Micromachines*, 11(1):7.
- [Zhu, 2017] Zhu, Y. (2017). Mechanics of crystalline nanowires: an experimental perspective. *Applied Mechanics Reviews*, 69(1):010802.
- [Zhu, 2023] Zhu, Y. (2023). MemS platforms for in-situ testing of mechanical properties of nanostructures.
- [Zhu and Chang, 2015] Zhu, Y. and Chang, T.-H. (2015). A review of microelectromechanical systems for nanoscale mechanical characterization. *Journal of Micromechanics and Microengineering*, 25(9):093001.
- [Zhu et al., 2009] Zhu, Y., Xu, F., Qin, Q., Fung, W. Y., and Lu, W. (2009). Mechanical properties of vapor- liquid- solid synthesized silicon nanowires. *Nano letters*, 9(11):3934–3939.
- [Zhuo and Beom, 2018] Zhuo, X. and Beom, H. (2018). Atomistic study of the bending properties of silicon nanowires. *Computational Materials Science*, 152:331–336.

- [Zhuo and Beom, 2019] Zhuo, X. R. and Beom, H. G. (2019). Effect of side surface orientation on the mechanical properties of silicon nanowires: A molecular dynamics study. *Crystals*, 9(2).
- [Zimmerman et al., 2004] Zimmerman, J. A., WebbIII, E. B., Hoyt, J., Jones, R. E., Klein, P., and Bammann, D. J. (2004). Calculation of stress in atomistic simulation. *Modelling and simulation in materials science and engineering*, 12(4):S319.
- [Zou et al., 2017] Zou, H., Wang, J., Chen, F., Bao, H., Jiao, D., Zhang, K., Song, Z., and Li, X. (2017). Monolithically integrated tri-axis shock accelerometers with mhz-level high resonant-frequency. *Journal of Micromechanics and Micro-engineering*, 27(7):075009.



## Appendix A

### **MACHINE LEARNING DATA**

The appendix contains the information pertaining to molecular dynamics simulations carried out on silicon nanowires. The tables contain data regarding critical dimension (CD), crystal orientation (ORNT), length (L), boundary condition (BC), temperature (T), interatomic potential (POT), surface state (SS), and modulus of elasticity (E).

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|---------|---------|---------|
| 2       | < 100 > | 14     | P-Tensile | 10    | Tersoff | 0       | 87.5    |
| 3       | < 100 > | 21     | P-Tensile | 10    | Tersoff | 0       | 84.8    |
| 4       | < 100 > | 28     | P-Tensile | 10    | Tersoff | 0       | 90.2    |
| 5       | < 100 > | 35     | P-Tensile | 10    | Tersoff | 0       | 88.8    |
| 6       | < 100 > | 42     | P-Tensile | 10    | Tersoff | 0       | 92.9    |
| 7       | < 100 > | 49     | P-Tensile | 10    | Tersoff | 0       | 91.2    |
| 8       | < 100 > | 56     | P-Tensile | 10    | Tersoff | 0       | 94.5    |
| 9       | < 100 > | 63     | P-Tensile | 10    | Tersoff | 0       | 92.0    |
| 10      | < 100 > | 70     | P-Tensile | 10    | Tersoff | 0       | 93.7    |
| 2       | < 110 > | 14     | P-Tensile | 10    | Tersoff | 0       | 180.0   |
| 3       | < 110 > | 21     | P-Tensile | 10    | Tersoff | 0       | 151.6   |
| 4       | < 110 > | 28     | P-Tensile | 10    | Tersoff | 0       | 151.1   |
| 5       | < 110 > | 35     | P-Tensile | 10    | Tersoff | 0       | 148.6   |
| 6       | < 110 > | 42     | P-Tensile | 10    | Tersoff | 0       | 152.9   |
| 7       | < 110 > | 49     | P-Tensile | 10    | Tersoff | 0       | 149.5   |
| 8       | < 110 > | 56     | P-Tensile | 10    | Tersoff | 0       | 144.1   |
| 9       | < 110 > | 63     | P-Tensile | 10    | Tersoff | 0       | 143.8   |
| 10      | < 110 > | 70     | P-Tensile | 10    | Tersoff | 0       | 150.9   |
| 2       | < 100 > | 16     | P-Tensile | 10    | Tersoff | 0       | 86.1    |
| 3       | < 100 > | 24     | P-Tensile | 10    | Tersoff | 0       | 85.5    |
| 4       | < 100 > | 32     | P-Tensile | 10    | Tersoff | 0       | 90.8    |
| 5       | < 100 > | 40     | P-Tensile | 10    | Tersoff | 0       | 88.3    |
| 6       | < 100 > | 48     | P-Tensile | 10    | Tersoff | 0       | 92.7    |
| 7       | < 100 > | 56     | P-Tensile | 10    | Tersoff | 0       | 91.1    |
| 8       | < 100 > | 64     | P-Tensile | 10    | Tersoff | 0       | 94.1    |
| 9       | < 100 > | 72     | P-Tensile | 10    | Tersoff | 0       | 92.1    |
| 10      | < 100 > | 80     | P-Tensile | 10    | Tersoff | 0       | 94.1    |
| 2       | < 110 > | 16     | P-Tensile | 10    | Tersoff | 0       | 180.3   |
| 3       | < 110 > | 24     | P-Tensile | 10    | Tersoff | 0       | 155.4   |
| 4       | < 110 > | 32     | P-Tensile | 10    | Tersoff | 0       | 150.5   |
| 5       | < 110 > | 40     | P-Tensile | 10    | Tersoff | 0       | 148.1   |
| 6       | < 110 > | 48     | P-Tensile | 10    | Tersoff | 0       | 151.0   |
| 7       | < 110 > | 56     | P-Tensile | 10    | Tersoff | 0       | 150.2   |
| 8       | < 110 > | 64     | P-Tensile | 10    | Tersoff | 0       | 143.4   |
| 9       | < 110 > | 72     | P-Tensile | 10    | Tersoff | 0       | 143.2   |
| 10      | < 110 > | 80     | P-Tensile | 10    | Tersoff | 0       | 149.5   |
| 2       | < 100 > | 18     | P-Tensile | 10    | Tersoff | 0       | 87.1    |
| 3       | < 100 > | 27     | P-Tensile | 10    | Tersoff | 0       | 83.4    |
| 4       | < 100 > | 36     | P-Tensile | 10    | Tersoff | 0       | 90.0    |
| 5       | < 100 > | 45     | P-Tensile | 10    | Tersoff | 0       | 88.0    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|---------|---------|---------|
| 6       | < 100 > | 54     | P-Tensile | 10    | Tersoff | 0       | 92.2    |
| 7       | < 100 > | 63     | P-Tensile | 10    | Tersoff | 0       | 90.3    |
| 8       | < 100 > | 72     | P-Tensile | 10    | Tersoff | 0       | 92.4    |
| 9       | < 100 > | 81     | P-Tensile | 10    | Tersoff | 0       | 91.9    |
| 10      | < 100 > | 90     | P-Tensile | 10    | Tersoff | 0       | 93.4    |
| 2       | < 110 > | 18     | P-Tensile | 10    | Tersoff | 0       | 182.8   |
| 3       | < 110 > | 27     | P-Tensile | 10    | Tersoff | 0       | 156.4   |
| 4       | < 110 > | 36     | P-Tensile | 10    | Tersoff | 0       | 151.3   |
| 5       | < 110 > | 45     | P-Tensile | 10    | Tersoff | 0       | 147.5   |
| 6       | < 110 > | 54     | P-Tensile | 10    | Tersoff | 0       | 151.5   |
| 7       | < 110 > | 63     | P-Tensile | 10    | Tersoff | 0       | 150.0   |
| 8       | < 110 > | 72     | P-Tensile | 10    | Tersoff | 0       | 143.7   |
| 9       | < 110 > | 81     | P-Tensile | 10    | Tersoff | 0       | 143.2   |
| 10      | < 110 > | 90     | P-Tensile | 10    | Tersoff | 0       | 148.0   |
| 2       | < 100 > | 20     | P-Tensile | 10    | Tersoff | 0       | 86.2    |
| 3       | < 100 > | 30     | P-Tensile | 10    | Tersoff | 0       | 84.6    |
| 4       | < 100 > | 40     | P-Tensile | 10    | Tersoff | 0       | 91.1    |
| 5       | < 100 > | 50     | P-Tensile | 10    | Tersoff | 0       | 89.4    |
| 6       | < 100 > | 60     | P-Tensile | 10    | Tersoff | 0       | 92.7    |
| 7       | < 100 > | 70     | P-Tensile | 10    | Tersoff | 0       | 91.2    |
| 8       | < 100 > | 80     | P-Tensile | 10    | Tersoff | 0       | 92.5    |
| 9       | < 100 > | 90     | P-Tensile | 10    | Tersoff | 0       | 91.0    |
| 10      | < 100 > | 100    | P-Tensile | 10    | Tersoff | 0       | 93.5    |
| 2       | < 110 > | 20     | P-Tensile | 10    | Tersoff | 0       | 174.7   |
| 3       | < 110 > | 30     | P-Tensile | 10    | Tersoff | 0       | 155.4   |
| 4       | < 110 > | 40     | P-Tensile | 10    | Tersoff | 0       | 150.7   |
| 5       | < 110 > | 50     | P-Tensile | 10    | Tersoff | 0       | 147.6   |
| 6       | < 110 > | 60     | P-Tensile | 10    | Tersoff | 0       | 150.2   |
| 7       | < 110 > | 70     | P-Tensile | 10    | Tersoff | 0       | 150.3   |
| 8       | < 110 > | 80     | P-Tensile | 10    | Tersoff | 0       | 143.3   |
| 9       | < 110 > | 90     | P-Tensile | 10    | Tersoff | 0       | 142.6   |
| 10      | < 110 > | 100    | P-Tensile | 10    | Tersoff | 0       | 148.3   |
| 2       | < 100 > | 24     | P-Tensile | 10    | Tersoff | 0       | 80.1    |
| 3       | < 100 > | 36     | P-Tensile | 10    | Tersoff | 0       | 84.6    |
| 4       | < 100 > | 48     | P-Tensile | 10    | Tersoff | 0       | 90.5    |
| 5       | < 100 > | 60     | P-Tensile | 10    | Tersoff | 0       | 87.6    |
| 6       | < 100 > | 72     | P-Tensile | 10    | Tersoff | 0       | 92.7    |
| 7       | < 100 > | 84     | P-Tensile | 10    | Tersoff | 0       | 90.3    |
| 8       | < 100 > | 96     | P-Tensile | 10    | Tersoff | 0       | 93.1    |
| 9       | < 100 > | 108    | P-Tensile | 10    | Tersoff | 0       | 91.6    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|---------|---------|---------|
| 10      | < 100 > | 120    | P-Tensile | 10    | Tersoff | 0       | 93.1    |
| 2       | < 110 > | 24     | P-Tensile | 10    | Tersoff | 0       | 179.0   |
| 3       | < 110 > | 36     | P-Tensile | 10    | Tersoff | 0       | 155.5   |
| 4       | < 110 > | 48     | P-Tensile | 10    | Tersoff | 0       | 150.6   |
| 5       | < 110 > | 60     | P-Tensile | 10    | Tersoff | 0       | 147.2   |
| 6       | < 110 > | 72     | P-Tensile | 10    | Tersoff | 0       | 150.0   |
| 7       | < 110 > | 84     | P-Tensile | 10    | Tersoff | 0       | 150.0   |
| 8       | < 110 > | 96     | P-Tensile | 10    | Tersoff | 0       | 143.5   |
| 9       | < 110 > | 108    | P-Tensile | 10    | Tersoff | 0       | 142.6   |
| 10      | < 110 > | 120    | P-Tensile | 10    | Tersoff | 0       | 147.5   |
| 2       | < 100 > | 28     | P-Tensile | 10    | Tersoff | 0       | 86.1    |
| 3       | < 100 > | 42     | P-Tensile | 10    | Tersoff | 0       | 84.3    |
| 4       | < 100 > | 56     | P-Tensile | 10    | Tersoff | 0       | 90.0    |
| 5       | < 100 > | 70     | P-Tensile | 10    | Tersoff | 0       | 88.4    |
| 6       | < 100 > | 84     | P-Tensile | 10    | Tersoff | 0       | 92.0    |
| 7       | < 100 > | 98     | P-Tensile | 10    | Tersoff | 0       | 90.0    |
| 8       | < 100 > | 112    | P-Tensile | 10    | Tersoff | 0       | 93.1    |
| 9       | < 100 > | 126    | P-Tensile | 10    | Tersoff | 0       | 90.7    |
| 10      | < 100 > | 140    | P-Tensile | 10    | Tersoff | 0       | 93.2    |
| 2       | < 110 > | 28     | P-Tensile | 10    | Tersoff | 0       | 183.4   |
| 3       | < 110 > | 42     | P-Tensile | 10    | Tersoff | 0       | 150.2   |
| 4       | < 110 > | 56     | P-Tensile | 10    | Tersoff | 0       | 150.7   |
| 5       | < 110 > | 70     | P-Tensile | 10    | Tersoff | 0       | 147.4   |
| 6       | < 110 > | 84     | P-Tensile | 10    | Tersoff | 0       | 150.9   |
| 7       | < 110 > | 98     | P-Tensile | 10    | Tersoff | 0       | 150.1   |
| 8       | < 110 > | 112    | P-Tensile | 10    | Tersoff | 0       | 143.8   |
| 9       | < 110 > | 126    | P-Tensile | 10    | Tersoff | 0       | 142.6   |
| 10      | < 110 > | 140    | P-Tensile | 10    | Tersoff | 0       | 148.2   |
| 2       | < 100 > | 32     | P-Tensile | 10    | Tersoff | 0       | 85.5    |
| 3       | < 100 > | 48     | P-Tensile | 10    | Tersoff | 0       | 84.5    |
| 4       | < 100 > | 64     | P-Tensile | 10    | Tersoff | 0       | 89.8    |
| 5       | < 100 > | 80     | P-Tensile | 10    | Tersoff | 0       | 89.1    |
| 6       | < 100 > | 96     | P-Tensile | 10    | Tersoff | 0       | 92.6    |
| 7       | < 100 > | 112    | P-Tensile | 10    | Tersoff | 0       | 90.4    |
| 8       | < 100 > | 128    | P-Tensile | 10    | Tersoff | 0       | 92.8    |
| 9       | < 100 > | 144    | P-Tensile | 10    | Tersoff | 0       | 90.9    |
| 10      | < 100 > | 160    | P-Tensile | 10    | Tersoff | 0       | 93.2    |
| 2       | < 110 > | 32     | P-Tensile | 10    | Tersoff | 0       | 183.9   |
| 3       | < 110 > | 48     | P-Tensile | 10    | Tersoff | 0       | 161.6   |
| 4       | < 110 > | 64     | P-Tensile | 10    | Tersoff | 0       | 151.3   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|---------|---------|---------|
| 5       | < 110 > | 80     | P-Tensile | 10    | Tersoff | 0       | 147.4   |
| 6       | < 110 > | 96     | P-Tensile | 10    | Tersoff | 0       | 150.7   |
| 7       | < 110 > | 112    | P-Tensile | 10    | Tersoff | 0       | 150.1   |
| 8       | < 110 > | 128    | P-Tensile | 10    | Tersoff | 0       | 143.8   |
| 9       | < 110 > | 144    | P-Tensile | 10    | Tersoff | 0       | 142.8   |
| 10      | < 110 > | 160    | P-Tensile | 10    | Tersoff | 0       | 148.1   |
| 2       | < 100 > | 36     | P-Tensile | 10    | Tersoff | 0       | 86.2    |
| 3       | < 100 > | 54     | P-Tensile | 10    | Tersoff | 0       | 82.7    |
| 4       | < 100 > | 72     | P-Tensile | 10    | Tersoff | 0       | 90.1    |
| 5       | < 100 > | 90     | P-Tensile | 10    | Tersoff | 0       | 88.9    |
| 6       | < 100 > | 108    | P-Tensile | 10    | Tersoff | 0       | 91.8    |
| 7       | < 100 > | 126    | P-Tensile | 10    | Tersoff | 0       | 90.1    |
| 8       | < 100 > | 144    | P-Tensile | 10    | Tersoff | 0       | 93.1    |
| 9       | < 100 > | 162    | P-Tensile | 10    | Tersoff | 0       | 90.9    |
| 10      | < 100 > | 180    | P-Tensile | 10    | Tersoff | 0       | 93.3    |
| 2       | < 110 > | 36     | P-Tensile | 10    | Tersoff | 0       | 167.3   |
| 3       | < 110 > | 54     | P-Tensile | 10    | Tersoff | 0       | 156.9   |
| 4       | < 110 > | 72     | P-Tensile | 10    | Tersoff | 0       | 147.9   |
| 5       | < 110 > | 90     | P-Tensile | 10    | Tersoff | 0       | 147.2   |
| 6       | < 110 > | 108    | P-Tensile | 10    | Tersoff | 0       | 150.5   |
| 7       | < 110 > | 126    | P-Tensile | 10    | Tersoff | 0       | 150.2   |
| 8       | < 110 > | 144    | P-Tensile | 10    | Tersoff | 0       | 144.2   |
| 9       | < 110 > | 162    | P-Tensile | 10    | Tersoff | 0       | 143.3   |
| 10      | < 110 > | 180    | P-Tensile | 10    | Tersoff | 0       | 148.7   |
| 2       | < 100 > | 40     | P-Tensile | 10    | Tersoff | 0       | 85.3    |
| 3       | < 100 > | 60     | P-Tensile | 10    | Tersoff | 0       | 75.6    |
| 4       | < 100 > | 80     | P-Tensile | 10    | Tersoff | 0       | 90.2    |
| 5       | < 100 > | 100    | P-Tensile | 10    | Tersoff | 0       | 88.6    |
| 6       | < 100 > | 120    | P-Tensile | 10    | Tersoff | 0       | 91.7    |
| 7       | < 100 > | 140    | P-Tensile | 10    | Tersoff | 0       | 91.2    |
| 8       | < 100 > | 160    | P-Tensile | 10    | Tersoff | 0       | 93.3    |
| 9       | < 100 > | 180    | P-Tensile | 10    | Tersoff | 0       | 90.9    |
| 10      | < 100 > | 200    | P-Tensile | 10    | Tersoff | 0       | 93.2    |
| 2       | < 110 > | 40     | P-Tensile | 10    | Tersoff | 0       | 174.3   |
| 3       | < 110 > | 60     | P-Tensile | 10    | Tersoff | 0       | 149.2   |
| 4       | < 110 > | 80     | P-Tensile | 10    | Tersoff | 0       | 148.3   |
| 5       | < 110 > | 100    | P-Tensile | 10    | Tersoff | 0       | 145.9   |
| 6       | < 110 > | 120    | P-Tensile | 10    | Tersoff | 0       | 151.3   |
| 7       | < 110 > | 140    | P-Tensile | 10    | Tersoff | 0       | 149.9   |
| 8       | < 110 > | 160    | P-Tensile | 10    | Tersoff | 0       | 144.1   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 9       | < 110 > | 180    | P-Tensile  | 10    | Tersoff | 0       | 142.6   |
| 10      | < 110 > | 200    | P-Tensile  | 10    | Tersoff | 0       | 149.2   |
| 2       | < 100 > | 14     | NP-Tensile | 10    | Tersoff | 0       | 103.1   |
| 3       | < 100 > | 21     | NP-Tensile | 10    | Tersoff | 0       | 112.6   |
| 4       | < 100 > | 28     | NP-Tensile | 10    | Tersoff | 0       | 117.7   |
| 5       | < 100 > | 35     | NP-Tensile | 10    | Tersoff | 0       | 120.9   |
| 6       | < 100 > | 42     | NP-Tensile | 10    | Tersoff | 0       | 123.8   |
| 7       | < 100 > | 49     | NP-Tensile | 10    | Tersoff | 0       | 125.0   |
| 8       | < 100 > | 56     | NP-Tensile | 10    | Tersoff | 0       | 126.2   |
| 9       | < 100 > | 63     | NP-Tensile | 10    | Tersoff | 0       | 126.8   |
| 10      | < 100 > | 70     | NP-Tensile | 10    | Tersoff | 0       | 127.8   |
| 2       | < 110 > | 14     | NP-Tensile | 10    | Tersoff | 0       | 210.5   |
| 3       | < 110 > | 21     | NP-Tensile | 10    | Tersoff | 0       | 205.4   |
| 4       | < 110 > | 28     | NP-Tensile | 10    | Tersoff | 0       | 188.2   |
| 5       | < 110 > | 35     | NP-Tensile | 10    | Tersoff | 0       | 189.1   |
| 6       | < 110 > | 42     | NP-Tensile | 10    | Tersoff | 0       | 199.1   |
| 7       | < 110 > | 49     | NP-Tensile | 10    | Tersoff | 0       | 197.9   |
| 8       | < 110 > | 56     | NP-Tensile | 10    | Tersoff | 0       | 191.3   |
| 9       | < 110 > | 63     | NP-Tensile | 10    | Tersoff | 0       | 191.3   |
| 10      | < 110 > | 70     | NP-Tensile | 10    | Tersoff | 0       | 197.1   |
| 2       | < 100 > | 16     | NP-Tensile | 10    | Tersoff | 0       | 103.2   |
| 3       | < 100 > | 24     | NP-Tensile | 10    | Tersoff | 0       | 113.0   |
| 4       | < 100 > | 32     | NP-Tensile | 10    | Tersoff | 0       | 117.3   |
| 5       | < 100 > | 40     | NP-Tensile | 10    | Tersoff | 0       | 120.5   |
| 6       | < 100 > | 48     | NP-Tensile | 10    | Tersoff | 0       | 123.6   |
| 7       | < 100 > | 56     | NP-Tensile | 10    | Tersoff | 0       | 125.0   |
| 8       | < 100 > | 64     | NP-Tensile | 10    | Tersoff | 0       | 125.9   |
| 9       | < 100 > | 72     | NP-Tensile | 10    | Tersoff | 0       | 126.8   |
| 10      | < 100 > | 80     | NP-Tensile | 10    | Tersoff | 0       | 127.8   |
| 2       | < 110 > | 16     | NP-Tensile | 10    | Tersoff | 0       | 209.2   |
| 3       | < 110 > | 24     | NP-Tensile | 10    | Tersoff | 0       | 204.7   |
| 4       | < 110 > | 32     | NP-Tensile | 10    | Tersoff | 0       | 187.4   |
| 5       | < 110 > | 40     | NP-Tensile | 10    | Tersoff | 0       | 189.0   |
| 6       | < 110 > | 48     | NP-Tensile | 10    | Tersoff | 0       | 199.1   |
| 7       | < 110 > | 56     | NP-Tensile | 10    | Tersoff | 0       | 198.1   |
| 8       | < 110 > | 64     | NP-Tensile | 10    | Tersoff | 0       | 191.7   |
| 9       | < 110 > | 72     | NP-Tensile | 10    | Tersoff | 0       | 192.3   |
| 10      | < 110 > | 80     | NP-Tensile | 10    | Tersoff | 0       | 197.1   |
| 2       | < 100 > | 18     | NP-Tensile | 10    | Tersoff | 0       | 103.7   |
| 3       | < 100 > | 27     | NP-Tensile | 10    | Tersoff | 0       | 112.6   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 4       | < 100 > | 36     | NP-Tensile | 10    | Tersoff | 0       | 117.5   |
| 5       | < 100 > | 45     | NP-Tensile | 10    | Tersoff | 0       | 120.6   |
| 6       | < 100 > | 54     | NP-Tensile | 10    | Tersoff | 0       | 123.3   |
| 7       | < 100 > | 63     | NP-Tensile | 10    | Tersoff | 0       | 124.6   |
| 8       | < 100 > | 72     | NP-Tensile | 10    | Tersoff | 0       | 125.9   |
| 9       | < 100 > | 81     | NP-Tensile | 10    | Tersoff | 0       | 126.8   |
| 10      | < 100 > | 90     | NP-Tensile | 10    | Tersoff | 0       | 127.6   |
| 2       | < 110 > | 18     | NP-Tensile | 10    | Tersoff | 0       | 209.3   |
| 3       | < 110 > | 27     | NP-Tensile | 10    | Tersoff | 0       | 205.5   |
| 4       | < 110 > | 36     | NP-Tensile | 10    | Tersoff | 0       | 185.9   |
| 5       | < 110 > | 45     | NP-Tensile | 10    | Tersoff | 0       | 187.3   |
| 6       | < 110 > | 54     | NP-Tensile | 10    | Tersoff | 0       | 199.0   |
| 7       | < 110 > | 63     | NP-Tensile | 10    | Tersoff | 0       | 197.9   |
| 8       | < 110 > | 72     | NP-Tensile | 10    | Tersoff | 0       | 192.0   |
| 9       | < 110 > | 81     | NP-Tensile | 10    | Tersoff | 0       | 192.1   |
| 10      | < 110 > | 90     | NP-Tensile | 10    | Tersoff | 0       | 197.0   |
| 2       | < 100 > | 20     | NP-Tensile | 10    | Tersoff | 0       | 102.8   |
| 3       | < 100 > | 30     | NP-Tensile | 10    | Tersoff | 0       | 112.5   |
| 4       | < 100 > | 40     | NP-Tensile | 10    | Tersoff | 0       | 117.2   |
| 5       | < 100 > | 50     | NP-Tensile | 10    | Tersoff | 0       | 120.7   |
| 6       | < 100 > | 60     | NP-Tensile | 10    | Tersoff | 0       | 123.3   |
| 7       | < 100 > | 70     | NP-Tensile | 10    | Tersoff | 0       | 124.7   |
| 8       | < 100 > | 80     | NP-Tensile | 10    | Tersoff | 0       | 125.8   |
| 9       | < 100 > | 90     | NP-Tensile | 10    | Tersoff | 0       | 126.6   |
| 10      | < 100 > | 100    | NP-Tensile | 10    | Tersoff | 0       | 127.6   |
| 2       | < 110 > | 20     | NP-Tensile | 10    | Tersoff | 0       | 210.7   |
| 3       | < 110 > | 30     | NP-Tensile | 10    | Tersoff | 0       | 205.5   |
| 4       | < 110 > | 40     | NP-Tensile | 10    | Tersoff | 0       | 185.0   |
| 5       | < 110 > | 50     | NP-Tensile | 10    | Tersoff | 0       | 186.9   |
| 6       | < 110 > | 60     | NP-Tensile | 10    | Tersoff | 0       | 199.0   |
| 7       | < 110 > | 70     | NP-Tensile | 10    | Tersoff | 0       | 198.4   |
| 8       | < 110 > | 80     | NP-Tensile | 10    | Tersoff | 0       | 192.3   |
| 9       | < 110 > | 90     | NP-Tensile | 10    | Tersoff | 0       | 192.4   |
| 10      | < 110 > | 100    | NP-Tensile | 10    | Tersoff | 0       | 196.6   |
| 2       | < 100 > | 24     | NP-Tensile | 10    | Tersoff | 0       | 103.8   |
| 3       | < 100 > | 36     | NP-Tensile | 10    | Tersoff | 0       | 112.4   |
| 4       | < 100 > | 48     | NP-Tensile | 10    | Tersoff | 0       | 117.5   |
| 5       | < 100 > | 60     | NP-Tensile | 10    | Tersoff | 0       | 120.4   |
| 6       | < 100 > | 72     | NP-Tensile | 10    | Tersoff | 0       | 123.2   |
| 7       | < 100 > | 84     | NP-Tensile | 10    | Tersoff | 0       | 124.6   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 8       | < 100 > | 96     | NP-Tensile | 10    | Tersoff | 0       | 125.6   |
| 9       | < 100 > | 108    | NP-Tensile | 10    | Tersoff | 0       | 126.4   |
| 10      | < 100 > | 120    | NP-Tensile | 10    | Tersoff | 0       | 127.4   |
| 2       | < 110 > | 24     | NP-Tensile | 10    | Tersoff | 0       | 209.5   |
| 3       | < 110 > | 36     | NP-Tensile | 10    | Tersoff | 0       | 204.8   |
| 4       | < 110 > | 48     | NP-Tensile | 10    | Tersoff | 0       | 183.3   |
| 5       | < 110 > | 60     | NP-Tensile | 10    | Tersoff | 0       | 186.7   |
| 6       | < 110 > | 72     | NP-Tensile | 10    | Tersoff | 0       | 198.6   |
| 7       | < 110 > | 84     | NP-Tensile | 10    | Tersoff | 0       | 198.4   |
| 8       | < 110 > | 96     | NP-Tensile | 10    | Tersoff | 0       | 191.6   |
| 9       | < 110 > | 108    | NP-Tensile | 10    | Tersoff | 0       | 191.8   |
| 10      | < 110 > | 120    | NP-Tensile | 10    | Tersoff | 0       | 196.6   |
| 2       | < 100 > | 28     | NP-Tensile | 10    | Tersoff | 0       | 103.1   |
| 3       | < 100 > | 42     | NP-Tensile | 10    | Tersoff | 0       | 112.5   |
| 4       | < 100 > | 56     | NP-Tensile | 10    | Tersoff | 0       | 117.3   |
| 5       | < 100 > | 70     | NP-Tensile | 10    | Tersoff | 0       | 120.3   |
| 6       | < 100 > | 84     | NP-Tensile | 10    | Tersoff | 0       | 123.1   |
| 7       | < 100 > | 98     | NP-Tensile | 10    | Tersoff | 0       | 124.5   |
| 8       | < 100 > | 112    | NP-Tensile | 10    | Tersoff | 0       | 125.6   |
| 9       | < 100 > | 126    | NP-Tensile | 10    | Tersoff | 0       | 126.3   |
| 10      | < 100 > | 140    | NP-Tensile | 10    | Tersoff | 0       | 127.3   |
| 2       | < 110 > | 28     | NP-Tensile | 10    | Tersoff | 0       | 208.9   |
| 3       | < 110 > | 42     | NP-Tensile | 10    | Tersoff | 0       | 205.3   |
| 4       | < 110 > | 56     | NP-Tensile | 10    | Tersoff | 0       | 181.6   |
| 5       | < 110 > | 70     | NP-Tensile | 10    | Tersoff | 0       | 190.5   |
| 6       | < 110 > | 84     | NP-Tensile | 10    | Tersoff | 0       | 198.8   |
| 7       | < 110 > | 98     | NP-Tensile | 10    | Tersoff | 0       | 197.9   |
| 8       | < 110 > | 112    | NP-Tensile | 10    | Tersoff | 0       | 191.5   |
| 9       | < 110 > | 126    | NP-Tensile | 10    | Tersoff | 0       | 191.7   |
| 10      | < 110 > | 140    | NP-Tensile | 10    | Tersoff | 0       | 196.4   |
| 2       | < 100 > | 32     | NP-Tensile | 10    | Tersoff | 0       | 103.0   |
| 3       | < 100 > | 48     | NP-Tensile | 10    | Tersoff | 0       | 112.5   |
| 4       | < 100 > | 64     | NP-Tensile | 10    | Tersoff | 0       | 117.1   |
| 5       | < 100 > | 80     | NP-Tensile | 10    | Tersoff | 0       | 120.3   |
| 6       | < 100 > | 96     | NP-Tensile | 10    | Tersoff | 0       | 123.1   |
| 7       | < 100 > | 112    | NP-Tensile | 10    | Tersoff | 0       | 124.5   |
| 8       | < 100 > | 128    | NP-Tensile | 10    | Tersoff | 0       | 125.5   |
| 9       | < 100 > | 144    | NP-Tensile | 10    | Tersoff | 0       | 126.3   |
| 10      | < 100 > | 160    | NP-Tensile | 10    | Tersoff | 0       | 127.2   |
| 2       | < 110 > | 32     | NP-Tensile | 10    | Tersoff | 0       | 211.3   |



Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 3       | < 110 > | 48     | NP-Tensile | 10    | Tersoff | 0       | 205.4   |
| 4       | < 110 > | 64     | NP-Tensile | 10    | Tersoff | 0       | 178.2   |
| 5       | < 110 > | 80     | NP-Tensile | 10    | Tersoff | 0       | 190.5   |
| 6       | < 110 > | 96     | NP-Tensile | 10    | Tersoff | 0       | 198.4   |
| 7       | < 110 > | 112    | NP-Tensile | 10    | Tersoff | 0       | 197.9   |
| 8       | < 110 > | 128    | NP-Tensile | 10    | Tersoff | 0       | 191.5   |
| 9       | < 110 > | 144    | NP-Tensile | 10    | Tersoff | 0       | 191.9   |
| 10      | < 110 > | 160    | NP-Tensile | 10    | Tersoff | 0       | 196.5   |
| 2       | < 100 > | 36     | NP-Tensile | 10    | Tersoff | 0       | 103.3   |
| 3       | < 100 > | 54     | NP-Tensile | 10    | Tersoff | 0       | 112.3   |
| 4       | < 100 > | 72     | NP-Tensile | 10    | Tersoff | 0       | 117.2   |
| 5       | < 100 > | 90     | NP-Tensile | 10    | Tersoff | 0       | 120.2   |
| 6       | < 100 > | 108    | NP-Tensile | 10    | Tersoff | 0       | 123.0   |
| 7       | < 100 > | 126    | NP-Tensile | 10    | Tersoff | 0       | 124.3   |
| 8       | < 100 > | 144    | NP-Tensile | 10    | Tersoff | 0       | 125.4   |
| 9       | < 100 > | 162    | NP-Tensile | 10    | Tersoff | 0       | 126.3   |
| 10      | < 100 > | 180    | NP-Tensile | 10    | Tersoff | 0       | 127.2   |
| 2       | < 110 > | 36     | NP-Tensile | 10    | Tersoff | 0       | 210.9   |
| 3       | < 110 > | 54     | NP-Tensile | 10    | Tersoff | 0       | 205.4   |
| 4       | < 110 > | 72     | NP-Tensile | 10    | Tersoff | 0       | 172.4   |
| 5       | < 110 > | 90     | NP-Tensile | 10    | Tersoff | 0       | 190.2   |
| 6       | < 110 > | 108    | NP-Tensile | 10    | Tersoff | 0       | 198.5   |
| 7       | < 110 > | 126    | NP-Tensile | 10    | Tersoff | 0       | 197.8   |
| 8       | < 110 > | 144    | NP-Tensile | 10    | Tersoff | 0       | 191.8   |
| 9       | < 110 > | 162    | NP-Tensile | 10    | Tersoff | 0       | 193.0   |
| 10      | < 110 > | 180    | NP-Tensile | 10    | Tersoff | 0       | 196.4   |
| 2       | < 100 > | 40     | NP-Tensile | 10    | Tersoff | 0       | 103.1   |
| 3       | < 100 > | 60     | NP-Tensile | 10    | Tersoff | 0       | 112.3   |
| 4       | < 100 > | 80     | NP-Tensile | 10    | Tersoff | 0       | 117.1   |
| 5       | < 100 > | 100    | NP-Tensile | 10    | Tersoff | 0       | 120.3   |
| 6       | < 100 > | 120    | NP-Tensile | 10    | Tersoff | 0       | 123.0   |
| 7       | < 100 > | 140    | NP-Tensile | 10    | Tersoff | 0       | 124.3   |
| 8       | < 100 > | 160    | NP-Tensile | 10    | Tersoff | 0       | 125.3   |
| 9       | < 100 > | 180    | NP-Tensile | 10    | Tersoff | 0       | 126.1   |
| 10      | < 100 > | 200    | NP-Tensile | 10    | Tersoff | 0       | 124.3   |
| 2       | < 110 > | 40     | NP-Tensile | 10    | Tersoff | 0       | 211.7   |
| 3       | < 110 > | 60     | NP-Tensile | 10    | Tersoff | 0       | 205.5   |
| 4       | < 110 > | 80     | NP-Tensile | 10    | Tersoff | 0       | 190.2   |
| 5       | < 110 > | 100    | NP-Tensile | 10    | Tersoff | 0       | 189.7   |
| 6       | < 110 > | 120    | NP-Tensile | 10    | Tersoff | 0       | 198.6   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 7       | < 110 > | 140    | NP-Tensile | 10    | Tersoff | 0       | 198.0   |
| 8       | < 110 > | 160    | NP-Tensile | 10    | Tersoff | 0       | 191.8   |
| 9       | < 110 > | 180    | NP-Tensile | 10    | Tersoff | 0       | 192.6   |
| 10      | < 110 > | 200    | NP-Tensile | 10    | Tersoff | 0       | 197.4   |
| 2       | < 100 > | 14     | NP-Tensile | 10    | SW      | 0       | 109.1   |
| 3       | < 100 > | 21     | NP-Tensile | 10    | SW      | 0       | 120.4   |
| 4       | < 100 > | 28     | NP-Tensile | 10    | SW      | 0       | 126.9   |
| 5       | < 100 > | 35     | NP-Tensile | 10    | SW      | 0       | 130.3   |
| 6       | < 100 > | 42     | NP-Tensile | 10    | SW      | 0       | 133.7   |
| 7       | < 100 > | 49     | NP-Tensile | 10    | SW      | 0       | 135.2   |
| 8       | < 100 > | 56     | NP-Tensile | 10    | SW      | 0       | 136.7   |
| 9       | < 100 > | 63     | NP-Tensile | 10    | SW      | 0       | 137.4   |
| 10      | < 100 > | 70     | NP-Tensile | 10    | SW      | 0       | 138.5   |
| 2       | < 110 > | 14     | NP-Tensile | 10    | SW      | 0       | 162.7   |
| 3       | < 110 > | 21     | NP-Tensile | 10    | SW      | 0       | 165.3   |
| 4       | < 110 > | 28     | NP-Tensile | 10    | SW      | 0       | 160.8   |
| 5       | < 110 > | 35     | NP-Tensile | 10    | SW      | 0       | 162.9   |
| 6       | < 110 > | 42     | NP-Tensile | 10    | SW      | 0       | 167.7   |
| 7       | < 110 > | 49     | NP-Tensile | 10    | SW      | 0       | 167.4   |
| 8       | < 110 > | 56     | NP-Tensile | 10    | SW      | 0       | 165.2   |
| 9       | < 110 > | 63     | NP-Tensile | 10    | SW      | 0       | 165.6   |
| 10      | < 110 > | 70     | NP-Tensile | 10    | SW      | 0       | 168.8   |
| 2       | < 100 > | 16     | NP-Tensile | 10    | SW      | 0       | 109.3   |
| 3       | < 100 > | 24     | NP-Tensile | 10    | SW      | 0       | 120.9   |
| 4       | < 100 > | 32     | NP-Tensile | 10    | SW      | 0       | 126.5   |
| 5       | < 100 > | 40     | NP-Tensile | 10    | SW      | 0       | 130.2   |
| 6       | < 100 > | 48     | NP-Tensile | 10    | SW      | 0       | 133.6   |
| 7       | < 100 > | 56     | NP-Tensile | 10    | SW      | 0       | 135.2   |
| 8       | < 100 > | 64     | NP-Tensile | 10    | SW      | 0       | 136.3   |
| 9       | < 100 > | 72     | NP-Tensile | 10    | SW      | 0       | 137.5   |
| 10      | < 100 > | 80     | NP-Tensile | 10    | SW      | 0       | 138.5   |
| 2       | < 110 > | 16     | NP-Tensile | 10    | SW      | 0       | 161.8   |
| 3       | < 110 > | 24     | NP-Tensile | 10    | SW      | 0       | 164.9   |
| 4       | < 110 > | 32     | NP-Tensile | 10    | SW      | 0       | 161.0   |
| 5       | < 110 > | 40     | NP-Tensile | 10    | SW      | 0       | 162.7   |
| 6       | < 110 > | 48     | NP-Tensile | 10    | SW      | 0       | 167.7   |
| 7       | < 110 > | 56     | NP-Tensile | 10    | SW      | 0       | 167.5   |
| 8       | < 110 > | 64     | NP-Tensile | 10    | SW      | 0       | 165.5   |
| 9       | < 110 > | 72     | NP-Tensile | 10    | SW      | 0       | 165.8   |
| 10      | < 110 > | 80     | NP-Tensile | 10    | SW      | 0       | 168.7   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 2       | < 100 > | 18     | NP-Tensile | 10    | SW  | 0       | 109.5   |
| 3       | < 100 > | 27     | NP-Tensile | 10    | SW  | 0       | 120.4   |
| 4       | < 100 > | 36     | NP-Tensile | 10    | SW  | 0       | 126.7   |
| 5       | < 100 > | 45     | NP-Tensile | 10    | SW  | 0       | 130.2   |
| 6       | < 100 > | 54     | NP-Tensile | 10    | SW  | 0       | 133.3   |
| 7       | < 100 > | 63     | NP-Tensile | 10    | SW  | 0       | 134.9   |
| 8       | < 100 > | 72     | NP-Tensile | 10    | SW  | 0       | 136.4   |
| 9       | < 100 > | 81     | NP-Tensile | 10    | SW  | 0       | 137.4   |
| 10      | < 100 > | 90     | NP-Tensile | 10    | SW  | 0       | 138.4   |
| 2       | < 110 > | 18     | NP-Tensile | 10    | SW  | 0       | 162.5   |
| 3       | < 110 > | 27     | NP-Tensile | 10    | SW  | 0       | 165.1   |
| 4       | < 110 > | 36     | NP-Tensile | 10    | SW  | 0       | 160.8   |
| 5       | < 110 > | 45     | NP-Tensile | 10    | SW  | 0       | 162.6   |
| 6       | < 110 > | 54     | NP-Tensile | 10    | SW  | 0       | 167.6   |
| 7       | < 110 > | 63     | NP-Tensile | 10    | SW  | 0       | 167.3   |
| 8       | < 110 > | 72     | NP-Tensile | 10    | SW  | 0       | 165.1   |
| 9       | < 110 > | 81     | NP-Tensile | 10    | SW  | 0       | 165.8   |
| 10      | < 110 > | 90     | NP-Tensile | 10    | SW  | 0       | 168.6   |
| 2       | < 100 > | 20     | NP-Tensile | 10    | SW  | 0       | 108.7   |
| 3       | < 100 > | 30     | NP-Tensile | 10    | SW  | 0       | 120.4   |
| 4       | < 100 > | 40     | NP-Tensile | 10    | SW  | 0       | 126.4   |
| 5       | < 100 > | 50     | NP-Tensile | 10    | SW  | 0       | 130.3   |
| 6       | < 100 > | 60     | NP-Tensile | 10    | SW  | 0       | 133.2   |
| 7       | < 100 > | 70     | NP-Tensile | 10    | SW  | 0       | 134.8   |
| 8       | < 100 > | 80     | NP-Tensile | 10    | SW  | 0       | 136.3   |
| 9       | < 100 > | 90     | NP-Tensile | 10    | SW  | 0       | 137.2   |
| 10      | < 100 > | 100    | NP-Tensile | 10    | SW  | 0       | 138.4   |
| 2       | < 110 > | 20     | NP-Tensile | 10    | SW  | 0       | 163.2   |
| 3       | < 110 > | 30     | NP-Tensile | 10    | SW  | 0       | 165.3   |
| 4       | < 110 > | 40     | NP-Tensile | 10    | SW  | 0       | 161.1   |
| 5       | < 110 > | 50     | NP-Tensile | 10    | SW  | 0       | 162.6   |
| 6       | < 110 > | 60     | NP-Tensile | 10    | SW  | 0       | 167.5   |
| 7       | < 110 > | 70     | NP-Tensile | 10    | SW  | 0       | 167.8   |
| 8       | < 110 > | 80     | NP-Tensile | 10    | SW  | 0       | 165.3   |
| 9       | < 110 > | 90     | NP-Tensile | 10    | SW  | 0       | 165.9   |
| 10      | < 110 > | 100    | NP-Tensile | 10    | SW  | 0       | 168.3   |
| 2       | < 100 > | 24     | NP-Tensile | 10    | SW  | 0       | 109.7   |
| 3       | < 100 > | 36     | NP-Tensile | 10    | SW  | 0       | 120.4   |
| 4       | < 100 > | 48     | NP-Tensile | 10    | SW  | 0       | 126.8   |
| 5       | < 100 > | 60     | NP-Tensile | 10    | SW  | 0       | 130.1   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 6       | < 100 > | 72     | NP-Tensile | 10    | SW  | 0       | 133.2   |
| 7       | < 100 > | 84     | NP-Tensile | 10    | SW  | 0       | 134.8   |
| 8       | < 100 > | 96     | NP-Tensile | 10    | SW  | 0       | 136.2   |
| 9       | < 100 > | 108    | NP-Tensile | 10    | SW  | 0       | 137.1   |
| 10      | < 100 > | 120    | NP-Tensile | 10    | SW  | 0       | 138.1   |
| 2       | < 110 > | 24     | NP-Tensile | 10    | SW  | 0       | 162.9   |
| 3       | < 110 > | 36     | NP-Tensile | 10    | SW  | 0       | 164.5   |
| 4       | < 110 > | 48     | NP-Tensile | 10    | SW  | 0       | 161.1   |
| 5       | < 110 > | 60     | NP-Tensile | 10    | SW  | 0       | 162.6   |
| 6       | < 110 > | 72     | NP-Tensile | 10    | SW  | 0       | 167.1   |
| 7       | < 110 > | 84     | NP-Tensile | 10    | SW  | 0       | 167.6   |
| 8       | < 110 > | 96     | NP-Tensile | 10    | SW  | 0       | 164.8   |
| 9       | < 110 > | 108    | NP-Tensile | 10    | SW  | 0       | 165.4   |
| 10      | < 110 > | 120    | NP-Tensile | 10    | SW  | 0       | 168.2   |
| 2       | < 100 > | 28     | NP-Tensile | 10    | SW  | 0       | 109.4   |
| 3       | < 100 > | 42     | NP-Tensile | 10    | SW  | 0       | 120.5   |
| 4       | < 100 > | 56     | NP-Tensile | 10    | SW  | 0       | 126.6   |
| 5       | < 100 > | 70     | NP-Tensile | 10    | SW  | 0       | 130.0   |
| 6       | < 100 > | 84     | NP-Tensile | 10    | SW  | 0       | 133.1   |
| 7       | < 100 > | 98     | NP-Tensile | 10    | SW  | 0       | 134.8   |
| 8       | < 100 > | 112    | NP-Tensile | 10    | SW  | 0       | 136.1   |
| 9       | < 100 > | 126    | NP-Tensile | 10    | SW  | 0       | 137.0   |
| 10      | < 100 > | 140    | NP-Tensile | 10    | SW  | 0       | 138.0   |
| 2       | < 110 > | 28     | NP-Tensile | 10    | SW  | 0       | 162.3   |
| 3       | < 110 > | 42     | NP-Tensile | 10    | SW  | 0       | 164.8   |
| 4       | < 110 > | 56     | NP-Tensile | 10    | SW  | 0       | 160.6   |
| 5       | < 110 > | 70     | NP-Tensile | 10    | SW  | 0       | 162.5   |
| 6       | < 110 > | 84     | NP-Tensile | 10    | SW  | 0       | 167.2   |
| 7       | < 110 > | 98     | NP-Tensile | 10    | SW  | 0       | 167.2   |
| 8       | < 110 > | 112    | NP-Tensile | 10    | SW  | 0       | 164.8   |
| 9       | < 110 > | 126    | NP-Tensile | 10    | SW  | 0       | 165.3   |
| 10      | < 110 > | 140    | NP-Tensile | 10    | SW  | 0       | 168.1   |
| 2       | < 100 > | 32     | NP-Tensile | 10    | SW  | 0       | 109.1   |
| 3       | < 100 > | 48     | NP-Tensile | 10    | SW  | 0       | 120.5   |
| 4       | < 100 > | 64     | NP-Tensile | 10    | SW  | 0       | 126.3   |
| 5       | < 100 > | 80     | NP-Tensile | 10    | SW  | 0       | 130.1   |
| 6       | < 100 > | 96     | NP-Tensile | 10    | SW  | 0       | 133.1   |
| 7       | < 100 > | 112    | NP-Tensile | 10    | SW  | 0       | 134.7   |
| 8       | < 100 > | 128    | NP-Tensile | 10    | SW  | 0       | 136.0   |
| 9       | < 100 > | 144    | NP-Tensile | 10    | SW  | 0       | 137.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 10      | < 100 > | 160    | NP-Tensile | 10    | SW  | 0       | 138.0   |
| 2       | < 110 > | 32     | NP-Tensile | 10    | SW  | 0       | 162.6   |
| 3       | < 110 > | 48     | NP-Tensile | 10    | SW  | 0       | 164.8   |
| 4       | < 110 > | 64     | NP-Tensile | 10    | SW  | 0       | 161.1   |
| 5       | < 110 > | 80     | NP-Tensile | 10    | SW  | 0       | 162.5   |
| 6       | < 110 > | 96     | NP-Tensile | 10    | SW  | 0       | 166.9   |
| 7       | < 110 > | 112    | NP-Tensile | 10    | SW  | 0       | 167.3   |
| 8       | < 110 > | 128    | NP-Tensile | 10    | SW  | 0       | 164.8   |
| 9       | < 110 > | 144    | NP-Tensile | 10    | SW  | 0       | 165.4   |
| 10      | < 110 > | 160    | NP-Tensile | 10    | SW  | 0       | 168.1   |
| 2       | < 100 > | 36     | NP-Tensile | 10    | SW  | 0       | 109.3   |
| 3       | < 100 > | 54     | NP-Tensile | 10    | SW  | 0       | 120.2   |
| 4       | < 100 > | 72     | NP-Tensile | 10    | SW  | 0       | 126.5   |
| 5       | < 100 > | 90     | NP-Tensile | 10    | SW  | 0       | 130.0   |
| 6       | < 100 > | 108    | NP-Tensile | 10    | SW  | 0       | 133.0   |
| 7       | < 100 > | 126    | NP-Tensile | 10    | SW  | 0       | 134.6   |
| 8       | < 100 > | 144    | NP-Tensile | 10    | SW  | 0       | 136.0   |
| 9       | < 100 > | 162    | NP-Tensile | 10    | SW  | 0       | 137.0   |
| 10      | < 100 > | 180    | NP-Tensile | 10    | SW  | 0       | 138.0   |
| 2       | < 110 > | 36     | NP-Tensile | 10    | SW  | 0       | 162.5   |
| 3       | < 110 > | 54     | NP-Tensile | 10    | SW  | 0       | 164.8   |
| 4       | < 110 > | 72     | NP-Tensile | 10    | SW  | 0       | 160.8   |
| 5       | < 110 > | 90     | NP-Tensile | 10    | SW  | 0       | 162.4   |
| 6       | < 110 > | 108    | NP-Tensile | 10    | SW  | 0       | 166.9   |
| 7       | < 110 > | 126    | NP-Tensile | 10    | SW  | 0       | 167.1   |
| 8       | < 110 > | 144    | NP-Tensile | 10    | SW  | 0       | 164.8   |
| 9       | < 110 > | 162    | NP-Tensile | 10    | SW  | 0       | 165.3   |
| 10      | < 110 > | 180    | NP-Tensile | 10    | SW  | 0       | 168.0   |
| 2       | < 100 > | 40     | NP-Tensile | 10    | SW  | 0       | 109.2   |
| 3       | < 100 > | 60     | NP-Tensile | 10    | SW  | 0       | 120.2   |
| 4       | < 100 > | 80     | NP-Tensile | 10    | SW  | 0       | 126.4   |
| 5       | < 100 > | 100    | NP-Tensile | 10    | SW  | 0       | 130.1   |
| 6       | < 100 > | 120    | NP-Tensile | 10    | SW  | 0       | 132.9   |
| 7       | < 100 > | 140    | NP-Tensile | 10    | SW  | 0       | 134.5   |
| 8       | < 100 > | 160    | NP-Tensile | 10    | SW  | 0       | 135.9   |
| 9       | < 100 > | 180    | NP-Tensile | 10    | SW  | 0       | 136.9   |
| 10      | < 100 > | 200    | NP-Tensile | 10    | SW  | 0       | 137.9   |
| 2       | < 110 > | 40     | NP-Tensile | 10    | SW  | 0       | 162.8   |
| 3       | < 110 > | 60     | NP-Tensile | 10    | SW  | 0       | 164.8   |
| 4       | < 110 > | 80     | NP-Tensile | 10    | SW  | 0       | 161.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 5       | < 110 > | 100    | NP-Tensile | 10    | SW  | 0       | 162.3   |
| 6       | < 110 > | 120    | NP-Tensile | 10    | SW  | 0       | 167.0   |
| 7       | < 110 > | 140    | NP-Tensile | 10    | SW  | 0       | 167.3   |
| 8       | < 110 > | 160    | NP-Tensile | 10    | SW  | 0       | 164.9   |
| 9       | < 110 > | 180    | NP-Tensile | 10    | SW  | 0       | 165.4   |
| 10      | < 110 > | 200    | NP-Tensile | 10    | SW  | 0       | 167.9   |
| 2       | < 100 > | 14     | P-Tensile  | 10    | SW  | 0       | 91.8    |
| 3       | < 100 > | 21     | P-Tensile  | 10    | SW  | 0       | 140.0   |
| 4       | < 100 > | 28     | P-Tensile  | 10    | SW  | 0       | 126.2   |
| 5       | < 100 > | 35     | P-Tensile  | 10    | SW  | 0       | 127.7   |
| 6       | < 100 > | 42     | P-Tensile  | 10    | SW  | 0       | 127.1   |
| 7       | < 100 > | 49     | P-Tensile  | 10    | SW  | 0       | 127.6   |
| 8       | < 100 > | 56     | P-Tensile  | 10    | SW  | 0       | 127.3   |
| 9       | < 100 > | 63     | P-Tensile  | 10    | SW  | 0       | 123.7   |
| 10      | < 100 > | 70     | P-Tensile  | 10    | SW  | 0       | 123.6   |
| 2       | < 110 > | 14     | P-Tensile  | 10    | SW  | 0       | 130.4   |
| 3       | < 110 > | 21     | P-Tensile  | 10    | SW  | 0       | 88.4    |
| 4       | < 110 > | 28     | P-Tensile  | 10    | SW  | 0       | 98.2    |
| 5       | < 110 > | 35     | P-Tensile  | 10    | SW  | 0       | 94.6    |
| 6       | < 110 > | 42     | P-Tensile  | 10    | SW  | 0       | 99.9    |
| 7       | < 110 > | 49     | P-Tensile  | 10    | SW  | 0       | 98.4    |
| 8       | < 110 > | 56     | P-Tensile  | 10    | SW  | 0       | 101.0   |
| 9       | < 110 > | 63     | P-Tensile  | 10    | SW  | 0       | 99.4    |
| 10      | < 110 > | 70     | P-Tensile  | 10    | SW  | 0       | 101.9   |
| 2       | < 100 > | 16     | P-Tensile  | 10    | SW  | 0       | 89.6    |
| 3       | < 100 > | 24     | P-Tensile  | 10    | SW  | 0       | 90.0    |
| 4       | < 100 > | 32     | P-Tensile  | 10    | SW  | 0       | 98.8    |
| 5       | < 100 > | 40     | P-Tensile  | 10    | SW  | 0       | 94.2    |
| 6       | < 100 > | 48     | P-Tensile  | 10    | SW  | 0       | 99.6    |
| 7       | < 100 > | 56     | P-Tensile  | 10    | SW  | 0       | 98.3    |
| 8       | < 100 > | 64     | P-Tensile  | 10    | SW  | 0       | 100.8   |
| 9       | < 100 > | 72     | P-Tensile  | 10    | SW  | 0       | 98.7    |
| 10      | < 100 > | 80     | P-Tensile  | 10    | SW  | 0       | 101.7   |
| 2       | < 110 > | 16     | P-Tensile  | 10    | SW  | 0       | 142.4   |
| 3       | < 110 > | 24     | P-Tensile  | 10    | SW  | 0       | 125.4   |
| 4       | < 110 > | 32     | P-Tensile  | 10    | SW  | 0       | 127.4   |
| 5       | < 110 > | 40     | P-Tensile  | 10    | SW  | 0       | 126.6   |
| 6       | < 110 > | 48     | P-Tensile  | 10    | SW  | 0       | 127.9   |
| 7       | < 110 > | 56     | P-Tensile  | 10    | SW  | 0       | 128.2   |
| 8       | < 110 > | 64     | P-Tensile  | 10    | SW  | 0       | 124.6   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|-----|---------|---------|
| 9       | < 110 > | 72     | P-Tensile | 10    | SW  | 0       | 124.2   |
| 10      | < 110 > | 80     | P-Tensile | 10    | SW  | 0       | 128.1   |
| 2       | < 100 > | 18     | P-Tensile | 10    | SW  | 0       | 91.3    |
| 3       | < 100 > | 27     | P-Tensile | 10    | SW  | 0       | 89.6    |
| 4       | < 100 > | 36     | P-Tensile | 10    | SW  | 0       | 96.3    |
| 5       | < 100 > | 45     | P-Tensile | 10    | SW  | 0       | 96.5    |
| 6       | < 100 > | 54     | P-Tensile | 10    | SW  | 0       | 99.7    |
| 7       | < 100 > | 63     | P-Tensile | 10    | SW  | 0       | 98.5    |
| 8       | < 100 > | 72     | P-Tensile | 10    | SW  | 0       | 100.4   |
| 9       | < 100 > | 81     | P-Tensile | 10    | SW  | 0       | 99.4    |
| 10      | < 100 > | 90     | P-Tensile | 10    | SW  | 0       | 101.1   |
| 2       | < 110 > | 18     | P-Tensile | 10    | SW  | 0       | 141.5   |
| 3       | < 110 > | 27     | P-Tensile | 10    | SW  | 0       | 126.5   |
| 4       | < 110 > | 36     | P-Tensile | 10    | SW  | 0       | 127.8   |
| 5       | < 110 > | 45     | P-Tensile | 10    | SW  | 0       | 126.6   |
| 6       | < 110 > | 54     | P-Tensile | 10    | SW  | 0       | 128.7   |
| 7       | < 110 > | 63     | P-Tensile | 10    | SW  | 0       | 127.6   |
| 8       | < 110 > | 72     | P-Tensile | 10    | SW  | 0       | 124.1   |
| 9       | < 110 > | 81     | P-Tensile | 10    | SW  | 0       | 124.5   |
| 10      | < 110 > | 90     | P-Tensile | 10    | SW  | 0       | 129.0   |
| 2       | < 100 > | 20     | P-Tensile | 10    | SW  | 0       | 90.9    |
| 3       | < 100 > | 30     | P-Tensile | 10    | SW  | 0       | 87.9    |
| 4       | < 100 > | 40     | P-Tensile | 10    | SW  | 0       | 98.0    |
| 5       | < 100 > | 50     | P-Tensile | 10    | SW  | 0       | 94.8    |
| 6       | < 100 > | 60     | P-Tensile | 10    | SW  | 0       | 99.9    |
| 7       | < 100 > | 70     | P-Tensile | 10    | SW  | 0       | 98.0    |
| 8       | < 100 > | 80     | P-Tensile | 10    | SW  | 0       | 100.8   |
| 9       | < 100 > | 90     | P-Tensile | 10    | SW  | 0       | 99.7    |
| 10      | < 100 > | 100    | P-Tensile | 10    | SW  | 0       | 101.9   |
| 2       | < 110 > | 20     | P-Tensile | 10    | SW  | 0       | 140.7   |
| 3       | < 110 > | 30     | P-Tensile | 10    | SW  | 0       | 126.6   |
| 4       | < 110 > | 40     | P-Tensile | 10    | SW  | 0       | 126.8   |
| 5       | < 110 > | 50     | P-Tensile | 10    | SW  | 0       | 126.8   |
| 6       | < 110 > | 60     | P-Tensile | 10    | SW  | 0       | 128.6   |
| 7       | < 110 > | 70     | P-Tensile | 10    | SW  | 0       | 128.3   |
| 8       | < 110 > | 80     | P-Tensile | 10    | SW  | 0       | 123.8   |
| 9       | < 110 > | 90     | P-Tensile | 10    | SW  | 0       | 124.5   |
| 10      | < 110 > | 100    | P-Tensile | 10    | SW  | 0       | 128.1   |
| 2       | < 100 > | 24     | P-Tensile | 10    | SW  | 0       | 90.5    |
| 3       | < 100 > | 36     | P-Tensile | 10    | SW  | 0       | 88.1    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|-----|---------|---------|
| 4       | < 100 > | 48     | P-Tensile | 10    | SW  | 0       | 98.7    |
| 5       | < 100 > | 60     | P-Tensile | 10    | SW  | 0       | 95.3    |
| 6       | < 100 > | 72     | P-Tensile | 10    | SW  | 0       | 99.9    |
| 7       | < 100 > | 84     | P-Tensile | 10    | SW  | 0       | 98.3    |
| 8       | < 100 > | 96     | P-Tensile | 10    | SW  | 0       | 100.8   |
| 9       | < 100 > | 108    | P-Tensile | 10    | SW  | 0       | 98.7    |
| 10      | < 100 > | 120    | P-Tensile | 10    | SW  | 0       | 101.1   |
| 2       | < 110 > | 24     | P-Tensile | 10    | SW  | 0       | 141.1   |
| 3       | < 110 > | 36     | P-Tensile | 10    | SW  | 0       | 125.8   |
| 4       | < 110 > | 48     | P-Tensile | 10    | SW  | 0       | 128.2   |
| 5       | < 110 > | 60     | P-Tensile | 10    | SW  | 0       | 126.4   |
| 6       | < 110 > | 72     | P-Tensile | 10    | SW  | 0       | 128.6   |
| 7       | < 110 > | 84     | P-Tensile | 10    | SW  | 0       | 127.9   |
| 8       | < 110 > | 96     | P-Tensile | 10    | SW  | 0       | 124.3   |
| 9       | < 110 > | 108    | P-Tensile | 10    | SW  | 0       | 124.6   |
| 10      | < 110 > | 120    | P-Tensile | 10    | SW  | 0       | 129.3   |
| 2       | < 100 > | 28     | P-Tensile | 10    | SW  | 0       | 140.6   |
| 3       | < 100 > | 42     | P-Tensile | 10    | SW  | 0       | 125.1   |
| 4       | < 100 > | 56     | P-Tensile | 10    | SW  | 0       | 127.3   |
| 5       | < 100 > | 70     | P-Tensile | 10    | SW  | 0       | 126.4   |
| 6       | < 100 > | 84     | P-Tensile | 10    | SW  | 0       | 128.0   |
| 7       | < 100 > | 98     | P-Tensile | 10    | SW  | 0       | 127.4   |
| 8       | < 100 > | 112    | P-Tensile | 10    | SW  | 0       | 124.4   |
| 9       | < 100 > | 126    | P-Tensile | 10    | SW  | 0       | 123.9   |
| 10      | < 100 > | 140    | P-Tensile | 10    | SW  | 0       | 128.0   |
| 2       | < 110 > | 28     | P-Tensile | 10    | SW  | 0       | 90.1    |
| 3       | < 110 > | 42     | P-Tensile | 10    | SW  | 0       | 89.4    |
| 4       | < 110 > | 56     | P-Tensile | 10    | SW  | 0       | 99.0    |
| 5       | < 110 > | 70     | P-Tensile | 10    | SW  | 0       | 95.0    |
| 6       | < 110 > | 84     | P-Tensile | 10    | SW  | 0       | 100.8   |
| 7       | < 110 > | 98     | P-Tensile | 10    | SW  | 0       | 98.5    |
| 8       | < 110 > | 112    | P-Tensile | 10    | SW  | 0       | 101.0   |
| 9       | < 110 > | 126    | P-Tensile | 10    | SW  | 0       | 99.4    |
| 10      | < 110 > | 140    | P-Tensile | 10    | SW  | 0       | 101.5   |
| 2       | < 100 > | 32     | P-Tensile | 10    | SW  | 0       | 89.1    |
| 3       | < 100 > | 48     | P-Tensile | 10    | SW  | 0       | 89.4    |
| 4       | < 100 > | 64     | P-Tensile | 10    | SW  | 0       | 98.1    |
| 5       | < 100 > | 80     | P-Tensile | 10    | SW  | 0       | 95.1    |
| 6       | < 100 > | 96     | P-Tensile | 10    | SW  | 0       | 100.6   |
| 7       | < 100 > | 112    | P-Tensile | 10    | SW  | 0       | 98.6    |



Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|-----|---------|---------|
| 8       | < 100 > | 128    | P-Tensile | 10    | SW  | 0       | 100.9   |
| 9       | < 100 > | 144    | P-Tensile | 10    | SW  | 0       | 99.3    |
| 10      | < 100 > | 160    | P-Tensile | 10    | SW  | 0       | 100.8   |
| 2       | < 110 > | 32     | P-Tensile | 10    | SW  | 0       | 141.6   |
| 3       | < 110 > | 48     | P-Tensile | 10    | SW  | 0       | 125.8   |
| 4       | < 110 > | 64     | P-Tensile | 10    | SW  | 0       | 126.8   |
| 5       | < 110 > | 80     | P-Tensile | 10    | SW  | 0       | 126.8   |
| 6       | < 110 > | 96     | P-Tensile | 10    | SW  | 0       | 128.8   |
| 7       | < 110 > | 112    | P-Tensile | 10    | SW  | 0       | 128.2   |
| 8       | < 110 > | 128    | P-Tensile | 10    | SW  | 0       | 124.4   |
| 9       | < 110 > | 144    | P-Tensile | 10    | SW  | 0       | 124.6   |
| 10      | < 110 > | 160    | P-Tensile | 10    | SW  | 0       | 128.4   |
| 2       | < 100 > | 36     | P-Tensile | 10    | SW  | 0       | 90.2    |
| 3       | < 100 > | 54     | P-Tensile | 10    | SW  | 0       | 90.4    |
| 4       | < 100 > | 72     | P-Tensile | 10    | SW  | 0       | 98.3    |
| 5       | < 100 > | 90     | P-Tensile | 10    | SW  | 0       | 95.7    |
| 6       | < 100 > | 108    | P-Tensile | 10    | SW  | 0       | 100.2   |
| 7       | < 100 > | 126    | P-Tensile | 10    | SW  | 0       | 98.1    |
| 8       | < 100 > | 144    | P-Tensile | 10    | SW  | 0       | 101.0   |
| 9       | < 100 > | 162    | P-Tensile | 10    | SW  | 0       | 99.2    |
| 10      | < 100 > | 180    | P-Tensile | 10    | SW  | 0       | 100.9   |
| 2       | < 110 > | 36     | P-Tensile | 10    | SW  | 0       | 140.7   |
| 3       | < 110 > | 54     | P-Tensile | 10    | SW  | 0       | 125.6   |
| 4       | < 110 > | 72     | P-Tensile | 10    | SW  | 0       | 127.1   |
| 5       | < 110 > | 90     | P-Tensile | 10    | SW  | 0       | 126.2   |
| 6       | < 110 > | 108    | P-Tensile | 10    | SW  | 0       | 127.8   |
| 7       | < 110 > | 126    | P-Tensile | 10    | SW  | 0       | 127.7   |
| 8       | < 110 > | 144    | P-Tensile | 10    | SW  | 0       | 123.8   |
| 9       | < 110 > | 162    | P-Tensile | 10    | SW  | 0       | 124.5   |
| 10      | < 110 > | 180    | P-Tensile | 10    | SW  | 0       | 128.2   |
| 2       | < 100 > | 40     | P-Tensile | 10    | SW  | 0       | 91.0    |
| 3       | < 100 > | 60     | P-Tensile | 10    | SW  | 0       | 90.5    |
| 4       | < 100 > | 80     | P-Tensile | 10    | SW  | 0       | 97.0    |
| 5       | < 100 > | 100    | P-Tensile | 10    | SW  | 0       | 96.5    |
| 6       | < 100 > | 120    | P-Tensile | 10    | SW  | 0       | 100.1   |
| 7       | < 100 > | 140    | P-Tensile | 10    | SW  | 0       | 98.4    |
| 8       | < 100 > | 160    | P-Tensile | 10    | SW  | 0       | 100.8   |
| 9       | < 100 > | 180    | P-Tensile | 10    | SW  | 0       | 99.0    |
| 10      | < 100 > | 200    | P-Tensile | 10    | SW  | 0       | 101.5   |
| 2       | < 110 > | 40     | P-Tensile | 10    | SW  | 0       | 141.3   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|---------|---------|---------|
| 3       | < 110 > | 60     | P-Tensile | 10    | SW      | 0       | 126.4   |
| 4       | < 110 > | 80     | P-Tensile | 10    | SW      | 0       | 127.1   |
| 5       | < 110 > | 100    | P-Tensile | 10    | SW      | 0       | 126.9   |
| 6       | < 110 > | 120    | P-Tensile | 10    | SW      | 0       | 128.8   |
| 7       | < 110 > | 140    | P-Tensile | 10    | SW      | 0       | 127.6   |
| 8       | < 110 > | 160    | P-Tensile | 10    | SW      | 0       | 124.1   |
| 9       | < 110 > | 180    | P-Tensile | 10    | SW      | 0       | 124.6   |
| 10      | < 110 > | 200    | P-Tensile | 10    | SW      | 0       | 129.2   |
| 2       | < 111 > | 14     | P-Tensile | 10    | Tersoff | 0       | 144.2   |
| 3       | < 111 > | 21     | P-Tensile | 10    | Tersoff | 0       | 162.4   |
| 4       | < 111 > | 28     | P-Tensile | 10    | Tersoff | 0       | 146.3   |
| 5       | < 111 > | 35     | P-Tensile | 10    | Tersoff | 0       | 145.1   |
| 6       | < 111 > | 42     | P-Tensile | 10    | Tersoff | 0       | 154.3   |
| 7       | < 111 > | 49     | P-Tensile | 10    | Tersoff | 0       | 158.5   |
| 8       | < 111 > | 56     | P-Tensile | 10    | Tersoff | 0       | 136.5   |
| 9       | < 111 > | 63     | P-Tensile | 10    | Tersoff | 0       | 155.5   |
| 10      | < 111 > | 70     | P-Tensile | 10    | Tersoff | 0       | 159.6   |
| 2       | < 111 > | 16     | P-Tensile | 10    | Tersoff | 0       | 159.9   |
| 3       | < 111 > | 24     | P-Tensile | 10    | Tersoff | 0       | 161.6   |
| 4       | < 111 > | 32     | P-Tensile | 10    | Tersoff | 0       | 157.4   |
| 5       | < 111 > | 40     | P-Tensile | 10    | Tersoff | 0       | 146.7   |
| 6       | < 111 > | 48     | P-Tensile | 10    | Tersoff | 0       | 142.2   |
| 7       | < 111 > | 56     | P-Tensile | 10    | Tersoff | 0       | 144.4   |
| 8       | < 111 > | 64     | P-Tensile | 10    | Tersoff | 0       | 154.1   |
| 9       | < 111 > | 72     | P-Tensile | 10    | Tersoff | 0       | 155.9   |
| 10      | < 111 > | 80     | P-Tensile | 10    | Tersoff | 0       | 156.5   |
| 2       | < 111 > | 18     | P-Tensile | 10    | Tersoff | 0       | 157.4   |
| 3       | < 111 > | 27     | P-Tensile | 10    | Tersoff | 0       | 158.5   |
| 4       | < 111 > | 36     | P-Tensile | 10    | Tersoff | 0       | 158.2   |
| 5       | < 111 > | 45     | P-Tensile | 10    | Tersoff | 0       | 162.0   |
| 6       | < 111 > | 54     | P-Tensile | 10    | Tersoff | 0       | 146.2   |
| 7       | < 111 > | 63     | P-Tensile | 10    | Tersoff | 0       | 151.1   |
| 8       | < 111 > | 72     | P-Tensile | 10    | Tersoff | 0       | 145.6   |
| 9       | < 111 > | 81     | P-Tensile | 10    | Tersoff | 0       | 142.9   |
| 10      | < 111 > | 90     | P-Tensile | 10    | Tersoff | 0       | 152.0   |
| 2       | < 111 > | 20     | P-Tensile | 10    | Tersoff | 0       | 157.6   |
| 3       | < 111 > | 30     | P-Tensile | 10    | Tersoff | 0       | 155.5   |
| 4       | < 111 > | 40     | P-Tensile | 10    | Tersoff | 0       | 158.7   |
| 5       | < 111 > | 50     | P-Tensile | 10    | Tersoff | 0       | 157.6   |
| 6       | < 111 > | 60     | P-Tensile | 10    | Tersoff | 0       | 159.4   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|---------|---------|---------|
| 7       | < 111 > | 70     | P-Tensile | 10    | Tersoff | 0       | 162.0   |
| 8       | < 111 > | 80     | P-Tensile | 10    | Tersoff | 0       | 153.2   |
| 9       | < 111 > | 90     | P-Tensile | 10    | Tersoff | 0       | 142.0   |
| 10      | < 111 > | 100    | P-Tensile | 10    | Tersoff | 0       | 143.3   |
| 2       | < 111 > | 24     | P-Tensile | 10    | Tersoff | 0       | 153.6   |
| 3       | < 111 > | 36     | P-Tensile | 10    | Tersoff | 0       | 156.9   |
| 4       | < 111 > | 48     | P-Tensile | 10    | Tersoff | 0       | 157.3   |
| 5       | < 111 > | 60     | P-Tensile | 10    | Tersoff | 0       | 155.4   |
| 6       | < 111 > | 72     | P-Tensile | 10    | Tersoff | 0       | 158.7   |
| 7       | < 111 > | 84     | P-Tensile | 10    | Tersoff | 0       | 156.2   |
| 8       | < 111 > | 96     | P-Tensile | 10    | Tersoff | 0       | 158.8   |
| 9       | < 111 > | 108    | P-Tensile | 10    | Tersoff | 0       | 161.6   |
| 10      | < 111 > | 120    | P-Tensile | 10    | Tersoff | 0       | 158.8   |
| 2       | < 111 > | 28     | P-Tensile | 10    | Tersoff | 0       | 156.0   |
| 3       | < 111 > | 42     | P-Tensile | 10    | Tersoff | 0       | 145.7   |
| 4       | < 111 > | 56     | P-Tensile | 10    | Tersoff | 0       | 145.7   |
| 5       | < 111 > | 70     | P-Tensile | 10    | Tersoff | 0       | 153.9   |
| 6       | < 111 > | 84     | P-Tensile | 10    | Tersoff | 0       | 158.5   |
| 7       | < 111 > | 98     | P-Tensile | 10    | Tersoff | 0       | 155.8   |
| 8       | < 111 > | 112    | P-Tensile | 10    | Tersoff | 0       | 157.1   |
| 9       | < 111 > | 126    | P-Tensile | 10    | Tersoff | 0       | 160.4   |
| 10      | < 111 > | 140    | P-Tensile | 10    | Tersoff | 0       | 158.1   |
| 2       | < 111 > | 32     | P-Tensile | 10    | Tersoff | 0       | 159.6   |
| 3       | < 111 > | 48     | P-Tensile | 10    | Tersoff | 0       | 156.0   |
| 4       | < 111 > | 64     | P-Tensile | 10    | Tersoff | 0       | 160.3   |
| 5       | < 111 > | 80     | P-Tensile | 10    | Tersoff | 0       | 156.2   |
| 6       | < 111 > | 96     | P-Tensile | 10    | Tersoff | 0       | 145.0   |
| 7       | < 111 > | 112    | P-Tensile | 10    | Tersoff | 0       | 143.8   |
| 8       | < 111 > | 128    | P-Tensile | 10    | Tersoff | 0       | 152.9   |
| 9       | < 111 > | 144    | P-Tensile | 10    | Tersoff | 0       | 158.4   |
| 10      | < 111 > | 160    | P-Tensile | 10    | Tersoff | 0       | 156.6   |
| 2       | < 111 > | 36     | P-Tensile | 10    | Tersoff | 0       | 158.9   |
| 3       | < 111 > | 54     | P-Tensile | 10    | Tersoff | 0       | 157.3   |
| 4       | < 111 > | 72     | P-Tensile | 10    | Tersoff | 0       | 159.9   |
| 5       | < 111 > | 90     | P-Tensile | 10    | Tersoff | 0       | 159.5   |
| 6       | < 111 > | 108    | P-Tensile | 10    | Tersoff | 0       | 158.8   |
| 7       | < 111 > | 126    | P-Tensile | 10    | Tersoff | 0       | 161.0   |
| 8       | < 111 > | 144    | P-Tensile | 10    | Tersoff | 0       | 160.5   |
| 9       | < 111 > | 162    | P-Tensile | 10    | Tersoff | 0       | 147.0   |
| 10      | < 111 > | 180    | P-Tensile | 10    | Tersoff | 0       | 145.7   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 2       | < 111 > | 40     | P-Tensile  | 10    | Tersoff | 0       | 154.1   |
| 3       | < 111 > | 60     | P-Tensile  | 10    | Tersoff | 0       | 159.5   |
| 4       | < 111 > | 80     | P-Tensile  | 10    | Tersoff | 0       | 156.4   |
| 5       | < 111 > | 100    | P-Tensile  | 10    | Tersoff | 0       | 160.0   |
| 6       | < 111 > | 120    | P-Tensile  | 10    | Tersoff | 0       | 157.1   |
| 7       | < 111 > | 140    | P-Tensile  | 10    | Tersoff | 0       | 157.2   |
| 8       | < 111 > | 160    | P-Tensile  | 10    | Tersoff | 0       | 159.2   |
| 9       | < 111 > | 180    | P-Tensile  | 10    | Tersoff | 0       | 161.3   |
| 10      | < 111 > | 200    | P-Tensile  | 10    | Tersoff | 0       | 159.5   |
| 2       | < 111 > | 14     | NP-Tensile | 10    | Tersoff | 0       | 187.8   |
| 3       | < 111 > | 21     | NP-Tensile | 10    | Tersoff | 0       | 198.7   |
| 4       | < 111 > | 28     | NP-Tensile | 10    | Tersoff | 0       | 205.1   |
| 5       | < 111 > | 35     | NP-Tensile | 10    | Tersoff | 0       | 208.2   |
| 6       | < 111 > | 42     | NP-Tensile | 10    | Tersoff | 0       | 210.8   |
| 7       | < 111 > | 49     | NP-Tensile | 10    | Tersoff | 0       | 213.0   |
| 8       | < 111 > | 56     | NP-Tensile | 10    | Tersoff | 0       | 213.4   |
| 9       | < 111 > | 63     | NP-Tensile | 10    | Tersoff | 0       | 214.8   |
| 10      | < 111 > | 70     | NP-Tensile | 10    | Tersoff | 0       | 215.5   |
| 2       | < 111 > | 16     | NP-Tensile | 10    | Tersoff | 0       | 185.6   |
| 3       | < 111 > | 24     | NP-Tensile | 10    | Tersoff | 0       | 200.7   |
| 4       | < 111 > | 32     | NP-Tensile | 10    | Tersoff | 0       | 205.1   |
| 5       | < 111 > | 40     | NP-Tensile | 10    | Tersoff | 0       | 208.3   |
| 6       | < 111 > | 48     | NP-Tensile | 10    | Tersoff | 0       | 210.9   |
| 7       | < 111 > | 56     | NP-Tensile | 10    | Tersoff | 0       | 212.1   |
| 8       | < 111 > | 64     | NP-Tensile | 10    | Tersoff | 0       | 213.5   |
| 9       | < 111 > | 72     | NP-Tensile | 10    | Tersoff | 0       | 214.7   |
| 10      | < 111 > | 80     | NP-Tensile | 10    | Tersoff | 0       | 215.3   |
| 2       | < 111 > | 18     | NP-Tensile | 10    | Tersoff | 0       | 187.7   |
| 3       | < 111 > | 27     | NP-Tensile | 10    | Tersoff | 0       | 199.0   |
| 4       | < 111 > | 36     | NP-Tensile | 10    | Tersoff | 0       | 204.7   |
| 5       | < 111 > | 45     | NP-Tensile | 10    | Tersoff | 0       | 208.3   |
| 6       | < 111 > | 54     | NP-Tensile | 10    | Tersoff | 0       | 211.2   |
| 7       | < 111 > | 63     | NP-Tensile | 10    | Tersoff | 0       | 212.5   |
| 8       | < 111 > | 72     | NP-Tensile | 10    | Tersoff | 0       | 213.6   |
| 9       | < 111 > | 81     | NP-Tensile | 10    | Tersoff | 0       | 214.6   |
| 10      | < 111 > | 90     | NP-Tensile | 10    | Tersoff | 0       | 215.3   |
| 2       | < 111 > | 20     | NP-Tensile | 10    | Tersoff | 0       | 188.0   |
| 3       | < 111 > | 30     | NP-Tensile | 10    | Tersoff | 0       | 199.0   |
| 4       | < 111 > | 40     | NP-Tensile | 10    | Tersoff | 0       | 204.8   |
| 5       | < 111 > | 50     | NP-Tensile | 10    | Tersoff | 0       | 208.5   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 6       | < 111 > | 60     | NP-Tensile | 10    | Tersoff | 0       | 210.9   |
| 7       | < 111 > | 70     | NP-Tensile | 10    | Tersoff | 0       | 212.4   |
| 8       | < 111 > | 80     | NP-Tensile | 10    | Tersoff | 0       | 213.4   |
| 9       | < 111 > | 90     | NP-Tensile | 10    | Tersoff | 0       | 214.5   |
| 10      | < 111 > | 100    | NP-Tensile | 10    | Tersoff | 0       | 215.6   |
| 2       | < 111 > | 24     | NP-Tensile | 10    | Tersoff | 0       | 188.9   |
| 3       | < 111 > | 36     | NP-Tensile | 10    | Tersoff | 0       | 198.8   |
| 4       | < 111 > | 48     | NP-Tensile | 10    | Tersoff | 0       | 204.9   |
| 5       | < 111 > | 60     | NP-Tensile | 10    | Tersoff | 0       | 208.6   |
| 6       | < 111 > | 72     | NP-Tensile | 10    | Tersoff | 0       | 210.7   |
| 7       | < 111 > | 84     | NP-Tensile | 10    | Tersoff | 0       | 212.5   |
| 8       | < 111 > | 96     | NP-Tensile | 10    | Tersoff | 0       | 213.9   |
| 9       | < 111 > | 108    | NP-Tensile | 10    | Tersoff | 0       | 215.0   |
| 10      | < 111 > | 120    | NP-Tensile | 10    | Tersoff | 0       | 215.6   |
| 2       | < 111 > | 28     | NP-Tensile | 10    | Tersoff | 0       | 188.6   |
| 3       | < 111 > | 42     | NP-Tensile | 10    | Tersoff | 0       | 199.0   |
| 4       | < 111 > | 56     | NP-Tensile | 10    | Tersoff | 0       | 204.6   |
| 5       | < 111 > | 70     | NP-Tensile | 10    | Tersoff | 0       | 208.3   |
| 6       | < 111 > | 84     | NP-Tensile | 10    | Tersoff | 0       | 210.8   |
| 7       | < 111 > | 98     | NP-Tensile | 10    | Tersoff | 0       | 212.9   |
| 8       | < 111 > | 112    | NP-Tensile | 10    | Tersoff | 0       | 214.0   |
| 9       | < 111 > | 126    | NP-Tensile | 10    | Tersoff | 0       | 214.8   |
| 10      | < 111 > | 140    | NP-Tensile | 10    | Tersoff | 0       | 215.5   |
| 2       | < 111 > | 32     | NP-Tensile | 10    | Tersoff | 0       | 188.3   |
| 3       | < 111 > | 48     | NP-Tensile | 10    | Tersoff | 0       | 199.1   |
| 4       | < 111 > | 64     | NP-Tensile | 10    | Tersoff | 0       | 204.6   |
| 5       | < 111 > | 80     | NP-Tensile | 10    | Tersoff | 0       | 208.2   |
| 6       | < 111 > | 96     | NP-Tensile | 10    | Tersoff | 0       | 210.9   |
| 7       | < 111 > | 112    | NP-Tensile | 10    | Tersoff | 0       | 212.6   |
| 8       | < 111 > | 128    | NP-Tensile | 10    | Tersoff | 0       | 213.7   |
| 9       | < 111 > | 144    | NP-Tensile | 10    | Tersoff | 0       | 214.6   |
| 10      | < 111 > | 160    | NP-Tensile | 10    | Tersoff | 0       | 215.6   |
| 2       | < 111 > | 36     | NP-Tensile | 10    | Tersoff | 0       | 187.8   |
| 3       | < 111 > | 54     | NP-Tensile | 10    | Tersoff | 0       | 199.4   |
| 4       | < 111 > | 72     | NP-Tensile | 10    | Tersoff | 0       | 204.8   |
| 5       | < 111 > | 90     | NP-Tensile | 10    | Tersoff | 0       | 208.3   |
| 6       | < 111 > | 108    | NP-Tensile | 10    | Tersoff | 0       | 211.0   |
| 7       | < 111 > | 126    | NP-Tensile | 10    | Tersoff | 0       | 212.6   |
| 8       | < 111 > | 144    | NP-Tensile | 10    | Tersoff | 0       | 213.5   |
| 9       | < 111 > | 162    | NP-Tensile | 10    | Tersoff | 0       | 215.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 10      | < 111 > | 180    | NP-Tensile | 10    | Tersoff | 0       | 215.7   |
| 2       | < 111 > | 40     | NP-Tensile | 10    | Tersoff | 0       | 188.2   |
| 3       | < 111 > | 60     | NP-Tensile | 10    | Tersoff | 0       | 198.9   |
| 4       | < 111 > | 80     | NP-Tensile | 10    | Tersoff | 0       | 204.7   |
| 5       | < 111 > | 100    | NP-Tensile | 10    | Tersoff | 0       | 208.4   |
| 6       | < 111 > | 120    | NP-Tensile | 10    | Tersoff | 0       | 210.8   |
| 7       | < 111 > | 140    | NP-Tensile | 10    | Tersoff | 0       | 212.4   |
| 8       | < 111 > | 160    | NP-Tensile | 10    | Tersoff | 0       | 213.6   |
| 9       | < 111 > | 180    | NP-Tensile | 10    | Tersoff | 0       | 214.9   |
| 10      | < 111 > | 200    | NP-Tensile | 10    | Tersoff | 0       | 217.9   |
| 2       | < 111 > | 14     | NP-Tensile | 10    | SW      | 0       | 164.9   |
| 3       | < 111 > | 21     | NP-Tensile | 10    | SW      | 0       | 176.8   |
| 4       | < 111 > | 28     | NP-Tensile | 10    | SW      | 0       | 183.9   |
| 5       | < 111 > | 35     | NP-Tensile | 10    | SW      | 0       | 187.3   |
| 6       | < 111 > | 42     | NP-Tensile | 10    | SW      | 0       | 189.8   |
| 7       | < 111 > | 49     | NP-Tensile | 10    | SW      | 0       | 192.3   |
| 8       | < 111 > | 56     | NP-Tensile | 10    | SW      | 0       | 192.8   |
| 9       | < 111 > | 63     | NP-Tensile | 10    | SW      | 0       | 194.5   |
| 10      | < 111 > | 70     | NP-Tensile | 10    | SW      | 0       | 195.3   |
| 2       | < 111 > | 16     | NP-Tensile | 10    | SW      | 0       | 163.3   |
| 3       | < 111 > | 24     | NP-Tensile | 10    | SW      | 0       | 178.3   |
| 4       | < 111 > | 32     | NP-Tensile | 10    | SW      | 0       | 183.6   |
| 5       | < 111 > | 40     | NP-Tensile | 10    | SW      | 0       | 187.4   |
| 6       | < 111 > | 48     | NP-Tensile | 10    | SW      | 0       | 189.9   |
| 7       | < 111 > | 56     | NP-Tensile | 10    | SW      | 0       | 191.5   |
| 8       | < 111 > | 64     | NP-Tensile | 10    | SW      | 0       | 193.0   |
| 9       | < 111 > | 72     | NP-Tensile | 10    | SW      | 0       | 194.2   |
| 10      | < 111 > | 80     | NP-Tensile | 10    | SW      | 0       | 195.0   |
| 2       | < 111 > | 18     | NP-Tensile | 10    | SW      | 0       | 164.9   |
| 3       | < 111 > | 27     | NP-Tensile | 10    | SW      | 0       | 177.0   |
| 4       | < 111 > | 36     | NP-Tensile | 10    | SW      | 0       | 183.1   |
| 5       | < 111 > | 45     | NP-Tensile | 10    | SW      | 0       | 187.4   |
| 6       | < 111 > | 54     | NP-Tensile | 10    | SW      | 0       | 190.2   |
| 7       | < 111 > | 63     | NP-Tensile | 10    | SW      | 0       | 191.8   |
| 8       | < 111 > | 72     | NP-Tensile | 10    | SW      | 0       | 193.0   |
| 9       | < 111 > | 81     | NP-Tensile | 10    | SW      | 0       | 194.2   |
| 10      | < 111 > | 90     | NP-Tensile | 10    | SW      | 0       | 194.9   |
| 2       | < 111 > | 20     | NP-Tensile | 10    | SW      | 0       | 165.2   |
| 3       | < 111 > | 30     | NP-Tensile | 10    | SW      | 0       | 176.8   |
| 4       | < 111 > | 40     | NP-Tensile | 10    | SW      | 0       | 183.6   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 5       | < 111 > | 50     | NP-Tensile | 10    | SW  | 0       | 187.5   |
| 6       | < 111 > | 60     | NP-Tensile | 10    | SW  | 0       | 190.0   |
| 7       | < 111 > | 70     | NP-Tensile | 10    | SW  | 0       | 191.8   |
| 8       | < 111 > | 80     | NP-Tensile | 10    | SW  | 0       | 192.8   |
| 9       | < 111 > | 90     | NP-Tensile | 10    | SW  | 0       | 194.0   |
| 10      | < 111 > | 100    | NP-Tensile | 10    | SW  | 0       | 195.1   |
| 2       | < 111 > | 24     | NP-Tensile | 10    | SW  | 0       | 166.1   |
| 3       | < 111 > | 36     | NP-Tensile | 10    | SW  | 0       | 176.6   |
| 4       | < 111 > | 48     | NP-Tensile | 10    | SW  | 0       | 183.4   |
| 5       | < 111 > | 60     | NP-Tensile | 10    | SW  | 0       | 187.4   |
| 6       | < 111 > | 72     | NP-Tensile | 10    | SW  | 0       | 189.7   |
| 7       | < 111 > | 84     | NP-Tensile | 10    | SW  | 0       | 191.8   |
| 8       | < 111 > | 96     | NP-Tensile | 10    | SW  | 0       | 193.2   |
| 9       | < 111 > | 108    | NP-Tensile | 10    | SW  | 0       | 194.5   |
| 10      | < 111 > | 120    | NP-Tensile | 10    | SW  | 0       | 195.1   |
| 2       | < 111 > | 28     | NP-Tensile | 10    | SW  | 0       | 165.7   |
| 3       | < 111 > | 42     | NP-Tensile | 10    | SW  | 0       | 176.8   |
| 4       | < 111 > | 56     | NP-Tensile | 10    | SW  | 0       | 183.1   |
| 5       | < 111 > | 70     | NP-Tensile | 10    | SW  | 0       | 187.3   |
| 6       | < 111 > | 84     | NP-Tensile | 10    | SW  | 0       | 189.8   |
| 7       | < 111 > | 98     | NP-Tensile | 10    | SW  | 0       | 192.1   |
| 8       | < 111 > | 112    | NP-Tensile | 10    | SW  | 0       | 193.2   |
| 9       | < 111 > | 126    | NP-Tensile | 10    | SW  | 0       | 194.2   |
| 10      | < 111 > | 140    | NP-Tensile | 10    | SW  | 0       | 195.0   |
| 2       | < 111 > | 32     | NP-Tensile | 10    | SW  | 0       | 165.4   |
| 3       | < 111 > | 48     | NP-Tensile | 10    | SW  | 0       | 176.9   |
| 4       | < 111 > | 64     | NP-Tensile | 10    | SW  | 0       | 183.2   |
| 5       | < 111 > | 80     | NP-Tensile | 10    | SW  | 0       | 187.1   |
| 6       | < 111 > | 96     | NP-Tensile | 10    | SW  | 0       | 190.0   |
| 7       | < 111 > | 112    | NP-Tensile | 10    | SW  | 0       | 191.9   |
| 8       | < 111 > | 128    | NP-Tensile | 10    | SW  | 0       | 193.0   |
| 9       | < 111 > | 144    | NP-Tensile | 10    | SW  | 0       | 194.0   |
| 10      | < 111 > | 160    | NP-Tensile | 10    | SW  | 0       | 195.1   |
| 2       | < 111 > | 36     | NP-Tensile | 10    | SW  | 0       | 165.0   |
| 3       | < 111 > | 54     | NP-Tensile | 10    | SW  | 0       | 177.3   |
| 4       | < 111 > | 72     | NP-Tensile | 10    | SW  | 0       | 183.3   |
| 5       | < 111 > | 90     | NP-Tensile | 10    | SW  | 0       | 187.1   |
| 6       | < 111 > | 108    | NP-Tensile | 10    | SW  | 0       | 190.0   |
| 7       | < 111 > | 126    | NP-Tensile | 10    | SW  | 0       | 191.8   |
| 8       | < 111 > | 144    | NP-Tensile | 10    | SW  | 0       | 192.9   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 9       | < 111 > | 162    | NP-Tensile | 10    | SW  | 0       | 194.4   |
| 10      | < 111 > | 180    | NP-Tensile | 10    | SW  | 0       | 195.2   |
| 2       | < 111 > | 40     | NP-Tensile | 10    | SW  | 0       | 165.4   |
| 3       | < 111 > | 60     | NP-Tensile | 10    | SW  | 0       | 177.0   |
| 4       | < 111 > | 80     | NP-Tensile | 10    | SW  | 0       | 183.2   |
| 5       | < 111 > | 100    | NP-Tensile | 10    | SW  | 0       | 187.3   |
| 6       | < 111 > | 120    | NP-Tensile | 10    | SW  | 0       | 189.8   |
| 7       | < 111 > | 140    | NP-Tensile | 10    | SW  | 0       | 191.6   |
| 8       | < 111 > | 160    | NP-Tensile | 10    | SW  | 0       | 193.0   |
| 9       | < 111 > | 180    | NP-Tensile | 10    | SW  | 0       | 194.3   |
| 10      | < 111 > | 200    | NP-Tensile | 10    | SW  | 0       | 195.1   |
| 2       | < 111 > | 14     | P-Tensile  | 10    | SW  | 0       | 123.8   |
| 3       | < 111 > | 21     | P-Tensile  | 10    | SW  | 0       | 123.8   |
| 4       | < 111 > | 28     | P-Tensile  | 10    | SW  | 0       | 124.7   |
| 5       | < 111 > | 35     | P-Tensile  | 10    | SW  | 0       | 133.3   |
| 6       | < 111 > | 42     | P-Tensile  | 10    | SW  | 0       | 137.7   |
| 7       | < 111 > | 49     | P-Tensile  | 10    | SW  | 0       | 136.4   |
| 8       | < 111 > | 56     | P-Tensile  | 10    | SW  | 0       | 141.3   |
| 9       | < 111 > | 63     | P-Tensile  | 10    | SW  | 0       | 138.1   |
| 10      | < 111 > | 70     | P-Tensile  | 10    | SW  | 0       | 140.2   |
| 2       | < 111 > | 16     | P-Tensile  | 10    | SW  | 0       | 126.4   |
| 3       | < 111 > | 24     | P-Tensile  | 10    | SW  | 0       | 125.2   |
| 4       | < 111 > | 32     | P-Tensile  | 10    | SW  | 0       | 133.7   |
| 5       | < 111 > | 40     | P-Tensile  | 10    | SW  | 0       | 138.7   |
| 6       | < 111 > | 48     | P-Tensile  | 10    | SW  | 0       | 137.3   |
| 7       | < 111 > | 56     | P-Tensile  | 10    | SW  | 0       | 139.9   |
| 8       | < 111 > | 64     | P-Tensile  | 10    | SW  | 0       | 139.6   |
| 9       | < 111 > | 72     | P-Tensile  | 10    | SW  | 0       | 140.4   |
| 10      | < 111 > | 80     | P-Tensile  | 10    | SW  | 0       | 143.2   |
| 2       | < 111 > | 18     | P-Tensile  | 10    | SW  | 0       | 124.5   |
| 3       | < 111 > | 27     | P-Tensile  | 10    | SW  | 0       | 122.5   |
| 4       | < 111 > | 36     | P-Tensile  | 10    | SW  | 0       | 134.6   |
| 5       | < 111 > | 45     | P-Tensile  | 10    | SW  | 0       | 138.6   |
| 6       | < 111 > | 54     | P-Tensile  | 10    | SW  | 0       | 137.3   |
| 7       | < 111 > | 63     | P-Tensile  | 10    | SW  | 0       | 141.0   |
| 8       | < 111 > | 72     | P-Tensile  | 10    | SW  | 0       | 138.7   |
| 9       | < 111 > | 81     | P-Tensile  | 10    | SW  | 0       | 141.4   |
| 10      | < 111 > | 90     | P-Tensile  | 10    | SW  | 0       | 143.4   |
| 2       | < 111 > | 20     | P-Tensile  | 10    | SW  | 0       | 124.1   |
| 3       | < 111 > | 30     | P-Tensile  | 10    | SW  | 0       | 126.9   |



Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|-----|---------|---------|
| 4       | < 111 > | 40     | P-Tensile | 10    | SW  | 0       | 135.0   |
| 5       | < 111 > | 50     | P-Tensile | 10    | SW  | 0       | 139.5   |
| 6       | < 111 > | 60     | P-Tensile | 10    | SW  | 0       | 137.6   |
| 7       | < 111 > | 70     | P-Tensile | 10    | SW  | 0       | 141.1   |
| 8       | < 111 > | 80     | P-Tensile | 10    | SW  | 0       | 139.6   |
| 9       | < 111 > | 90     | P-Tensile | 10    | SW  | 0       | 141.3   |
| 10      | < 111 > | 100    | P-Tensile | 10    | SW  | 0       | 142.7   |
| 2       | < 111 > | 24     | P-Tensile | 10    | SW  | 0       | 121.5   |
| 3       | < 111 > | 36     | P-Tensile | 10    | SW  | 0       | 127.0   |
| 4       | < 111 > | 48     | P-Tensile | 10    | SW  | 0       | 134.5   |
| 5       | < 111 > | 60     | P-Tensile | 10    | SW  | 0       | 139.6   |
| 6       | < 111 > | 72     | P-Tensile | 10    | SW  | 0       | 137.6   |
| 7       | < 111 > | 84     | P-Tensile | 10    | SW  | 0       | 141.1   |
| 8       | < 111 > | 96     | P-Tensile | 10    | SW  | 0       | 139.9   |
| 9       | < 111 > | 108    | P-Tensile | 10    | SW  | 0       | 140.5   |
| 10      | < 111 > | 120    | P-Tensile | 10    | SW  | 0       | 142.6   |
| 2       | < 111 > | 28     | P-Tensile | 10    | SW  | 0       | 127.0   |
| 3       | < 111 > | 42     | P-Tensile | 10    | SW  | 0       | 126.5   |
| 4       | < 111 > | 56     | P-Tensile | 10    | SW  | 0       | 135.2   |
| 5       | < 111 > | 70     | P-Tensile | 10    | SW  | 0       | 140.5   |
| 6       | < 111 > | 84     | P-Tensile | 10    | SW  | 0       | 138.0   |
| 7       | < 111 > | 98     | P-Tensile | 10    | SW  | 0       | 141.4   |
| 8       | < 111 > | 112    | P-Tensile | 10    | SW  | 0       | 139.8   |
| 9       | < 111 > | 126    | P-Tensile | 10    | SW  | 0       | 141.5   |
| 10      | < 111 > | 140    | P-Tensile | 10    | SW  | 0       | 143.4   |
| 2       | < 111 > | 32     | P-Tensile | 10    | SW  | 0       | 124.4   |
| 3       | < 111 > | 48     | P-Tensile | 10    | SW  | 0       | 126.9   |
| 4       | < 111 > | 64     | P-Tensile | 10    | SW  | 0       | 134.8   |
| 5       | < 111 > | 80     | P-Tensile | 10    | SW  | 0       | 140.1   |
| 6       | < 111 > | 96     | P-Tensile | 10    | SW  | 0       | 137.7   |
| 7       | < 111 > | 112    | P-Tensile | 10    | SW  | 0       | 141.0   |
| 8       | < 111 > | 128    | P-Tensile | 10    | SW  | 0       | 139.9   |
| 9       | < 111 > | 144    | P-Tensile | 10    | SW  | 0       | 141.1   |
| 10      | < 111 > | 160    | P-Tensile | 10    | SW  | 0       | 143.9   |
| 2       | < 111 > | 36     | P-Tensile | 10    | SW  | 0       | 124.9   |
| 3       | < 111 > | 54     | P-Tensile | 10    | SW  | 0       | 125.8   |
| 4       | < 111 > | 72     | P-Tensile | 10    | SW  | 0       | 135.5   |
| 5       | < 111 > | 90     | P-Tensile | 10    | SW  | 0       | 139.7   |
| 6       | < 111 > | 108    | P-Tensile | 10    | SW  | 0       | 137.7   |
| 7       | < 111 > | 126    | P-Tensile | 10    | SW  | 0       | 140.8   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 8       | < 111 > | 144    | P-Tensile  | 10    | SW      | 0       | 139.8   |
| 9       | < 111 > | 162    | P-Tensile  | 10    | SW      | 0       | 141.6   |
| 10      | < 111 > | 180    | P-Tensile  | 10    | SW      | 0       | 143.5   |
| 2       | < 111 > | 40     | P-Tensile  | 10    | SW      | 0       | 125.5   |
| 3       | < 111 > | 60     | P-Tensile  | 10    | SW      | 0       | 125.3   |
| 4       | < 111 > | 80     | P-Tensile  | 10    | SW      | 0       | 133.8   |
| 5       | < 111 > | 100    | P-Tensile  | 10    | SW      | 0       | 138.7   |
| 6       | < 111 > | 120    | P-Tensile  | 10    | SW      | 0       | 137.4   |
| 7       | < 111 > | 140    | P-Tensile  | 10    | SW      | 0       | 140.6   |
| 8       | < 111 > | 160    | P-Tensile  | 10    | SW      | 0       | 139.6   |
| 9       | < 111 > | 180    | P-Tensile  | 10    | SW      | 0       | 141.2   |
| 10      | < 111 > | 200    | P-Tensile  | 10    | SW      | 0       | 142.7   |
| 2       | < 100 > | 14     | NP-Tensile | 300   | Tersoff | 0       | 103.0   |
| 3       | < 100 > | 21     | NP-Tensile | 300   | Tersoff | 0       | 109.1   |
| 4       | < 100 > | 28     | NP-Tensile | 300   | Tersoff | 0       | 114.9   |
| 5       | < 100 > | 35     | NP-Tensile | 300   | Tersoff | 0       | 118.3   |
| 6       | < 100 > | 42     | NP-Tensile | 300   | Tersoff | 0       | 120.9   |
| 7       | < 100 > | 49     | NP-Tensile | 300   | Tersoff | 0       | 122.4   |
| 8       | < 100 > | 56     | NP-Tensile | 300   | Tersoff | 0       | 123.5   |
| 9       | < 100 > | 63     | NP-Tensile | 300   | Tersoff | 0       | 123.9   |
| 10      | < 100 > | 70     | NP-Tensile | 300   | Tersoff | 0       | 124.8   |
| 2       | < 100 > | 16     | NP-Tensile | 300   | Tersoff | 0       | 104.0   |
| 3       | < 100 > | 24     | NP-Tensile | 300   | Tersoff | 0       | 110.6   |
| 4       | < 100 > | 32     | NP-Tensile | 300   | Tersoff | 0       | 113.5   |
| 5       | < 100 > | 40     | NP-Tensile | 300   | Tersoff | 0       | 117.2   |
| 6       | < 100 > | 48     | NP-Tensile | 300   | Tersoff | 0       | 121.3   |
| 7       | < 100 > | 56     | NP-Tensile | 300   | Tersoff | 0       | 122.2   |
| 8       | < 100 > | 64     | NP-Tensile | 300   | Tersoff | 0       | 122.8   |
| 9       | < 100 > | 72     | NP-Tensile | 300   | Tersoff | 0       | 123.8   |
| 10      | < 100 > | 80     | NP-Tensile | 300   | Tersoff | 0       | 124.8   |
| 2       | < 100 > | 18     | NP-Tensile | 300   | Tersoff | 0       | 99.4    |
| 3       | < 100 > | 27     | NP-Tensile | 300   | Tersoff | 0       | 109.6   |
| 4       | < 100 > | 36     | NP-Tensile | 300   | Tersoff | 0       | 114.4   |
| 5       | < 100 > | 45     | NP-Tensile | 300   | Tersoff | 0       | 117.6   |
| 6       | < 100 > | 54     | NP-Tensile | 300   | Tersoff | 0       | 120.7   |
| 7       | < 100 > | 63     | NP-Tensile | 300   | Tersoff | 0       | 121.5   |
| 8       | < 100 > | 72     | NP-Tensile | 300   | Tersoff | 0       | 122.8   |
| 9       | < 100 > | 81     | NP-Tensile | 300   | Tersoff | 0       | 123.8   |
| 10      | < 100 > | 90     | NP-Tensile | 300   | Tersoff | 0       | 124.9   |
| 2       | < 100 > | 20     | NP-Tensile | 300   | Tersoff | 0       | 100.7   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 3       | < 100 > | 30     | NP-Tensile | 300   | Tersoff | 0       | 109.3   |
| 4       | < 100 > | 40     | NP-Tensile | 300   | Tersoff | 0       | 114.1   |
| 5       | < 100 > | 50     | NP-Tensile | 300   | Tersoff | 0       | 117.9   |
| 6       | < 100 > | 60     | NP-Tensile | 300   | Tersoff | 0       | 120.6   |
| 7       | < 100 > | 70     | NP-Tensile | 300   | Tersoff | 0       | 121.3   |
| 8       | < 100 > | 80     | NP-Tensile | 300   | Tersoff | 0       | 122.8   |
| 9       | < 100 > | 90     | NP-Tensile | 300   | Tersoff | 0       | 123.9   |
| 10      | < 100 > | 100    | NP-Tensile | 300   | Tersoff | 0       | 125.0   |
| 2       | < 100 > | 24     | NP-Tensile | 300   | Tersoff | 0       | 104.0   |
| 3       | < 100 > | 36     | NP-Tensile | 300   | Tersoff | 0       | 109.3   |
| 4       | < 100 > | 48     | NP-Tensile | 300   | Tersoff | 0       | 114.9   |
| 5       | < 100 > | 60     | NP-Tensile | 300   | Tersoff | 0       | 118.3   |
| 6       | < 100 > | 72     | NP-Tensile | 300   | Tersoff | 0       | 120.5   |
| 7       | < 100 > | 84     | NP-Tensile | 300   | Tersoff | 0       | 121.6   |
| 8       | < 100 > | 96     | NP-Tensile | 300   | Tersoff | 0       | 123.0   |
| 9       | < 100 > | 108    | NP-Tensile | 300   | Tersoff | 0       | 123.9   |
| 10      | < 100 > | 120    | NP-Tensile | 300   | Tersoff | 0       | 123.0   |
| 2       | < 100 > | 28     | NP-Tensile | 300   | Tersoff | 0       | 101.5   |
| 3       | < 100 > | 42     | NP-Tensile | 300   | Tersoff | 0       | 110.4   |
| 4       | < 100 > | 56     | NP-Tensile | 300   | Tersoff | 0       | 114.6   |
| 5       | < 100 > | 70     | NP-Tensile | 300   | Tersoff | 0       | 117.7   |
| 6       | < 100 > | 84     | NP-Tensile | 300   | Tersoff | 0       | 120.4   |
| 7       | < 100 > | 98     | NP-Tensile | 300   | Tersoff | 0       | 121.8   |
| 8       | < 100 > | 112    | NP-Tensile | 300   | Tersoff | 0       | 123.0   |
| 9       | < 100 > | 126    | NP-Tensile | 300   | Tersoff | 0       | 123.4   |
| 10      | < 100 > | 140    | NP-Tensile | 300   | Tersoff | 0       | 124.8   |
| 2       | < 100 > | 32     | NP-Tensile | 300   | Tersoff | 0       | 101.1   |
| 3       | < 100 > | 48     | NP-Tensile | 300   | Tersoff | 0       | 110.0   |
| 4       | < 100 > | 64     | NP-Tensile | 300   | Tersoff | 0       | 114.4   |
| 5       | < 100 > | 80     | NP-Tensile | 300   | Tersoff | 0       | 117.7   |
| 6       | < 100 > | 96     | NP-Tensile | 300   | Tersoff | 0       | 120.3   |
| 7       | < 100 > | 112    | NP-Tensile | 300   | Tersoff | 0       | 121.9   |
| 8       | < 100 > | 128    | NP-Tensile | 300   | Tersoff | 0       | 123.0   |
| 9       | < 100 > | 144    | NP-Tensile | 300   | Tersoff | 0       | 124.0   |
| 10      | < 100 > | 160    | NP-Tensile | 300   | Tersoff | 0       | 118.0   |
| 2       | < 100 > | 36     | NP-Tensile | 300   | Tersoff | 0       | 101.7   |
| 3       | < 100 > | 54     | NP-Tensile | 300   | Tersoff | 0       | 109.5   |
| 4       | < 100 > | 72     | NP-Tensile | 300   | Tersoff | 0       | 114.3   |
| 5       | < 100 > | 90     | NP-Tensile | 300   | Tersoff | 0       | 118.3   |
| 6       | < 100 > | 108    | NP-Tensile | 300   | Tersoff | 0       | 120.4   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 7       | < 100 > | 126    | NP-Tensile | 300   | Tersoff | 0       | 121.9   |
| 8       | < 100 > | 144    | NP-Tensile | 300   | Tersoff | 0       | 123.0   |
| 9       | < 100 > | 162    | NP-Tensile | 300   | Tersoff | 0       | 122.6   |
| 10      | < 100 > | 180    | NP-Tensile | 300   | Tersoff | 0       | 121.1   |
| 2       | < 100 > | 40     | NP-Tensile | 300   | Tersoff | 0       | 101.0   |
| 3       | < 100 > | 60     | NP-Tensile | 300   | Tersoff | 0       | 109.4   |
| 4       | < 100 > | 80     | NP-Tensile | 300   | Tersoff | 0       | 114.4   |
| 5       | < 100 > | 100    | NP-Tensile | 300   | Tersoff | 0       | 117.9   |
| 6       | < 100 > | 120    | NP-Tensile | 300   | Tersoff | 0       | 120.4   |
| 7       | < 100 > | 140    | NP-Tensile | 300   | Tersoff | 0       | 121.8   |
| 8       | < 100 > | 160    | NP-Tensile | 300   | Tersoff | 0       | 120.8   |
| 9       | < 100 > | 180    | NP-Tensile | 300   | Tersoff | 0       | 118.9   |
| 10      | < 100 > | 200    | NP-Tensile | 300   | Tersoff | 0       | 120.0   |
| 2       | < 100 > | 14     | P-Tensile  | 300   | Tersoff | 0       | 94.1    |
| 3       | < 100 > | 21     | P-Tensile  | 300   | Tersoff | 0       | 94.1    |
| 4       | < 100 > | 28     | P-Tensile  | 300   | Tersoff | 0       | 85.2    |
| 5       | < 100 > | 35     | P-Tensile  | 300   | Tersoff | 0       | 91.9    |
| 6       | < 100 > | 42     | P-Tensile  | 300   | Tersoff | 0       | 89.2    |
| 7       | < 100 > | 49     | P-Tensile  | 300   | Tersoff | 0       | 90.5    |
| 8       | < 100 > | 56     | P-Tensile  | 300   | Tersoff | 0       | 89.7    |
| 9       | < 100 > | 63     | P-Tensile  | 300   | Tersoff | 0       | 91.5    |
| 10      | < 100 > | 70     | P-Tensile  | 300   | Tersoff | 0       | 89.1    |
| 2       | < 100 > | 16     | P-Tensile  | 300   | Tersoff | 0       | 92.0    |
| 3       | < 100 > | 24     | P-Tensile  | 300   | Tersoff | 0       | 89.3    |
| 4       | < 100 > | 32     | P-Tensile  | 300   | Tersoff | 0       | 89.9    |
| 5       | < 100 > | 40     | P-Tensile  | 300   | Tersoff | 0       | 89.6    |
| 6       | < 100 > | 48     | P-Tensile  | 300   | Tersoff | 0       | 89.0    |
| 7       | < 100 > | 56     | P-Tensile  | 300   | Tersoff | 0       | 91.3    |
| 8       | < 100 > | 64     | P-Tensile  | 300   | Tersoff | 0       | 92.3    |
| 9       | < 100 > | 72     | P-Tensile  | 300   | Tersoff | 0       | 88.9    |
| 10      | < 100 > | 80     | P-Tensile  | 300   | Tersoff | 0       | 89.6    |
| 2       | < 100 > | 18     | P-Tensile  | 300   | Tersoff | 0       | 93.0    |
| 3       | < 100 > | 27     | P-Tensile  | 300   | Tersoff | 0       | 83.2    |
| 4       | < 100 > | 36     | P-Tensile  | 300   | Tersoff | 0       | 91.2    |
| 5       | < 100 > | 45     | P-Tensile  | 300   | Tersoff | 0       | 93.0    |
| 6       | < 100 > | 54     | P-Tensile  | 300   | Tersoff | 0       | 93.2    |
| 7       | < 100 > | 63     | P-Tensile  | 300   | Tersoff | 0       | 89.4    |
| 8       | < 100 > | 72     | P-Tensile  | 300   | Tersoff | 0       | 92.2    |
| 9       | < 100 > | 81     | P-Tensile  | 300   | Tersoff | 0       | 92.4    |
| 10      | < 100 > | 90     | P-Tensile  | 300   | Tersoff | 0       | 91.1    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|---------|---------|---------|
| 2       | < 100 > | 20     | P-Tensile | 300   | Tersoff | 0       | 91.1    |
| 3       | < 100 > | 30     | P-Tensile | 300   | Tersoff | 0       | 86.0    |
| 4       | < 100 > | 40     | P-Tensile | 300   | Tersoff | 0       | 90.0    |
| 5       | < 100 > | 50     | P-Tensile | 300   | Tersoff | 0       | 90.5    |
| 6       | < 100 > | 60     | P-Tensile | 300   | Tersoff | 0       | 88.6    |
| 7       | < 100 > | 70     | P-Tensile | 300   | Tersoff | 0       | 86.9    |
| 8       | < 100 > | 80     | P-Tensile | 300   | Tersoff | 0       | 90.3    |
| 9       | < 100 > | 90     | P-Tensile | 300   | Tersoff | 0       | 90.4    |
| 10      | < 100 > | 100    | P-Tensile | 300   | Tersoff | 0       | 93.1    |
| 2       | < 100 > | 24     | P-Tensile | 300   | Tersoff | 0       | 88.3    |
| 3       | < 100 > | 36     | P-Tensile | 300   | Tersoff | 0       | 83.2    |
| 4       | < 100 > | 48     | P-Tensile | 300   | Tersoff | 0       | 92.7    |
| 5       | < 100 > | 60     | P-Tensile | 300   | Tersoff | 0       | 80.7    |
| 6       | < 100 > | 72     | P-Tensile | 300   | Tersoff | 0       | 90.2    |
| 7       | < 100 > | 84     | P-Tensile | 300   | Tersoff | 0       | 88.5    |
| 8       | < 100 > | 96     | P-Tensile | 300   | Tersoff | 0       | 90.8    |
| 9       | < 100 > | 108    | P-Tensile | 300   | Tersoff | 0       | 88.3    |
| 10      | < 100 > | 120    | P-Tensile | 300   | Tersoff | 0       | 93.9    |
| 2       | < 100 > | 28     | P-Tensile | 300   | Tersoff | 0       | 93.6    |
| 3       | < 100 > | 42     | P-Tensile | 300   | Tersoff | 0       | 83.6    |
| 4       | < 100 > | 56     | P-Tensile | 300   | Tersoff | 0       | 89.0    |
| 5       | < 100 > | 70     | P-Tensile | 300   | Tersoff | 0       | 81.5    |
| 6       | < 100 > | 84     | P-Tensile | 300   | Tersoff | 0       | 93.0    |
| 7       | < 100 > | 98     | P-Tensile | 300   | Tersoff | 0       | 88.3    |
| 8       | < 100 > | 112    | P-Tensile | 300   | Tersoff | 0       | 90.2    |
| 9       | < 100 > | 126    | P-Tensile | 300   | Tersoff | 0       | 89.4    |
| 10      | < 100 > | 140    | P-Tensile | 300   | Tersoff | 0       | 91.1    |
| 2       | < 100 > | 32     | P-Tensile | 300   | Tersoff | 0       | 91.2    |
| 3       | < 100 > | 48     | P-Tensile | 300   | Tersoff | 0       | 84.6    |
| 4       | < 100 > | 64     | P-Tensile | 300   | Tersoff | 0       | 88.4    |
| 5       | < 100 > | 80     | P-Tensile | 300   | Tersoff | 0       | 89.8    |
| 6       | < 100 > | 96     | P-Tensile | 300   | Tersoff | 0       | 90.9    |
| 7       | < 100 > | 112    | P-Tensile | 300   | Tersoff | 0       | 88.6    |
| 8       | < 100 > | 128    | P-Tensile | 300   | Tersoff | 0       | 91.4    |
| 9       | < 100 > | 144    | P-Tensile | 300   | Tersoff | 0       | 85.5    |
| 10      | < 100 > | 160    | P-Tensile | 300   | Tersoff | 0       | 90.3    |
| 2       | < 100 > | 36     | P-Tensile | 300   | Tersoff | 0       | 83.1    |
| 3       | < 100 > | 54     | P-Tensile | 300   | Tersoff | 0       | 87.0    |
| 4       | < 100 > | 72     | P-Tensile | 300   | Tersoff | 0       | 91.1    |
| 5       | < 100 > | 90     | P-Tensile | 300   | Tersoff | 0       | 92.4    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 6       | < 100 > | 108    | P-Tensile  | 300   | Tersoff | 0       | 90.7    |
| 7       | < 100 > | 126    | P-Tensile  | 300   | Tersoff | 0       | 88.6    |
| 8       | < 100 > | 144    | P-Tensile  | 300   | Tersoff | 0       | 91.8    |
| 9       | < 100 > | 162    | P-Tensile  | 300   | Tersoff | 0       | 90.5    |
| 10      | < 100 > | 180    | P-Tensile  | 300   | Tersoff | 0       | 91.1    |
| 2       | < 100 > | 40     | P-Tensile  | 300   | Tersoff | 0       | 94.9    |
| 3       | < 100 > | 60     | P-Tensile  | 300   | Tersoff | 0       | 87.7    |
| 4       | < 100 > | 80     | P-Tensile  | 300   | Tersoff | 0       | 91.3    |
| 5       | < 100 > | 100    | P-Tensile  | 300   | Tersoff | 0       | 92.1    |
| 6       | < 100 > | 120    | P-Tensile  | 300   | Tersoff | 0       | 91.5    |
| 7       | < 100 > | 140    | P-Tensile  | 300   | Tersoff | 0       | 88.9    |
| 8       | < 100 > | 160    | P-Tensile  | 300   | Tersoff | 0       | 91.2    |
| 9       | < 100 > | 180    | P-Tensile  | 300   | Tersoff | 0       | 89.5    |
| 10      | < 100 > | 200    | P-Tensile  | 300   | Tersoff | 0       | 91.1    |
| 2       | < 100 > | 14     | NP-Tensile | 300   | SW      | 0       | 104.2   |
| 3       | < 100 > | 21     | NP-Tensile | 300   | SW      | 0       | 117.1   |
| 4       | < 100 > | 28     | NP-Tensile | 300   | SW      | 0       | 124.0   |
| 5       | < 100 > | 35     | NP-Tensile | 300   | SW      | 0       | 127.9   |
| 6       | < 100 > | 42     | NP-Tensile | 300   | SW      | 0       | 131.1   |
| 7       | < 100 > | 49     | NP-Tensile | 300   | SW      | 0       | 132.8   |
| 8       | < 100 > | 56     | NP-Tensile | 300   | SW      | 0       | 133.8   |
| 9       | < 100 > | 63     | NP-Tensile | 300   | SW      | 0       | 134.2   |
| 10      | < 100 > | 70     | NP-Tensile | 300   | SW      | 0       | 135.4   |
| 2       | < 100 > | 16     | NP-Tensile | 300   | SW      | 0       | 103.7   |
| 3       | < 100 > | 24     | NP-Tensile | 300   | SW      | 0       | 118.7   |
| 4       | < 100 > | 32     | NP-Tensile | 300   | SW      | 0       | 123.6   |
| 5       | < 100 > | 40     | NP-Tensile | 300   | SW      | 0       | 128.0   |
| 6       | < 100 > | 48     | NP-Tensile | 300   | SW      | 0       | 130.9   |
| 7       | < 100 > | 56     | NP-Tensile | 300   | SW      | 0       | 132.8   |
| 8       | < 100 > | 64     | NP-Tensile | 300   | SW      | 0       | 133.5   |
| 9       | < 100 > | 72     | NP-Tensile | 300   | SW      | 0       | 134.4   |
| 10      | < 100 > | 80     | NP-Tensile | 300   | SW      | 0       | 135.4   |
| 2       | < 100 > | 18     | NP-Tensile | 300   | SW      | 0       | 104.9   |
| 3       | < 100 > | 27     | NP-Tensile | 300   | SW      | 0       | 117.1   |
| 4       | < 100 > | 36     | NP-Tensile | 300   | SW      | 0       | 124.5   |
| 5       | < 100 > | 45     | NP-Tensile | 300   | SW      | 0       | 127.3   |
| 6       | < 100 > | 54     | NP-Tensile | 300   | SW      | 0       | 130.6   |
| 7       | < 100 > | 63     | NP-Tensile | 300   | SW      | 0       | 132.4   |
| 8       | < 100 > | 72     | NP-Tensile | 300   | SW      | 0       | 133.5   |
| 9       | < 100 > | 81     | NP-Tensile | 300   | SW      | 0       | 134.4   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 10      | < 100 > | 90     | NP-Tensile | 300   | SW  | 0       | 135.2   |
| 2       | < 100 > | 20     | NP-Tensile | 300   | SW  | 0       | 101.8   |
| 3       | < 100 > | 30     | NP-Tensile | 300   | SW  | 0       | 118.0   |
| 4       | < 100 > | 40     | NP-Tensile | 300   | SW  | 0       | 123.5   |
| 5       | < 100 > | 50     | NP-Tensile | 300   | SW  | 0       | 127.2   |
| 6       | < 100 > | 60     | NP-Tensile | 300   | SW  | 0       | 130.6   |
| 7       | < 100 > | 70     | NP-Tensile | 300   | SW  | 0       | 132.4   |
| 8       | < 100 > | 80     | NP-Tensile | 300   | SW  | 0       | 133.4   |
| 9       | < 100 > | 90     | NP-Tensile | 300   | SW  | 0       | 134.1   |
| 10      | < 100 > | 100    | NP-Tensile | 300   | SW  | 0       | 135.2   |
| 2       | < 100 > | 24     | NP-Tensile | 300   | SW  | 0       | 102.5   |
| 3       | < 100 > | 36     | NP-Tensile | 300   | SW  | 0       | 115.7   |
| 4       | < 100 > | 48     | NP-Tensile | 300   | SW  | 0       | 123.4   |
| 5       | < 100 > | 60     | NP-Tensile | 300   | SW  | 0       | 127.5   |
| 6       | < 100 > | 72     | NP-Tensile | 300   | SW  | 0       | 130.7   |
| 7       | < 100 > | 84     | NP-Tensile | 300   | SW  | 0       | 132.1   |
| 8       | < 100 > | 96     | NP-Tensile | 300   | SW  | 0       | 133.1   |
| 9       | < 100 > | 108    | NP-Tensile | 300   | SW  | 0       | 133.8   |
| 10      | < 100 > | 120    | NP-Tensile | 300   | SW  | 0       | 134.9   |
| 2       | < 100 > | 28     | NP-Tensile | 300   | SW  | 0       | 102.0   |
| 3       | < 100 > | 42     | NP-Tensile | 300   | SW  | 0       | 116.9   |
| 4       | < 100 > | 56     | NP-Tensile | 300   | SW  | 0       | 123.5   |
| 5       | < 100 > | 70     | NP-Tensile | 300   | SW  | 0       | 127.3   |
| 6       | < 100 > | 84     | NP-Tensile | 300   | SW  | 0       | 130.4   |
| 7       | < 100 > | 98     | NP-Tensile | 300   | SW  | 0       | 131.9   |
| 8       | < 100 > | 112    | NP-Tensile | 300   | SW  | 0       | 132.9   |
| 9       | < 100 > | 126    | NP-Tensile | 300   | SW  | 0       | 133.7   |
| 10      | < 100 > | 140    | NP-Tensile | 300   | SW  | 0       | 133.8   |
| 2       | < 100 > | 32     | NP-Tensile | 300   | SW  | 0       | 100.8   |
| 3       | < 100 > | 48     | NP-Tensile | 300   | SW  | 0       | 116.9   |
| 4       | < 100 > | 64     | NP-Tensile | 300   | SW  | 0       | 123.3   |
| 5       | < 100 > | 80     | NP-Tensile | 300   | SW  | 0       | 126.4   |
| 6       | < 100 > | 96     | NP-Tensile | 300   | SW  | 0       | 130.0   |
| 7       | < 100 > | 112    | NP-Tensile | 300   | SW  | 0       | 131.9   |
| 8       | < 100 > | 128    | NP-Tensile | 300   | SW  | 0       | 132.8   |
| 9       | < 100 > | 144    | NP-Tensile | 300   | SW  | 0       | 133.5   |
| 10      | < 100 > | 160    | NP-Tensile | 300   | SW  | 0       | 132.8   |
| 2       | < 100 > | 36     | NP-Tensile | 300   | SW  | 0       | 102.2   |
| 3       | < 100 > | 54     | NP-Tensile | 300   | SW  | 0       | 116.5   |
| 4       | < 100 > | 72     | NP-Tensile | 300   | SW  | 0       | 123.4   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 5       | < 100 > | 90     | NP-Tensile | 300   | SW  | 0       | 126.6   |
| 6       | < 100 > | 108    | NP-Tensile | 300   | SW  | 0       | 129.9   |
| 7       | < 100 > | 126    | NP-Tensile | 300   | SW  | 0       | 131.7   |
| 8       | < 100 > | 144    | NP-Tensile | 300   | SW  | 0       | 132.6   |
| 9       | < 100 > | 162    | NP-Tensile | 300   | SW  | 0       | 132.8   |
| 10      | < 100 > | 180    | NP-Tensile | 300   | SW  | 0       | 131.8   |
| 2       | < 100 > | 40     | NP-Tensile | 300   | SW  | 0       | 98.4    |
| 3       | < 100 > | 60     | NP-Tensile | 300   | SW  | 0       | 115.7   |
| 4       | < 100 > | 80     | NP-Tensile | 300   | SW  | 0       | 122.6   |
| 5       | < 100 > | 100    | NP-Tensile | 300   | SW  | 0       | 126.4   |
| 6       | < 100 > | 120    | NP-Tensile | 300   | SW  | 0       | 129.7   |
| 7       | < 100 > | 140    | NP-Tensile | 300   | SW  | 0       | 131.4   |
| 8       | < 100 > | 160    | NP-Tensile | 300   | SW  | 0       | 132.6   |
| 9       | < 100 > | 180    | NP-Tensile | 300   | SW  | 0       | 131.8   |
| 10      | < 100 > | 200    | NP-Tensile | 300   | SW  | 0       | 131.3   |
| 2       | < 100 > | 14     | P-Tensile  | 300   | SW  | 0       | 94.4    |
| 3       | < 100 > | 21     | P-Tensile  | 300   | SW  | 0       | 94.4    |
| 4       | < 100 > | 28     | P-Tensile  | 300   | SW  | 0       | 85.9    |
| 5       | < 100 > | 35     | P-Tensile  | 300   | SW  | 0       | 95.6    |
| 6       | < 100 > | 42     | P-Tensile  | 300   | SW  | 0       | 94.8    |
| 7       | < 100 > | 49     | P-Tensile  | 300   | SW  | 0       | 98.8    |
| 8       | < 100 > | 56     | P-Tensile  | 300   | SW  | 0       | 96.7    |
| 9       | < 100 > | 63     | P-Tensile  | 300   | SW  | 0       | 99.0    |
| 10      | < 100 > | 70     | P-Tensile  | 300   | SW  | 0       | 97.4    |
| 2       | < 100 > | 16     | P-Tensile  | 300   | SW  | 0       | 88.8    |
| 3       | < 100 > | 24     | P-Tensile  | 300   | SW  | 0       | 88.9    |
| 4       | < 100 > | 32     | P-Tensile  | 300   | SW  | 0       | 98.5    |
| 5       | < 100 > | 40     | P-Tensile  | 300   | SW  | 0       | 92.4    |
| 6       | < 100 > | 48     | P-Tensile  | 300   | SW  | 0       | 96.4    |
| 7       | < 100 > | 56     | P-Tensile  | 300   | SW  | 0       | 96.9    |
| 8       | < 100 > | 64     | P-Tensile  | 300   | SW  | 0       | 99.0    |
| 9       | < 100 > | 72     | P-Tensile  | 300   | SW  | 0       | 96.3    |
| 10      | < 100 > | 80     | P-Tensile  | 300   | SW  | 0       | 99.6    |
| 2       | < 100 > | 18     | P-Tensile  | 300   | SW  | 0       | 89.6    |
| 3       | < 100 > | 27     | P-Tensile  | 300   | SW  | 0       | 88.0    |
| 4       | < 100 > | 36     | P-Tensile  | 300   | SW  | 0       | 95.5    |
| 5       | < 100 > | 45     | P-Tensile  | 300   | SW  | 0       | 95.2    |
| 6       | < 100 > | 54     | P-Tensile  | 300   | SW  | 0       | 97.7    |
| 7       | < 100 > | 63     | P-Tensile  | 300   | SW  | 0       | 97.0    |
| 8       | < 100 > | 72     | P-Tensile  | 300   | SW  | 0       | 98.1    |



Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|-----|---------|---------|
| 9       | < 100 > | 81     | P-Tensile | 300   | SW  | 0       | 97.5    |
| 10      | < 100 > | 90     | P-Tensile | 300   | SW  | 0       | 99.9    |
| 2       | < 100 > | 20     | P-Tensile | 300   | SW  | 0       | 90.7    |
| 3       | < 100 > | 30     | P-Tensile | 300   | SW  | 0       | 90.4    |
| 4       | < 100 > | 40     | P-Tensile | 300   | SW  | 0       | 95.6    |
| 5       | < 100 > | 50     | P-Tensile | 300   | SW  | 0       | 91.9    |
| 6       | < 100 > | 60     | P-Tensile | 300   | SW  | 0       | 96.4    |
| 7       | < 100 > | 70     | P-Tensile | 300   | SW  | 0       | 96.0    |
| 8       | < 100 > | 80     | P-Tensile | 300   | SW  | 0       | 99.1    |
| 9       | < 100 > | 90     | P-Tensile | 300   | SW  | 0       | 98.0    |
| 10      | < 100 > | 100    | P-Tensile | 300   | SW  | 0       | 98.7    |
| 2       | < 100 > | 24     | P-Tensile | 300   | SW  | 0       | 86.7    |
| 3       | < 100 > | 36     | P-Tensile | 300   | SW  | 0       | 89.7    |
| 4       | < 100 > | 48     | P-Tensile | 300   | SW  | 0       | 97.5    |
| 5       | < 100 > | 60     | P-Tensile | 300   | SW  | 0       | 94.0    |
| 6       | < 100 > | 72     | P-Tensile | 300   | SW  | 0       | 97.3    |
| 7       | < 100 > | 84     | P-Tensile | 300   | SW  | 0       | 95.4    |
| 8       | < 100 > | 96     | P-Tensile | 300   | SW  | 0       | 99.0    |
| 9       | < 100 > | 108    | P-Tensile | 300   | SW  | 0       | 95.7    |
| 10      | < 100 > | 120    | P-Tensile | 300   | SW  | 0       | 99.7    |
| 2       | < 100 > | 28     | P-Tensile | 300   | SW  | 0       | 92.3    |
| 3       | < 100 > | 42     | P-Tensile | 300   | SW  | 0       | 89.3    |
| 4       | < 100 > | 56     | P-Tensile | 300   | SW  | 0       | 98.5    |
| 5       | < 100 > | 70     | P-Tensile | 300   | SW  | 0       | 92.1    |
| 6       | < 100 > | 84     | P-Tensile | 300   | SW  | 0       | 96.4    |
| 7       | < 100 > | 98     | P-Tensile | 300   | SW  | 0       | 96.1    |
| 8       | < 100 > | 112    | P-Tensile | 300   | SW  | 0       | 98.8    |
| 9       | < 100 > | 126    | P-Tensile | 300   | SW  | 0       | 96.7    |
| 10      | < 100 > | 140    | P-Tensile | 300   | SW  | 0       | 97.5    |
| 2       | < 100 > | 32     | P-Tensile | 300   | SW  | 0       | 87.5    |
| 3       | < 100 > | 48     | P-Tensile | 300   | SW  | 0       | 90.6    |
| 4       | < 100 > | 64     | P-Tensile | 300   | SW  | 0       | 95.7    |
| 5       | < 100 > | 80     | P-Tensile | 300   | SW  | 0       | 93.4    |
| 6       | < 100 > | 96     | P-Tensile | 300   | SW  | 0       | 97.1    |
| 7       | < 100 > | 112    | P-Tensile | 300   | SW  | 0       | 96.5    |
| 8       | < 100 > | 128    | P-Tensile | 300   | SW  | 0       | 99.5    |
| 9       | < 100 > | 144    | P-Tensile | 300   | SW  | 0       | 97.8    |
| 10      | < 100 > | 160    | P-Tensile | 300   | SW  | 0       | 97.9    |
| 2       | < 100 > | 36     | P-Tensile | 300   | SW  | 0       | 89.2    |
| 3       | < 100 > | 54     | P-Tensile | 300   | SW  | 0       | 89.5    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 4       | < 100 > | 72     | P-Tensile  | 300   | SW      | 0       | 96.8    |
| 5       | < 100 > | 90     | P-Tensile  | 300   | SW      | 0       | 93.9    |
| 6       | < 100 > | 108    | P-Tensile  | 300   | SW      | 0       | 96.4    |
| 7       | < 100 > | 126    | P-Tensile  | 300   | SW      | 0       | 95.2    |
| 8       | < 100 > | 144    | P-Tensile  | 300   | SW      | 0       | 99.1    |
| 9       | < 100 > | 162    | P-Tensile  | 300   | SW      | 0       | 94.8    |
| 10      | < 100 > | 180    | P-Tensile  | 300   | SW      | 0       | 97.9    |
| 2       | < 100 > | 40     | P-Tensile  | 300   | SW      | 0       | 93.2    |
| 3       | < 100 > | 60     | P-Tensile  | 300   | SW      | 0       | 87.1    |
| 4       | < 100 > | 80     | P-Tensile  | 300   | SW      | 0       | 94.9    |
| 5       | < 100 > | 100    | P-Tensile  | 300   | SW      | 0       | 93.6    |
| 6       | < 100 > | 120    | P-Tensile  | 300   | SW      | 0       | 96.5    |
| 7       | < 100 > | 140    | P-Tensile  | 300   | SW      | 0       | 95.2    |
| 8       | < 100 > | 160    | P-Tensile  | 300   | SW      | 0       | 98.4    |
| 9       | < 100 > | 180    | P-Tensile  | 300   | SW      | 0       | 97.2    |
| 10      | < 100 > | 200    | P-Tensile  | 300   | SW      | 0       | 100.3   |
| 2       | < 110 > | 14     | NP-Tensile | 300   | Tersoff | 0       | 200.7   |
| 3       | < 110 > | 21     | NP-Tensile | 300   | Tersoff | 0       | 200.3   |
| 4       | < 110 > | 28     | NP-Tensile | 300   | Tersoff | 0       | 182.4   |
| 5       | < 110 > | 35     | NP-Tensile | 300   | Tersoff | 0       | 183.5   |
| 6       | < 110 > | 42     | NP-Tensile | 300   | Tersoff | 0       | 194.6   |
| 7       | < 110 > | 49     | NP-Tensile | 300   | Tersoff | 0       | 193.9   |
| 8       | < 110 > | 56     | NP-Tensile | 300   | Tersoff | 0       | 187.4   |
| 9       | < 110 > | 63     | NP-Tensile | 300   | Tersoff | 0       | 187.5   |
| 10      | < 110 > | 70     | NP-Tensile | 300   | Tersoff | 0       | 193.3   |
| 2       | < 110 > | 16     | NP-Tensile | 300   | Tersoff | 0       | 201.6   |
| 3       | < 110 > | 24     | NP-Tensile | 300   | Tersoff | 0       | 200.5   |
| 4       | < 110 > | 32     | NP-Tensile | 300   | Tersoff | 0       | 182.4   |
| 5       | < 110 > | 40     | NP-Tensile | 300   | Tersoff | 0       | 183.0   |
| 6       | < 110 > | 48     | NP-Tensile | 300   | Tersoff | 0       | 194.8   |
| 7       | < 110 > | 56     | NP-Tensile | 300   | Tersoff | 0       | 194.2   |
| 8       | < 110 > | 64     | NP-Tensile | 300   | Tersoff | 0       | 187.6   |
| 9       | < 110 > | 72     | NP-Tensile | 300   | Tersoff | 0       | 188.4   |
| 10      | < 110 > | 80     | NP-Tensile | 300   | Tersoff | 0       | 193.4   |
| 2       | < 110 > | 18     | NP-Tensile | 300   | Tersoff | 0       | 202.3   |
| 3       | < 110 > | 27     | NP-Tensile | 300   | Tersoff | 0       | 200.5   |
| 4       | < 110 > | 36     | NP-Tensile | 300   | Tersoff | 0       | 181.6   |
| 5       | < 110 > | 45     | NP-Tensile | 300   | Tersoff | 0       | 181.7   |
| 6       | < 110 > | 54     | NP-Tensile | 300   | Tersoff | 0       | 194.9   |
| 7       | < 110 > | 63     | NP-Tensile | 300   | Tersoff | 0       | 194.1   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 8       | < 110 > | 72     | NP-Tensile | 300   | Tersoff | 0       | 188.2   |
| 9       | < 110 > | 81     | NP-Tensile | 300   | Tersoff | 0       | 188.3   |
| 10      | < 110 > | 90     | NP-Tensile | 300   | Tersoff | 0       | 193.2   |
| 2       | < 110 > | 20     | NP-Tensile | 300   | Tersoff | 0       | 204.6   |
| 3       | < 110 > | 30     | NP-Tensile | 300   | Tersoff | 0       | 199.8   |
| 4       | < 110 > | 40     | NP-Tensile | 300   | Tersoff | 0       | 181.6   |
| 5       | < 110 > | 50     | NP-Tensile | 300   | Tersoff | 0       | 181.6   |
| 6       | < 110 > | 60     | NP-Tensile | 300   | Tersoff | 0       | 195.1   |
| 7       | < 110 > | 70     | NP-Tensile | 300   | Tersoff | 0       | 194.5   |
| 8       | < 110 > | 80     | NP-Tensile | 300   | Tersoff | 0       | 188.4   |
| 9       | < 110 > | 90     | NP-Tensile | 300   | Tersoff | 0       | 188.5   |
| 10      | < 110 > | 100    | NP-Tensile | 300   | Tersoff | 0       | 192.9   |
| 2       | < 110 > | 24     | NP-Tensile | 300   | Tersoff | 0       | 201.0   |
| 3       | < 110 > | 36     | NP-Tensile | 300   | Tersoff | 0       | 199.7   |
| 4       | < 110 > | 48     | NP-Tensile | 300   | Tersoff | 0       | 179.7   |
| 5       | < 110 > | 60     | NP-Tensile | 300   | Tersoff | 0       | 180.2   |
| 6       | < 110 > | 72     | NP-Tensile | 300   | Tersoff | 0       | 194.7   |
| 7       | < 110 > | 84     | NP-Tensile | 300   | Tersoff | 0       | 194.5   |
| 8       | < 110 > | 96     | NP-Tensile | 300   | Tersoff | 0       | 187.7   |
| 9       | < 110 > | 108    | NP-Tensile | 300   | Tersoff | 0       | 187.9   |
| 10      | < 110 > | 120    | NP-Tensile | 300   | Tersoff | 0       | 194.6   |
| 2       | < 110 > | 28     | NP-Tensile | 300   | Tersoff | 0       | 202.5   |
| 3       | < 110 > | 42     | NP-Tensile | 300   | Tersoff | 0       | 200.4   |
| 4       | < 110 > | 56     | NP-Tensile | 300   | Tersoff | 0       | 176.1   |
| 5       | < 110 > | 70     | NP-Tensile | 300   | Tersoff | 0       | 185.1   |
| 6       | < 110 > | 84     | NP-Tensile | 300   | Tersoff | 0       | 194.7   |
| 7       | < 110 > | 98     | NP-Tensile | 300   | Tersoff | 0       | 194.0   |
| 8       | < 110 > | 112    | NP-Tensile | 300   | Tersoff | 0       | 187.7   |
| 9       | < 110 > | 126    | NP-Tensile | 300   | Tersoff | 0       | 189.1   |
| 10      | < 110 > | 140    | NP-Tensile | 300   | Tersoff | 0       | 194.0   |
| 2       | < 110 > | 32     | NP-Tensile | 300   | Tersoff | 0       | 204.4   |
| 3       | < 110 > | 48     | NP-Tensile | 300   | Tersoff | 0       | 199.4   |
| 4       | < 110 > | 64     | NP-Tensile | 300   | Tersoff | 0       | 186.0   |
| 5       | < 110 > | 80     | NP-Tensile | 300   | Tersoff | 0       | 184.8   |
| 6       | < 110 > | 96     | NP-Tensile | 300   | Tersoff | 0       | 194.4   |
| 7       | < 110 > | 112    | NP-Tensile | 300   | Tersoff | 0       | 193.9   |
| 8       | < 110 > | 128    | NP-Tensile | 300   | Tersoff | 0       | 187.7   |
| 9       | < 110 > | 144    | NP-Tensile | 300   | Tersoff | 0       | 188.4   |
| 10      | < 110 > | 160    | NP-Tensile | 300   | Tersoff | 0       | 193.8   |
| 2       | < 110 > | 36     | NP-Tensile | 300   | Tersoff | 0       | 203.8   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 3       | < 110 > | 54     | NP-Tensile | 300   | Tersoff | 0       | 199.7   |
| 4       | < 110 > | 72     | NP-Tensile | 300   | Tersoff | 0       | 185.4   |
| 5       | < 110 > | 90     | NP-Tensile | 300   | Tersoff | 0       | 184.7   |
| 6       | < 110 > | 108    | NP-Tensile | 300   | Tersoff | 0       | 194.6   |
| 7       | < 110 > | 126    | NP-Tensile | 300   | Tersoff | 0       | 193.8   |
| 8       | < 110 > | 144    | NP-Tensile | 300   | Tersoff | 0       | 188.0   |
| 9       | < 110 > | 162    | NP-Tensile | 300   | Tersoff | 0       | 189.7   |
| 10      | < 110 > | 180    | NP-Tensile | 300   | Tersoff | 0       | 194.7   |
| 2       | < 110 > | 40     | NP-Tensile | 300   | Tersoff | 0       | 205.3   |
| 3       | < 110 > | 60     | NP-Tensile | 300   | Tersoff | 0       | 200.0   |
| 4       | < 110 > | 80     | NP-Tensile | 300   | Tersoff | 0       | 185.7   |
| 5       | < 110 > | 100    | NP-Tensile | 300   | Tersoff | 0       | 184.6   |
| 6       | < 110 > | 120    | NP-Tensile | 300   | Tersoff | 0       | 194.6   |
| 7       | < 110 > | 140    | NP-Tensile | 300   | Tersoff | 0       | 194.0   |
| 8       | < 110 > | 160    | NP-Tensile | 300   | Tersoff | 0       | 188.1   |
| 9       | < 110 > | 180    | NP-Tensile | 300   | Tersoff | 0       | 189.5   |
| 10      | < 110 > | 200    | NP-Tensile | 300   | Tersoff | 0       | 193.7   |
| 2       | < 110 > | 14     | P-Tensile  | 300   | Tersoff | 0       | 163.3   |
| 3       | < 110 > | 21     | P-Tensile  | 300   | Tersoff | 0       | 163.3   |
| 4       | < 110 > | 28     | P-Tensile  | 300   | Tersoff | 0       | 147.1   |
| 5       | < 110 > | 35     | P-Tensile  | 300   | Tersoff | 0       | 146.3   |
| 6       | < 110 > | 42     | P-Tensile  | 300   | Tersoff | 0       | 142.9   |
| 7       | < 110 > | 49     | P-Tensile  | 300   | Tersoff | 0       | 143.8   |
| 8       | < 110 > | 56     | P-Tensile  | 300   | Tersoff | 0       | 146.8   |
| 9       | < 110 > | 63     | P-Tensile  | 300   | Tersoff | 0       | 139.1   |
| 10      | < 110 > | 70     | P-Tensile  | 300   | Tersoff | 0       | 138.3   |
| 2       | < 110 > | 16     | P-Tensile  | 300   | Tersoff | 0       | 163.6   |
| 3       | < 110 > | 24     | P-Tensile  | 300   | Tersoff | 0       | 145.6   |
| 4       | < 110 > | 32     | P-Tensile  | 300   | Tersoff | 0       | 143.4   |
| 5       | < 110 > | 40     | P-Tensile  | 300   | Tersoff | 0       | 143.1   |
| 6       | < 110 > | 48     | P-Tensile  | 300   | Tersoff | 0       | 142.8   |
| 7       | < 110 > | 56     | P-Tensile  | 300   | Tersoff | 0       | 143.1   |
| 8       | < 110 > | 64     | P-Tensile  | 300   | Tersoff | 0       | 139.1   |
| 9       | < 110 > | 72     | P-Tensile  | 300   | Tersoff | 0       | 138.9   |
| 10      | < 110 > | 80     | P-Tensile  | 300   | Tersoff | 0       | 142.5   |
| 2       | < 110 > | 18     | P-Tensile  | 300   | Tersoff | 0       | 162.3   |
| 3       | < 110 > | 27     | P-Tensile  | 300   | Tersoff | 0       | 144.1   |
| 4       | < 110 > | 36     | P-Tensile  | 300   | Tersoff | 0       | 140.9   |
| 5       | < 110 > | 45     | P-Tensile  | 300   | Tersoff | 0       | 133.0   |
| 6       | < 110 > | 54     | P-Tensile  | 300   | Tersoff | 0       | 141.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|---------|---------|---------|
| 7       | < 110 > | 63     | P-Tensile | 300   | Tersoff | 0       | 141.5   |
| 8       | < 110 > | 72     | P-Tensile | 300   | Tersoff | 0       | 137.2   |
| 9       | < 110 > | 81     | P-Tensile | 300   | Tersoff | 0       | 138.2   |
| 10      | < 110 > | 90     | P-Tensile | 300   | Tersoff | 0       | 140.9   |
| 2       | < 110 > | 20     | P-Tensile | 300   | Tersoff | 0       | 162.9   |
| 3       | < 110 > | 30     | P-Tensile | 300   | Tersoff | 0       | 141.7   |
| 4       | < 110 > | 40     | P-Tensile | 300   | Tersoff | 0       | 140.8   |
| 5       | < 110 > | 50     | P-Tensile | 300   | Tersoff | 0       | 142.8   |
| 6       | < 110 > | 60     | P-Tensile | 300   | Tersoff | 0       | 142.7   |
| 7       | < 110 > | 70     | P-Tensile | 300   | Tersoff | 0       | 142.7   |
| 8       | < 110 > | 80     | P-Tensile | 300   | Tersoff | 0       | 138.3   |
| 9       | < 110 > | 90     | P-Tensile | 300   | Tersoff | 0       | 139.1   |
| 10      | < 110 > | 100    | P-Tensile | 300   | Tersoff | 0       | 142.2   |
| 2       | < 110 > | 24     | P-Tensile | 300   | Tersoff | 0       | 167.2   |
| 3       | < 110 > | 36     | P-Tensile | 300   | Tersoff | 0       | 147.5   |
| 4       | < 110 > | 48     | P-Tensile | 300   | Tersoff | 0       | 144.1   |
| 5       | < 110 > | 60     | P-Tensile | 300   | Tersoff | 0       | 142.0   |
| 6       | < 110 > | 72     | P-Tensile | 300   | Tersoff | 0       | 143.6   |
| 7       | < 110 > | 84     | P-Tensile | 300   | Tersoff | 0       | 141.9   |
| 8       | < 110 > | 96     | P-Tensile | 300   | Tersoff | 0       | 139.8   |
| 9       | < 110 > | 108    | P-Tensile | 300   | Tersoff | 0       | 138.1   |
| 10      | < 110 > | 120    | P-Tensile | 300   | Tersoff | 0       | 144.3   |
| 2       | < 110 > | 28     | P-Tensile | 300   | Tersoff | 0       | 161.1   |
| 3       | < 110 > | 42     | P-Tensile | 300   | Tersoff | 0       | 150.0   |
| 4       | < 110 > | 56     | P-Tensile | 300   | Tersoff | 0       | 139.9   |
| 5       | < 110 > | 70     | P-Tensile | 300   | Tersoff | 0       | 143.1   |
| 6       | < 110 > | 84     | P-Tensile | 300   | Tersoff | 0       | 141.9   |
| 7       | < 110 > | 98     | P-Tensile | 300   | Tersoff | 0       | 146.5   |
| 8       | < 110 > | 112    | P-Tensile | 300   | Tersoff | 0       | 137.9   |
| 9       | < 110 > | 126    | P-Tensile | 300   | Tersoff | 0       | 137.1   |
| 10      | < 110 > | 140    | P-Tensile | 300   | Tersoff | 0       | 143.2   |
| 2       | < 110 > | 32     | P-Tensile | 300   | Tersoff | 0       | 163.0   |
| 3       | < 110 > | 48     | P-Tensile | 300   | Tersoff | 0       | 153.7   |
| 4       | < 110 > | 64     | P-Tensile | 300   | Tersoff | 0       | 141.2   |
| 5       | < 110 > | 80     | P-Tensile | 300   | Tersoff | 0       | 142.4   |
| 6       | < 110 > | 96     | P-Tensile | 300   | Tersoff | 0       | 145.4   |
| 7       | < 110 > | 112    | P-Tensile | 300   | Tersoff | 0       | 143.0   |
| 8       | < 110 > | 128    | P-Tensile | 300   | Tersoff | 0       | 138.5   |
| 9       | < 110 > | 144    | P-Tensile | 300   | Tersoff | 0       | 138.7   |
| 10      | < 110 > | 160    | P-Tensile | 300   | Tersoff | 0       | 143.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 2       | < 110 > | 36     | P-Tensile  | 300   | Tersoff | 0       | 152.6   |
| 3       | < 110 > | 54     | P-Tensile  | 300   | Tersoff | 0       | 149.2   |
| 4       | < 110 > | 72     | P-Tensile  | 300   | Tersoff | 0       | 144.0   |
| 5       | < 110 > | 90     | P-Tensile  | 300   | Tersoff | 0       | 143.0   |
| 6       | < 110 > | 108    | P-Tensile  | 300   | Tersoff | 0       | 143.2   |
| 7       | < 110 > | 126    | P-Tensile  | 300   | Tersoff | 0       | 146.3   |
| 8       | < 110 > | 144    | P-Tensile  | 300   | Tersoff | 0       | 139.0   |
| 9       | < 110 > | 162    | P-Tensile  | 300   | Tersoff | 0       | 137.5   |
| 10      | < 110 > | 180    | P-Tensile  | 300   | Tersoff | 0       | 143.1   |
| 2       | < 110 > | 40     | P-Tensile  | 300   | Tersoff | 0       | 162.4   |
| 3       | < 110 > | 60     | P-Tensile  | 300   | Tersoff | 0       | 147.0   |
| 4       | < 110 > | 80     | P-Tensile  | 300   | Tersoff | 0       | 144.9   |
| 5       | < 110 > | 100    | P-Tensile  | 300   | Tersoff | 0       | 143.3   |
| 6       | < 110 > | 120    | P-Tensile  | 300   | Tersoff | 0       | 143.2   |
| 7       | < 110 > | 140    | P-Tensile  | 300   | Tersoff | 0       | 142.6   |
| 8       | < 110 > | 160    | P-Tensile  | 300   | Tersoff | 0       | 137.5   |
| 9       | < 110 > | 180    | P-Tensile  | 300   | Tersoff | 0       | 139.9   |
| 10      | < 110 > | 200    | P-Tensile  | 300   | Tersoff | 0       | 143.5   |
| 2       | < 110 > | 14     | NP-Tensile | 300   | SW      | 0       | 158.7   |
| 3       | < 110 > | 21     | NP-Tensile | 300   | SW      | 0       | 160.6   |
| 4       | < 110 > | 28     | NP-Tensile | 300   | SW      | 0       | 156.5   |
| 5       | < 110 > | 35     | NP-Tensile | 300   | SW      | 0       | 159.1   |
| 6       | < 110 > | 42     | NP-Tensile | 300   | SW      | 0       | 163.6   |
| 7       | < 110 > | 49     | NP-Tensile | 300   | SW      | 0       | 163.7   |
| 8       | < 110 > | 56     | NP-Tensile | 300   | SW      | 0       | 161.9   |
| 9       | < 110 > | 63     | NP-Tensile | 300   | SW      | 0       | 162.5   |
| 10      | < 110 > | 70     | NP-Tensile | 300   | SW      | 0       | 165.6   |
| 2       | < 110 > | 16     | NP-Tensile | 300   | SW      | 0       | 157.8   |
| 3       | < 110 > | 24     | NP-Tensile | 300   | SW      | 0       | 159.7   |
| 4       | < 110 > | 32     | NP-Tensile | 300   | SW      | 0       | 157.7   |
| 5       | < 110 > | 40     | NP-Tensile | 300   | SW      | 0       | 159.0   |
| 6       | < 110 > | 48     | NP-Tensile | 300   | SW      | 0       | 163.7   |
| 7       | < 110 > | 56     | NP-Tensile | 300   | SW      | 0       | 163.6   |
| 8       | < 110 > | 64     | NP-Tensile | 300   | SW      | 0       | 162.1   |
| 9       | < 110 > | 72     | NP-Tensile | 300   | SW      | 0       | 162.8   |
| 10      | < 110 > | 80     | NP-Tensile | 300   | SW      | 0       | 165.5   |
| 2       | < 110 > | 18     | NP-Tensile | 300   | SW      | 0       | 157.1   |
| 3       | < 110 > | 27     | NP-Tensile | 300   | SW      | 0       | 159.6   |
| 4       | < 110 > | 36     | NP-Tensile | 300   | SW      | 0       | 157.4   |
| 5       | < 110 > | 45     | NP-Tensile | 300   | SW      | 0       | 157.7   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 6       | < 110 > | 54     | NP-Tensile | 300   | SW  | 0       | 163.1   |
| 7       | < 110 > | 63     | NP-Tensile | 300   | SW  | 0       | 163.3   |
| 8       | < 110 > | 72     | NP-Tensile | 300   | SW  | 0       | 161.6   |
| 9       | < 110 > | 81     | NP-Tensile | 300   | SW  | 0       | 162.7   |
| 10      | < 110 > | 90     | NP-Tensile | 300   | SW  | 0       | 165.5   |
| 2       | < 110 > | 20     | NP-Tensile | 300   | SW  | 0       | 156.0   |
| 3       | < 110 > | 30     | NP-Tensile | 300   | SW  | 0       | 160.3   |
| 4       | < 110 > | 40     | NP-Tensile | 300   | SW  | 0       | 157.5   |
| 5       | < 110 > | 50     | NP-Tensile | 300   | SW  | 0       | 157.5   |
| 6       | < 110 > | 60     | NP-Tensile | 300   | SW  | 0       | 163.3   |
| 7       | < 110 > | 70     | NP-Tensile | 300   | SW  | 0       | 164.1   |
| 8       | < 110 > | 80     | NP-Tensile | 300   | SW  | 0       | 162.0   |
| 9       | < 110 > | 90     | NP-Tensile | 300   | SW  | 0       | 162.8   |
| 10      | < 110 > | 100    | NP-Tensile | 300   | SW  | 0       | 165.2   |
| 2       | < 110 > | 24     | NP-Tensile | 300   | SW  | 0       | 158.2   |
| 3       | < 110 > | 36     | NP-Tensile | 300   | SW  | 0       | 159.5   |
| 4       | < 110 > | 48     | NP-Tensile | 300   | SW  | 0       | 156.7   |
| 5       | < 110 > | 60     | NP-Tensile | 300   | SW  | 0       | 157.2   |
| 6       | < 110 > | 72     | NP-Tensile | 300   | SW  | 0       | 162.9   |
| 7       | < 110 > | 84     | NP-Tensile | 300   | SW  | 0       | 163.9   |
| 8       | < 110 > | 96     | NP-Tensile | 300   | SW  | 0       | 161.4   |
| 9       | < 110 > | 108    | NP-Tensile | 300   | SW  | 0       | 162.4   |
| 10      | < 110 > | 120    | NP-Tensile | 300   | SW  | 0       | 164.9   |
| 2       | < 110 > | 28     | NP-Tensile | 300   | SW  | 0       | 157.1   |
| 3       | < 110 > | 42     | NP-Tensile | 300   | SW  | 0       | 160.4   |
| 4       | < 110 > | 56     | NP-Tensile | 300   | SW  | 0       | 156.3   |
| 5       | < 110 > | 70     | NP-Tensile | 300   | SW  | 0       | 157.4   |
| 6       | < 110 > | 84     | NP-Tensile | 300   | SW  | 0       | 163.2   |
| 7       | < 110 > | 98     | NP-Tensile | 300   | SW  | 0       | 163.6   |
| 8       | < 110 > | 112    | NP-Tensile | 300   | SW  | 0       | 161.5   |
| 9       | < 110 > | 126    | NP-Tensile | 300   | SW  | 0       | 162.4   |
| 10      | < 110 > | 140    | NP-Tensile | 300   | SW  | 0       | 164.8   |
| 2       | < 110 > | 32     | NP-Tensile | 300   | SW  | 0       | 155.0   |
| 3       | < 110 > | 48     | NP-Tensile | 300   | SW  | 0       | 159.2   |
| 4       | < 110 > | 64     | NP-Tensile | 300   | SW  | 0       | 157.0   |
| 5       | < 110 > | 80     | NP-Tensile | 300   | SW  | 0       | 157.3   |
| 6       | < 110 > | 96     | NP-Tensile | 300   | SW  | 0       | 162.8   |
| 7       | < 110 > | 112    | NP-Tensile | 300   | SW  | 0       | 163.4   |
| 8       | < 110 > | 128    | NP-Tensile | 300   | SW  | 0       | 161.6   |
| 9       | < 110 > | 144    | NP-Tensile | 300   | SW  | 0       | 162.5   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 10      | < 110 > | 160    | NP-Tensile | 300   | SW  | 0       | 164.7   |
| 2       | < 110 > | 36     | NP-Tensile | 300   | SW  | 0       | 155.2   |
| 3       | < 110 > | 54     | NP-Tensile | 300   | SW  | 0       | 158.4   |
| 4       | < 110 > | 72     | NP-Tensile | 300   | SW  | 0       | 156.8   |
| 5       | < 110 > | 90     | NP-Tensile | 300   | SW  | 0       | 157.3   |
| 6       | < 110 > | 108    | NP-Tensile | 300   | SW  | 0       | 162.8   |
| 7       | < 110 > | 126    | NP-Tensile | 300   | SW  | 0       | 163.3   |
| 8       | < 110 > | 144    | NP-Tensile | 300   | SW  | 0       | 161.5   |
| 9       | < 110 > | 162    | NP-Tensile | 300   | SW  | 0       | 164.0   |
| 10      | < 110 > | 180    | NP-Tensile | 300   | SW  | 0       | 169.8   |
| 2       | < 110 > | 40     | NP-Tensile | 300   | SW  | 0       | 156.7   |
| 3       | < 110 > | 60     | NP-Tensile | 300   | SW  | 0       | 158.7   |
| 4       | < 110 > | 80     | NP-Tensile | 300   | SW  | 0       | 157.4   |
| 5       | < 110 > | 100    | NP-Tensile | 300   | SW  | 0       | 157.2   |
| 6       | < 110 > | 120    | NP-Tensile | 300   | SW  | 0       | 162.8   |
| 7       | < 110 > | 140    | NP-Tensile | 300   | SW  | 0       | 163.4   |
| 8       | < 110 > | 160    | NP-Tensile | 300   | SW  | 0       | 161.5   |
| 9       | < 110 > | 180    | NP-Tensile | 300   | SW  | 0       | 162.4   |
| 10      | < 110 > | 200    | NP-Tensile | 300   | SW  | 0       | 167.1   |
| 2       | < 110 > | 14     | P-Tensile  | 300   | SW  | 0       | 126.3   |
| 3       | < 110 > | 21     | P-Tensile  | 300   | SW  | 0       | 126.3   |
| 4       | < 110 > | 28     | P-Tensile  | 300   | SW  | 0       | 126.5   |
| 5       | < 110 > | 35     | P-Tensile  | 300   | SW  | 0       | 125.9   |
| 6       | < 110 > | 42     | P-Tensile  | 300   | SW  | 0       | 123.8   |
| 7       | < 110 > | 49     | P-Tensile  | 300   | SW  | 0       | 124.5   |
| 8       | < 110 > | 56     | P-Tensile  | 300   | SW  | 0       | 122.3   |
| 9       | < 110 > | 63     | P-Tensile  | 300   | SW  | 0       | 121.5   |
| 10      | < 110 > | 70     | P-Tensile  | 300   | SW  | 0       | 122.8   |
| 2       | < 110 > | 16     | P-Tensile  | 300   | SW  | 0       | 137.1   |
| 3       | < 110 > | 24     | P-Tensile  | 300   | SW  | 0       | 119.4   |
| 4       | < 110 > | 32     | P-Tensile  | 300   | SW  | 0       | 121.3   |
| 5       | < 110 > | 40     | P-Tensile  | 300   | SW  | 0       | 120.6   |
| 6       | < 110 > | 48     | P-Tensile  | 300   | SW  | 0       | 126.1   |
| 7       | < 110 > | 56     | P-Tensile  | 300   | SW  | 0       | 122.6   |
| 8       | < 110 > | 64     | P-Tensile  | 300   | SW  | 0       | 121.7   |
| 9       | < 110 > | 72     | P-Tensile  | 300   | SW  | 0       | 121.0   |
| 10      | < 110 > | 80     | P-Tensile  | 300   | SW  | 0       | 124.3   |
| 2       | < 110 > | 18     | P-Tensile  | 300   | SW  | 0       | 138.5   |
| 3       | < 110 > | 27     | P-Tensile  | 300   | SW  | 0       | 121.2   |
| 4       | < 110 > | 36     | P-Tensile  | 300   | SW  | 0       | 125.8   |



Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT                  | L (nm) | BC        | T (K) | POT | SS (nm) | E (GPa) |
|---------|-----------------------|--------|-----------|-------|-----|---------|---------|
| 5       | $\langle 110 \rangle$ | 45     | P-Tensile | 300   | SW  | 0       | 120.8   |
| 6       | $\langle 110 \rangle$ | 54     | P-Tensile | 300   | SW  | 0       | 124.7   |
| 7       | $\langle 110 \rangle$ | 63     | P-Tensile | 300   | SW  | 0       | 122.4   |
| 8       | $\langle 110 \rangle$ | 72     | P-Tensile | 300   | SW  | 0       | 119.7   |
| 9       | $\langle 110 \rangle$ | 81     | P-Tensile | 300   | SW  | 0       | 121.8   |
| 10      | $\langle 110 \rangle$ | 90     | P-Tensile | 300   | SW  | 0       | 126.2   |
| 2       | $\langle 110 \rangle$ | 20     | P-Tensile | 300   | SW  | 0       | 128.9   |
| 3       | $\langle 110 \rangle$ | 30     | P-Tensile | 300   | SW  | 0       | 126.8   |
| 4       | $\langle 110 \rangle$ | 40     | P-Tensile | 300   | SW  | 0       | 122.7   |
| 5       | $\langle 110 \rangle$ | 50     | P-Tensile | 300   | SW  | 0       | 120.5   |
| 6       | $\langle 110 \rangle$ | 60     | P-Tensile | 300   | SW  | 0       | 122.1   |
| 7       | $\langle 110 \rangle$ | 70     | P-Tensile | 300   | SW  | 0       | 124.9   |
| 8       | $\langle 110 \rangle$ | 80     | P-Tensile | 300   | SW  | 0       | 120.4   |
| 9       | $\langle 110 \rangle$ | 90     | P-Tensile | 300   | SW  | 0       | 119.9   |
| 10      | $\langle 110 \rangle$ | 100    | P-Tensile | 300   | SW  | 0       | 124.3   |
| 2       | $\langle 110 \rangle$ | 24     | P-Tensile | 300   | SW  | 0       | 134.5   |
| 3       | $\langle 110 \rangle$ | 36     | P-Tensile | 300   | SW  | 0       | 118.8   |
| 4       | $\langle 110 \rangle$ | 48     | P-Tensile | 300   | SW  | 0       | 125.0   |
| 5       | $\langle 110 \rangle$ | 60     | P-Tensile | 300   | SW  | 0       | 120.8   |
| 6       | $\langle 110 \rangle$ | 72     | P-Tensile | 300   | SW  | 0       | 124.5   |
| 7       | $\langle 110 \rangle$ | 84     | P-Tensile | 300   | SW  | 0       | 123.5   |
| 8       | $\langle 110 \rangle$ | 96     | P-Tensile | 300   | SW  | 0       | 120.7   |
| 9       | $\langle 110 \rangle$ | 108    | P-Tensile | 300   | SW  | 0       | 120.9   |
| 10      | $\langle 110 \rangle$ | 120    | P-Tensile | 300   | SW  | 0       | 125.2   |
| 2       | $\langle 110 \rangle$ | 28     | P-Tensile | 300   | SW  | 0       | 133.1   |
| 3       | $\langle 110 \rangle$ | 42     | P-Tensile | 300   | SW  | 0       | 121.7   |
| 4       | $\langle 110 \rangle$ | 56     | P-Tensile | 300   | SW  | 0       | 125.0   |
| 5       | $\langle 110 \rangle$ | 70     | P-Tensile | 300   | SW  | 0       | 121.1   |
| 6       | $\langle 110 \rangle$ | 84     | P-Tensile | 300   | SW  | 0       | 122.6   |
| 7       | $\langle 110 \rangle$ | 98     | P-Tensile | 300   | SW  | 0       | 124.1   |
| 8       | $\langle 110 \rangle$ | 112    | P-Tensile | 300   | SW  | 0       | 120.4   |
| 9       | $\langle 110 \rangle$ | 126    | P-Tensile | 300   | SW  | 0       | 120.6   |
| 10      | $\langle 110 \rangle$ | 140    | P-Tensile | 300   | SW  | 0       | 125.8   |
| 2       | $\langle 110 \rangle$ | 32     | P-Tensile | 300   | SW  | 0       | 133.5   |
| 3       | $\langle 110 \rangle$ | 48     | P-Tensile | 300   | SW  | 0       | 119.8   |
| 4       | $\langle 110 \rangle$ | 64     | P-Tensile | 300   | SW  | 0       | 122.1   |
| 5       | $\langle 110 \rangle$ | 80     | P-Tensile | 300   | SW  | 0       | 121.9   |
| 6       | $\langle 110 \rangle$ | 96     | P-Tensile | 300   | SW  | 0       | 123.6   |
| 7       | $\langle 110 \rangle$ | 112    | P-Tensile | 300   | SW  | 0       | 122.5   |
| 8       | $\langle 110 \rangle$ | 128    | P-Tensile | 300   | SW  | 0       | 121.4   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 9       | < 110 > | 144    | P-Tensile  | 300   | SW      | 0       | 121.8   |
| 10      | < 110 > | 160    | P-Tensile  | 300   | SW      | 0       | 124.2   |
| 2       | < 110 > | 36     | P-Tensile  | 300   | SW      | 0       | 131.5   |
| 3       | < 110 > | 54     | P-Tensile  | 300   | SW      | 0       | 121.3   |
| 4       | < 110 > | 72     | P-Tensile  | 300   | SW      | 0       | 123.0   |
| 5       | < 110 > | 90     | P-Tensile  | 300   | SW      | 0       | 121.7   |
| 6       | < 110 > | 108    | P-Tensile  | 300   | SW      | 0       | 124.0   |
| 7       | < 110 > | 126    | P-Tensile  | 300   | SW      | 0       | 123.5   |
| 8       | < 110 > | 144    | P-Tensile  | 300   | SW      | 0       | 121.0   |
| 9       | < 110 > | 162    | P-Tensile  | 300   | SW      | 0       | 121.0   |
| 10      | < 110 > | 180    | P-Tensile  | 300   | SW      | 0       | 125.4   |
| 2       | < 110 > | 40     | P-Tensile  | 300   | SW      | 0       | 126.7   |
| 3       | < 110 > | 60     | P-Tensile  | 300   | SW      | 0       | 119.9   |
| 4       | < 110 > | 80     | P-Tensile  | 300   | SW      | 0       | 122.7   |
| 5       | < 110 > | 100    | P-Tensile  | 300   | SW      | 0       | 121.0   |
| 6       | < 110 > | 120    | P-Tensile  | 300   | SW      | 0       | 123.4   |
| 7       | < 110 > | 140    | P-Tensile  | 300   | SW      | 0       | 124.2   |
| 8       | < 110 > | 160    | P-Tensile  | 300   | SW      | 0       | 118.9   |
| 9       | < 110 > | 180    | P-Tensile  | 300   | SW      | 0       | 120.5   |
| 10      | < 110 > | 200    | P-Tensile  | 300   | SW      | 0       | 124.1   |
| 2       | < 111 > | 14     | NP-Tensile | 300   | Tersoff | 0       | 181.2   |
| 3       | < 111 > | 21     | NP-Tensile | 300   | Tersoff | 0       | 193.6   |
| 4       | < 111 > | 28     | NP-Tensile | 300   | Tersoff | 0       | 199.5   |
| 5       | < 111 > | 35     | NP-Tensile | 300   | Tersoff | 0       | 203.4   |
| 6       | < 111 > | 42     | NP-Tensile | 300   | Tersoff | 0       | 206.1   |
| 7       | < 111 > | 49     | NP-Tensile | 300   | Tersoff | 0       | 209.0   |
| 8       | < 111 > | 56     | NP-Tensile | 300   | Tersoff | 0       | 209.1   |
| 9       | < 111 > | 63     | NP-Tensile | 300   | Tersoff | 0       | 210.8   |
| 10      | < 111 > | 70     | NP-Tensile | 300   | Tersoff | 0       | 211.5   |
| 2       | < 111 > | 16     | NP-Tensile | 300   | Tersoff | 0       | 178.6   |
| 3       | < 111 > | 24     | NP-Tensile | 300   | Tersoff | 0       | 194.6   |
| 4       | < 111 > | 32     | NP-Tensile | 300   | Tersoff | 0       | 201.2   |
| 5       | < 111 > | 40     | NP-Tensile | 300   | Tersoff | 0       | 204.2   |
| 6       | < 111 > | 48     | NP-Tensile | 300   | Tersoff | 0       | 206.6   |
| 7       | < 111 > | 56     | NP-Tensile | 300   | Tersoff | 0       | 207.9   |
| 8       | < 111 > | 64     | NP-Tensile | 300   | Tersoff | 0       | 209.4   |
| 9       | < 111 > | 72     | NP-Tensile | 300   | Tersoff | 0       | 210.7   |
| 10      | < 111 > | 80     | NP-Tensile | 300   | Tersoff | 0       | 211.5   |
| 2       | < 111 > | 18     | NP-Tensile | 300   | Tersoff | 0       | 182.4   |
| 3       | < 111 > | 27     | NP-Tensile | 300   | Tersoff | 0       | 194.5   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 4       | < 111 > | 36     | NP-Tensile | 300   | Tersoff | 0       | 200.6   |
| 5       | < 111 > | 45     | NP-Tensile | 300   | Tersoff | 0       | 204.3   |
| 6       | < 111 > | 54     | NP-Tensile | 300   | Tersoff | 0       | 207.1   |
| 7       | < 111 > | 63     | NP-Tensile | 300   | Tersoff | 0       | 208.3   |
| 8       | < 111 > | 72     | NP-Tensile | 300   | Tersoff | 0       | 209.6   |
| 9       | < 111 > | 81     | NP-Tensile | 300   | Tersoff | 0       | 210.8   |
| 10      | < 111 > | 90     | NP-Tensile | 300   | Tersoff | 0       | 211.6   |
| 2       | < 111 > | 20     | NP-Tensile | 300   | Tersoff | 0       | 184.0   |
| 3       | < 111 > | 30     | NP-Tensile | 300   | Tersoff | 0       | 194.0   |
| 4       | < 111 > | 40     | NP-Tensile | 300   | Tersoff | 0       | 200.4   |
| 5       | < 111 > | 50     | NP-Tensile | 300   | Tersoff | 0       | 204.7   |
| 6       | < 111 > | 60     | NP-Tensile | 300   | Tersoff | 0       | 206.8   |
| 7       | < 111 > | 70     | NP-Tensile | 300   | Tersoff | 0       | 208.1   |
| 8       | < 111 > | 80     | NP-Tensile | 300   | Tersoff | 0       | 209.4   |
| 9       | < 111 > | 90     | NP-Tensile | 300   | Tersoff | 0       | 210.7   |
| 10      | < 111 > | 100    | NP-Tensile | 300   | Tersoff | 0       | 211.9   |
| 2       | < 111 > | 24     | NP-Tensile | 300   | Tersoff | 0       | 183.8   |
| 3       | < 111 > | 36     | NP-Tensile | 300   | Tersoff | 0       | 194.0   |
| 4       | < 111 > | 48     | NP-Tensile | 300   | Tersoff | 0       | 200.7   |
| 5       | < 111 > | 60     | NP-Tensile | 300   | Tersoff | 0       | 203.7   |
| 6       | < 111 > | 72     | NP-Tensile | 300   | Tersoff | 0       | 206.4   |
| 7       | < 111 > | 84     | NP-Tensile | 300   | Tersoff | 0       | 208.5   |
| 8       | < 111 > | 96     | NP-Tensile | 300   | Tersoff | 0       | 210.0   |
| 9       | < 111 > | 108    | NP-Tensile | 300   | Tersoff | 0       | 211.2   |
| 10      | < 111 > | 120    | NP-Tensile | 300   | Tersoff | 0       | 211.9   |
| 2       | < 111 > | 28     | NP-Tensile | 300   | Tersoff | 0       | 183.9   |
| 3       | < 111 > | 42     | NP-Tensile | 300   | Tersoff | 0       | 194.3   |
| 4       | < 111 > | 56     | NP-Tensile | 300   | Tersoff | 0       | 200.2   |
| 5       | < 111 > | 70     | NP-Tensile | 300   | Tersoff | 0       | 203.7   |
| 6       | < 111 > | 84     | NP-Tensile | 300   | Tersoff | 0       | 206.7   |
| 7       | < 111 > | 98     | NP-Tensile | 300   | Tersoff | 0       | 208.9   |
| 8       | < 111 > | 112    | NP-Tensile | 300   | Tersoff | 0       | 210.0   |
| 9       | < 111 > | 126    | NP-Tensile | 300   | Tersoff | 0       | 210.9   |
| 10      | < 111 > | 140    | NP-Tensile | 300   | Tersoff | 0       | 211.7   |
| 2       | < 111 > | 32     | NP-Tensile | 300   | Tersoff | 0       | 184.0   |
| 3       | < 111 > | 48     | NP-Tensile | 300   | Tersoff | 0       | 194.2   |
| 4       | < 111 > | 64     | NP-Tensile | 300   | Tersoff | 0       | 200.0   |
| 5       | < 111 > | 80     | NP-Tensile | 300   | Tersoff | 0       | 203.7   |
| 6       | < 111 > | 96     | NP-Tensile | 300   | Tersoff | 0       | 206.8   |
| 7       | < 111 > | 112    | NP-Tensile | 300   | Tersoff | 0       | 208.8   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 8       | < 111 > | 128    | NP-Tensile | 300   | Tersoff | 0       | 210.0   |
| 9       | < 111 > | 144    | NP-Tensile | 300   | Tersoff | 0       | 214.9   |
| 10      | < 111 > | 160    | NP-Tensile | 300   | Tersoff | 0       | 218.2   |
| 2       | < 111 > | 36     | NP-Tensile | 300   | Tersoff | 0       | 182.9   |
| 3       | < 111 > | 54     | NP-Tensile | 300   | Tersoff | 0       | 194.8   |
| 4       | < 111 > | 72     | NP-Tensile | 300   | Tersoff | 0       | 200.4   |
| 5       | < 111 > | 90     | NP-Tensile | 300   | Tersoff | 0       | 203.6   |
| 6       | < 111 > | 108    | NP-Tensile | 300   | Tersoff | 0       | 206.9   |
| 7       | < 111 > | 126    | NP-Tensile | 300   | Tersoff | 0       | 208.7   |
| 8       | < 111 > | 144    | NP-Tensile | 300   | Tersoff | 0       | 210.7   |
| 9       | < 111 > | 162    | NP-Tensile | 300   | Tersoff | 0       | 212.4   |
| 10      | < 111 > | 180    | NP-Tensile | 300   | Tersoff | 0       | 217.1   |
| 2       | < 111 > | 40     | NP-Tensile | 300   | Tersoff | 0       | 183.1   |
| 3       | < 111 > | 60     | NP-Tensile | 300   | Tersoff | 0       | 194.1   |
| 4       | < 111 > | 80     | NP-Tensile | 300   | Tersoff | 0       | 200.5   |
| 5       | < 111 > | 100    | NP-Tensile | 300   | Tersoff | 0       | 204.5   |
| 6       | < 111 > | 120    | NP-Tensile | 300   | Tersoff | 0       | 206.8   |
| 7       | < 111 > | 140    | NP-Tensile | 300   | Tersoff | 0       | 208.5   |
| 8       | < 111 > | 160    | NP-Tensile | 300   | Tersoff | 0       | 209.8   |
| 9       | < 111 > | 180    | NP-Tensile | 300   | Tersoff | 0       | 217.2   |
| 10      | < 111 > | 200    | NP-Tensile | 300   | Tersoff | 0       | 220.3   |
| 2       | < 111 > | 14     | P-Tensile  | 300   | Tersoff | 0       | 135.0   |
| 3       | < 111 > | 21     | P-Tensile  | 300   | Tersoff | 0       | 135.0   |
| 4       | < 111 > | 28     | P-Tensile  | 300   | Tersoff | 0       | 141.1   |
| 5       | < 111 > | 35     | P-Tensile  | 300   | Tersoff | 0       | 147.9   |
| 6       | < 111 > | 42     | P-Tensile  | 300   | Tersoff | 0       | 153.0   |
| 7       | < 111 > | 49     | P-Tensile  | 300   | Tersoff | 0       | 147.1   |
| 8       | < 111 > | 56     | P-Tensile  | 300   | Tersoff | 0       | 152.6   |
| 9       | < 111 > | 63     | P-Tensile  | 300   | Tersoff | 0       | 153.1   |
| 10      | < 111 > | 70     | P-Tensile  | 300   | Tersoff | 0       | 153.2   |
| 2       | < 111 > | 16     | P-Tensile  | 300   | Tersoff | 0       | 144.2   |
| 3       | < 111 > | 24     | P-Tensile  | 300   | Tersoff | 0       | 140.3   |
| 4       | < 111 > | 32     | P-Tensile  | 300   | Tersoff | 0       | 149.6   |
| 5       | < 111 > | 40     | P-Tensile  | 300   | Tersoff | 0       | 155.7   |
| 6       | < 111 > | 48     | P-Tensile  | 300   | Tersoff | 0       | 151.9   |
| 7       | < 111 > | 56     | P-Tensile  | 300   | Tersoff | 0       | 153.9   |
| 8       | < 111 > | 64     | P-Tensile  | 300   | Tersoff | 0       | 152.9   |
| 9       | < 111 > | 72     | P-Tensile  | 300   | Tersoff | 0       | 156.3   |
| 10      | < 111 > | 80     | P-Tensile  | 300   | Tersoff | 0       | 157.8   |
| 2       | < 111 > | 18     | P-Tensile  | 300   | Tersoff | 0       | 140.9   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|---------|---------|---------|
| 3       | < 111 > | 27     | P-Tensile | 300   | Tersoff | 0       | 107.9   |
| 4       | < 111 > | 36     | P-Tensile | 300   | Tersoff | 0       | 145.7   |
| 5       | < 111 > | 45     | P-Tensile | 300   | Tersoff | 0       | 152.1   |
| 6       | < 111 > | 54     | P-Tensile | 300   | Tersoff | 0       | 149.8   |
| 7       | < 111 > | 63     | P-Tensile | 300   | Tersoff | 0       | 154.5   |
| 8       | < 111 > | 72     | P-Tensile | 300   | Tersoff | 0       | 149.1   |
| 9       | < 111 > | 81     | P-Tensile | 300   | Tersoff | 0       | 157.3   |
| 10      | < 111 > | 90     | P-Tensile | 300   | Tersoff | 0       | 156.7   |
| 2       | < 111 > | 20     | P-Tensile | 300   | Tersoff | 0       | 138.6   |
| 3       | < 111 > | 30     | P-Tensile | 300   | Tersoff | 0       | 136.1   |
| 4       | < 111 > | 40     | P-Tensile | 300   | Tersoff | 0       | 149.2   |
| 5       | < 111 > | 50     | P-Tensile | 300   | Tersoff | 0       | 150.8   |
| 6       | < 111 > | 60     | P-Tensile | 300   | Tersoff | 0       | 149.5   |
| 7       | < 111 > | 70     | P-Tensile | 300   | Tersoff | 0       | 154.5   |
| 8       | < 111 > | 80     | P-Tensile | 300   | Tersoff | 0       | 152.6   |
| 9       | < 111 > | 90     | P-Tensile | 300   | Tersoff | 0       | 153.6   |
| 10      | < 111 > | 100    | P-Tensile | 300   | Tersoff | 0       | 155.9   |
| 2       | < 111 > | 24     | P-Tensile | 300   | Tersoff | 0       | 128.3   |
| 3       | < 111 > | 36     | P-Tensile | 300   | Tersoff | 0       | 142.2   |
| 4       | < 111 > | 48     | P-Tensile | 300   | Tersoff | 0       | 149.6   |
| 5       | < 111 > | 60     | P-Tensile | 300   | Tersoff | 0       | 152.7   |
| 6       | < 111 > | 72     | P-Tensile | 300   | Tersoff | 0       | 153.2   |
| 7       | < 111 > | 84     | P-Tensile | 300   | Tersoff | 0       | 155.0   |
| 8       | < 111 > | 96     | P-Tensile | 300   | Tersoff | 0       | 152.7   |
| 9       | < 111 > | 108    | P-Tensile | 300   | Tersoff | 0       | 154.5   |
| 10      | < 111 > | 120    | P-Tensile | 300   | Tersoff | 0       | 153.0   |
| 2       | < 111 > | 28     | P-Tensile | 300   | Tersoff | 0       | 115.6   |
| 3       | < 111 > | 42     | P-Tensile | 300   | Tersoff | 0       | 141.3   |
| 4       | < 111 > | 56     | P-Tensile | 300   | Tersoff | 0       | 148.4   |
| 5       | < 111 > | 70     | P-Tensile | 300   | Tersoff | 0       | 154.7   |
| 6       | < 111 > | 84     | P-Tensile | 300   | Tersoff | 0       | 153.3   |
| 7       | < 111 > | 98     | P-Tensile | 300   | Tersoff | 0       | 155.1   |
| 8       | < 111 > | 112    | P-Tensile | 300   | Tersoff | 0       | 152.9   |
| 9       | < 111 > | 126    | P-Tensile | 300   | Tersoff | 0       | 155.5   |
| 10      | < 111 > | 140    | P-Tensile | 300   | Tersoff | 0       | 157.0   |
| 2       | < 111 > | 32     | P-Tensile | 300   | Tersoff | 0       | 126.4   |
| 3       | < 111 > | 48     | P-Tensile | 300   | Tersoff | 0       | 132.4   |
| 4       | < 111 > | 64     | P-Tensile | 300   | Tersoff | 0       | 149.4   |
| 5       | < 111 > | 80     | P-Tensile | 300   | Tersoff | 0       | 154.7   |
| 6       | < 111 > | 96     | P-Tensile | 300   | Tersoff | 0       | 141.3   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 7       | < 111 > | 112    | P-Tensile  | 300   | Tersoff | 0       | 154.9   |
| 8       | < 111 > | 128    | P-Tensile  | 300   | Tersoff | 0       | 152.3   |
| 9       | < 111 > | 144    | P-Tensile  | 300   | Tersoff | 0       | 155.0   |
| 10      | < 111 > | 160    | P-Tensile  | 300   | Tersoff | 0       | 158.3   |
| 2       | < 111 > | 36     | P-Tensile  | 300   | Tersoff | 0       | 105.8   |
| 3       | < 111 > | 54     | P-Tensile  | 300   | Tersoff | 0       | 135.9   |
| 4       | < 111 > | 72     | P-Tensile  | 300   | Tersoff | 0       | 150.6   |
| 5       | < 111 > | 90     | P-Tensile  | 300   | Tersoff | 0       | 154.6   |
| 6       | < 111 > | 108    | P-Tensile  | 300   | Tersoff | 0       | 152.4   |
| 7       | < 111 > | 126    | P-Tensile  | 300   | Tersoff | 0       | 154.1   |
| 8       | < 111 > | 144    | P-Tensile  | 300   | Tersoff | 0       | 153.7   |
| 9       | < 111 > | 162    | P-Tensile  | 300   | Tersoff | 0       | 156.0   |
| 10      | < 111 > | 180    | P-Tensile  | 300   | Tersoff | 0       | 157.8   |
| 2       | < 111 > | 40     | P-Tensile  | 300   | Tersoff | 0       | 102.3   |
| 3       | < 111 > | 60     | P-Tensile  | 300   | Tersoff | 0       | 138.5   |
| 4       | < 111 > | 80     | P-Tensile  | 300   | Tersoff | 0       | 149.7   |
| 5       | < 111 > | 100    | P-Tensile  | 300   | Tersoff | 0       | 153.4   |
| 6       | < 111 > | 120    | P-Tensile  | 300   | Tersoff | 0       | 149.8   |
| 7       | < 111 > | 140    | P-Tensile  | 300   | Tersoff | 0       | 152.2   |
| 8       | < 111 > | 160    | P-Tensile  | 300   | Tersoff | 0       | 152.8   |
| 9       | < 111 > | 180    | P-Tensile  | 300   | Tersoff | 0       | 155.0   |
| 10      | < 111 > | 200    | P-Tensile  | 300   | Tersoff | 0       | 152.7   |
| 2       | < 111 > | 14     | NP-Tensile | 300   | SW      | 0       | 152.3   |
| 3       | < 111 > | 21     | NP-Tensile | 300   | SW      | 0       | 169.5   |
| 4       | < 111 > | 28     | NP-Tensile | 300   | SW      | 0       | 177.9   |
| 5       | < 111 > | 35     | NP-Tensile | 300   | SW      | 0       | 183.7   |
| 6       | < 111 > | 42     | NP-Tensile | 300   | SW      | 0       | 185.4   |
| 7       | < 111 > | 49     | NP-Tensile | 300   | SW      | 0       | 188.9   |
| 8       | < 111 > | 56     | NP-Tensile | 300   | SW      | 0       | 189.6   |
| 9       | < 111 > | 63     | NP-Tensile | 300   | SW      | 0       | 191.7   |
| 10      | < 111 > | 70     | NP-Tensile | 300   | SW      | 0       | 192.2   |
| 2       | < 111 > | 16     | NP-Tensile | 300   | SW      | 0       | 155.1   |
| 3       | < 111 > | 24     | NP-Tensile | 300   | SW      | 0       | 170.8   |
| 4       | < 111 > | 32     | NP-Tensile | 300   | SW      | 0       | 178.9   |
| 5       | < 111 > | 40     | NP-Tensile | 300   | SW      | 0       | 184.2   |
| 6       | < 111 > | 48     | NP-Tensile | 300   | SW      | 0       | 186.1   |
| 7       | < 111 > | 56     | NP-Tensile | 300   | SW      | 0       | 188.1   |
| 8       | < 111 > | 64     | NP-Tensile | 300   | SW      | 0       | 189.9   |
| 9       | < 111 > | 72     | NP-Tensile | 300   | SW      | 0       | 191.2   |
| 10      | < 111 > | 80     | NP-Tensile | 300   | SW      | 0       | 191.8   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 2       | < 111 > | 18     | NP-Tensile | 300   | SW  | 0       | 157.4   |
| 3       | < 111 > | 27     | NP-Tensile | 300   | SW  | 0       | 170.5   |
| 4       | < 111 > | 36     | NP-Tensile | 300   | SW  | 0       | 178.9   |
| 5       | < 111 > | 45     | NP-Tensile | 300   | SW  | 0       | 183.1   |
| 6       | < 111 > | 54     | NP-Tensile | 300   | SW  | 0       | 186.7   |
| 7       | < 111 > | 63     | NP-Tensile | 300   | SW  | 0       | 188.9   |
| 8       | < 111 > | 72     | NP-Tensile | 300   | SW  | 0       | 189.9   |
| 9       | < 111 > | 81     | NP-Tensile | 300   | SW  | 0       | 191.0   |
| 10      | < 111 > | 90     | NP-Tensile | 300   | SW  | 0       | 191.7   |
| 2       | < 111 > | 20     | NP-Tensile | 300   | SW  | 0       | 155.2   |
| 3       | < 111 > | 30     | NP-Tensile | 300   | SW  | 0       | 170.7   |
| 4       | < 111 > | 40     | NP-Tensile | 300   | SW  | 0       | 178.8   |
| 5       | < 111 > | 50     | NP-Tensile | 300   | SW  | 0       | 183.3   |
| 6       | < 111 > | 60     | NP-Tensile | 300   | SW  | 0       | 186.4   |
| 7       | < 111 > | 70     | NP-Tensile | 300   | SW  | 0       | 188.2   |
| 8       | < 111 > | 80     | NP-Tensile | 300   | SW  | 0       | 189.4   |
| 9       | < 111 > | 90     | NP-Tensile | 300   | SW  | 0       | 190.7   |
| 10      | < 111 > | 100    | NP-Tensile | 300   | SW  | 0       | 192.0   |
| 2       | < 111 > | 24     | NP-Tensile | 300   | SW  | 0       | 159.3   |
| 3       | < 111 > | 36     | NP-Tensile | 300   | SW  | 0       | 170.6   |
| 4       | < 111 > | 48     | NP-Tensile | 300   | SW  | 0       | 178.5   |
| 5       | < 111 > | 60     | NP-Tensile | 300   | SW  | 0       | 183.7   |
| 6       | < 111 > | 72     | NP-Tensile | 300   | SW  | 0       | 186.0   |
| 7       | < 111 > | 84     | NP-Tensile | 300   | SW  | 0       | 188.1   |
| 8       | < 111 > | 96     | NP-Tensile | 300   | SW  | 0       | 189.8   |
| 9       | < 111 > | 108    | NP-Tensile | 300   | SW  | 0       | 191.4   |
| 10      | < 111 > | 120    | NP-Tensile | 300   | SW  | 0       | 192.1   |
| 2       | < 111 > | 28     | NP-Tensile | 300   | SW  | 0       | 154.2   |
| 3       | < 111 > | 42     | NP-Tensile | 300   | SW  | 0       | 170.0   |
| 4       | < 111 > | 56     | NP-Tensile | 300   | SW  | 0       | 178.5   |
| 5       | < 111 > | 70     | NP-Tensile | 300   | SW  | 0       | 183.4   |
| 6       | < 111 > | 84     | NP-Tensile | 300   | SW  | 0       | 185.8   |
| 7       | < 111 > | 98     | NP-Tensile | 300   | SW  | 0       | 188.5   |
| 8       | < 111 > | 112    | NP-Tensile | 300   | SW  | 0       | 190.0   |
| 9       | < 111 > | 126    | NP-Tensile | 300   | SW  | 0       | 191.3   |
| 10      | < 111 > | 140    | NP-Tensile | 300   | SW  | 0       | 192.3   |
| 2       | < 111 > | 32     | NP-Tensile | 300   | SW  | 0       | 154.8   |
| 3       | < 111 > | 48     | NP-Tensile | 300   | SW  | 0       | 170.3   |
| 4       | < 111 > | 64     | NP-Tensile | 300   | SW  | 0       | 178.8   |
| 5       | < 111 > | 80     | NP-Tensile | 300   | SW  | 0       | 183.2   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 6       | < 111 > | 96     | NP-Tensile | 300   | SW  | 0       | 186.1   |
| 7       | < 111 > | 112    | NP-Tensile | 300   | SW  | 0       | 188.5   |
| 8       | < 111 > | 128    | NP-Tensile | 300   | SW  | 0       | 190.0   |
| 9       | < 111 > | 144    | NP-Tensile | 300   | SW  | 0       | 191.2   |
| 10      | < 111 > | 160    | NP-Tensile | 300   | SW  | 0       | 192.5   |
| 2       | < 111 > | 36     | NP-Tensile | 300   | SW  | 0       | 155.0   |
| 3       | < 111 > | 54     | NP-Tensile | 300   | SW  | 0       | 172.0   |
| 4       | < 111 > | 72     | NP-Tensile | 300   | SW  | 0       | 178.6   |
| 5       | < 111 > | 90     | NP-Tensile | 300   | SW  | 0       | 182.9   |
| 6       | < 111 > | 108    | NP-Tensile | 300   | SW  | 0       | 186.4   |
| 7       | < 111 > | 126    | NP-Tensile | 300   | SW  | 0       | 188.5   |
| 8       | < 111 > | 144    | NP-Tensile | 300   | SW  | 0       | 189.9   |
| 9       | < 111 > | 162    | NP-Tensile | 300   | SW  | 0       | 191.7   |
| 10      | < 111 > | 180    | NP-Tensile | 300   | SW  | 0       | 190.6   |
| 2       | < 111 > | 40     | NP-Tensile | 300   | SW  | 0       | 156.9   |
| 3       | < 111 > | 60     | NP-Tensile | 300   | SW  | 0       | 171.4   |
| 4       | < 111 > | 80     | NP-Tensile | 300   | SW  | 0       | 178.2   |
| 5       | < 111 > | 100    | NP-Tensile | 300   | SW  | 0       | 182.9   |
| 6       | < 111 > | 120    | NP-Tensile | 300   | SW  | 0       | 186.1   |
| 7       | < 111 > | 140    | NP-Tensile | 300   | SW  | 0       | 188.5   |
| 8       | < 111 > | 160    | NP-Tensile | 300   | SW  | 0       | 190.1   |
| 9       | < 111 > | 180    | NP-Tensile | 300   | SW  | 0       | 191.6   |
| 10      | < 111 > | 200    | NP-Tensile | 300   | SW  | 0       | 191.5   |
| 2       | < 111 > | 14     | P-Tensile  | 300   | SW  | 0       | 111.4   |
| 3       | < 111 > | 21     | P-Tensile  | 300   | SW  | 0       | 111.4   |
| 4       | < 111 > | 28     | P-Tensile  | 300   | SW  | 0       | 115.0   |
| 5       | < 111 > | 35     | P-Tensile  | 300   | SW  | 0       | 127.5   |
| 6       | < 111 > | 42     | P-Tensile  | 300   | SW  | 0       | 135.5   |
| 7       | < 111 > | 49     | P-Tensile  | 300   | SW  | 0       | 132.7   |
| 8       | < 111 > | 56     | P-Tensile  | 300   | SW  | 0       | 136.0   |
| 9       | < 111 > | 63     | P-Tensile  | 300   | SW  | 0       | 133.8   |
| 10      | < 111 > | 70     | P-Tensile  | 300   | SW  | 0       | 138.1   |
| 2       | < 111 > | 16     | P-Tensile  | 300   | SW  | 0       | 118.5   |
| 3       | < 111 > | 24     | P-Tensile  | 300   | SW  | 0       | 115.5   |
| 4       | < 111 > | 32     | P-Tensile  | 300   | SW  | 0       | 127.1   |
| 5       | < 111 > | 40     | P-Tensile  | 300   | SW  | 0       | 129.8   |
| 6       | < 111 > | 48     | P-Tensile  | 300   | SW  | 0       | 131.8   |
| 7       | < 111 > | 56     | P-Tensile  | 300   | SW  | 0       | 134.8   |
| 8       | < 111 > | 64     | P-Tensile  | 300   | SW  | 0       | 134.9   |
| 9       | < 111 > | 72     | P-Tensile  | 300   | SW  | 0       | 136.3   |



Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|-----|---------|---------|
| 10      | < 111 > | 80     | P-Tensile | 300   | SW  | 0       | 139.1   |
| 2       | < 111 > | 18     | P-Tensile | 300   | SW  | 0       | 110.6   |
| 3       | < 111 > | 27     | P-Tensile | 300   | SW  | 0       | 118.2   |
| 4       | < 111 > | 36     | P-Tensile | 300   | SW  | 0       | 129.2   |
| 5       | < 111 > | 45     | P-Tensile | 300   | SW  | 0       | 129.7   |
| 6       | < 111 > | 54     | P-Tensile | 300   | SW  | 0       | 130.0   |
| 7       | < 111 > | 63     | P-Tensile | 300   | SW  | 0       | 137.0   |
| 8       | < 111 > | 72     | P-Tensile | 300   | SW  | 0       | 133.2   |
| 9       | < 111 > | 81     | P-Tensile | 300   | SW  | 0       | 136.8   |
| 10      | < 111 > | 90     | P-Tensile | 300   | SW  | 0       | 138.9   |
| 2       | < 111 > | 20     | P-Tensile | 300   | SW  | 0       | 111.9   |
| 3       | < 111 > | 30     | P-Tensile | 300   | SW  | 0       | 119.9   |
| 4       | < 111 > | 40     | P-Tensile | 300   | SW  | 0       | 128.7   |
| 5       | < 111 > | 50     | P-Tensile | 300   | SW  | 0       | 131.7   |
| 6       | < 111 > | 60     | P-Tensile | 300   | SW  | 0       | 132.2   |
| 7       | < 111 > | 70     | P-Tensile | 300   | SW  | 0       | 136.5   |
| 8       | < 111 > | 80     | P-Tensile | 300   | SW  | 0       | 134.9   |
| 9       | < 111 > | 90     | P-Tensile | 300   | SW  | 0       | 137.8   |
| 10      | < 111 > | 100    | P-Tensile | 300   | SW  | 0       | 139.3   |
| 2       | < 111 > | 24     | P-Tensile | 300   | SW  | 0       | 110.0   |
| 3       | < 111 > | 36     | P-Tensile | 300   | SW  | 0       | 119.3   |
| 4       | < 111 > | 48     | P-Tensile | 300   | SW  | 0       | 126.2   |
| 5       | < 111 > | 60     | P-Tensile | 300   | SW  | 0       | 131.2   |
| 6       | < 111 > | 72     | P-Tensile | 300   | SW  | 0       | 132.9   |
| 7       | < 111 > | 84     | P-Tensile | 300   | SW  | 0       | 136.0   |
| 8       | < 111 > | 96     | P-Tensile | 300   | SW  | 0       | 134.9   |
| 9       | < 111 > | 108    | P-Tensile | 300   | SW  | 0       | 137.8   |
| 10      | < 111 > | 120    | P-Tensile | 300   | SW  | 0       | 142.4   |
| 2       | < 111 > | 28     | P-Tensile | 300   | SW  | 0       | 114.5   |
| 3       | < 111 > | 42     | P-Tensile | 300   | SW  | 0       | 119.1   |
| 4       | < 111 > | 56     | P-Tensile | 300   | SW  | 0       | 129.8   |
| 5       | < 111 > | 70     | P-Tensile | 300   | SW  | 0       | 133.2   |
| 6       | < 111 > | 84     | P-Tensile | 300   | SW  | 0       | 132.6   |
| 7       | < 111 > | 98     | P-Tensile | 300   | SW  | 0       | 136.7   |
| 8       | < 111 > | 112    | P-Tensile | 300   | SW  | 0       | 134.4   |
| 9       | < 111 > | 126    | P-Tensile | 300   | SW  | 0       | 137.3   |
| 10      | < 111 > | 140    | P-Tensile | 300   | SW  | 0       | 137.9   |
| 2       | < 111 > | 32     | P-Tensile | 300   | SW  | 0       | 112.6   |
| 3       | < 111 > | 48     | P-Tensile | 300   | SW  | 0       | 117.9   |
| 4       | < 111 > | 64     | P-Tensile | 300   | SW  | 0       | 125.1   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 5       | < 111 > | 80     | P-Tensile  | 300   | SW      | 0       | 132.7   |
| 6       | < 111 > | 96     | P-Tensile  | 300   | SW      | 0       | 132.3   |
| 7       | < 111 > | 112    | P-Tensile  | 300   | SW      | 0       | 130.5   |
| 8       | < 111 > | 128    | P-Tensile  | 300   | SW      | 0       | 134.6   |
| 9       | < 111 > | 144    | P-Tensile  | 300   | SW      | 0       | 139.1   |
| 10      | < 111 > | 160    | P-Tensile  | 300   | SW      | 0       | 141.4   |
| 2       | < 111 > | 36     | P-Tensile  | 300   | SW      | 0       | 110.4   |
| 3       | < 111 > | 54     | P-Tensile  | 300   | SW      | 0       | 116.1   |
| 4       | < 111 > | 72     | P-Tensile  | 300   | SW      | 0       | 129.5   |
| 5       | < 111 > | 90     | P-Tensile  | 300   | SW      | 0       | 135.5   |
| 6       | < 111 > | 108    | P-Tensile  | 300   | SW      | 0       | 134.1   |
| 7       | < 111 > | 126    | P-Tensile  | 300   | SW      | 0       | 138.7   |
| 8       | < 111 > | 144    | P-Tensile  | 300   | SW      | 0       | 134.2   |
| 9       | < 111 > | 162    | P-Tensile  | 300   | SW      | 0       | 137.1   |
| 10      | < 111 > | 180    | P-Tensile  | 300   | SW      | 0       | 140.8   |
| 2       | < 111 > | 40     | P-Tensile  | 300   | SW      | 0       | 111.3   |
| 3       | < 111 > | 60     | P-Tensile  | 300   | SW      | 0       | 115.5   |
| 4       | < 111 > | 80     | P-Tensile  | 300   | SW      | 0       | 126.2   |
| 5       | < 111 > | 100    | P-Tensile  | 300   | SW      | 0       | 131.9   |
| 6       | < 111 > | 120    | P-Tensile  | 300   | SW      | 0       | 131.6   |
| 7       | < 111 > | 140    | P-Tensile  | 300   | SW      | 0       | 134.1   |
| 8       | < 111 > | 160    | P-Tensile  | 300   | SW      | 0       | 135.1   |
| 9       | < 111 > | 180    | P-Tensile  | 300   | SW      | 0       | 137.2   |
| 10      | < 111 > | 200    | P-Tensile  | 300   | SW      | 0       | 136.8   |
| 2       | < 100 > | 14     | NP-Tensile | 600   | Tersoff | 0       | 110.0   |
| 3       | < 100 > | 21     | NP-Tensile | 600   | Tersoff | 0       | 113.4   |
| 4       | < 100 > | 28     | NP-Tensile | 600   | Tersoff | 0       | 119.1   |
| 5       | < 100 > | 35     | NP-Tensile | 600   | Tersoff | 0       | 121.3   |
| 6       | < 100 > | 42     | NP-Tensile | 600   | Tersoff | 0       | 121.5   |
| 7       | < 100 > | 49     | NP-Tensile | 600   | Tersoff | 0       | 123.0   |
| 8       | < 100 > | 56     | NP-Tensile | 600   | Tersoff | 0       | 123.9   |
| 9       | < 100 > | 63     | NP-Tensile | 600   | Tersoff | 0       | 123.2   |
| 10      | < 100 > | 70     | NP-Tensile | 600   | Tersoff | 0       | 123.9   |
| 2       | < 100 > | 16     | NP-Tensile | 600   | Tersoff | 0       | 107.9   |
| 3       | < 100 > | 24     | NP-Tensile | 600   | Tersoff | 0       | 115.8   |
| 4       | < 100 > | 32     | NP-Tensile | 600   | Tersoff | 0       | 117.1   |
| 5       | < 100 > | 40     | NP-Tensile | 600   | Tersoff | 0       | 121.1   |
| 6       | < 100 > | 48     | NP-Tensile | 600   | Tersoff | 0       | 121.7   |
| 7       | < 100 > | 56     | NP-Tensile | 600   | Tersoff | 0       | 122.2   |
| 8       | < 100 > | 64     | NP-Tensile | 600   | Tersoff | 0       | 123.4   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 9       | < 100 > | 72     | NP-Tensile | 600   | Tersoff | 0       | 123.4   |
| 10      | < 100 > | 80     | NP-Tensile | 600   | Tersoff | 0       | 124.4   |
| 2       | < 100 > | 18     | NP-Tensile | 600   | Tersoff | 0       | 114.3   |
| 3       | < 100 > | 27     | NP-Tensile | 600   | Tersoff | 0       | 114.5   |
| 4       | < 100 > | 36     | NP-Tensile | 600   | Tersoff | 0       | 118.0   |
| 5       | < 100 > | 45     | NP-Tensile | 600   | Tersoff | 0       | 120.9   |
| 6       | < 100 > | 54     | NP-Tensile | 600   | Tersoff | 0       | 121.6   |
| 7       | < 100 > | 63     | NP-Tensile | 600   | Tersoff | 0       | 121.9   |
| 8       | < 100 > | 72     | NP-Tensile | 600   | Tersoff | 0       | 123.4   |
| 9       | < 100 > | 81     | NP-Tensile | 600   | Tersoff | 0       | 123.7   |
| 10      | < 100 > | 90     | NP-Tensile | 600   | Tersoff | 0       | 124.5   |
| 2       | < 100 > | 20     | NP-Tensile | 600   | Tersoff | 0       | 109.4   |
| 3       | < 100 > | 30     | NP-Tensile | 600   | Tersoff | 0       | 115.3   |
| 4       | < 100 > | 40     | NP-Tensile | 600   | Tersoff | 0       | 117.4   |
| 5       | < 100 > | 50     | NP-Tensile | 600   | Tersoff | 0       | 121.0   |
| 6       | < 100 > | 60     | NP-Tensile | 600   | Tersoff | 0       | 121.3   |
| 7       | < 100 > | 70     | NP-Tensile | 600   | Tersoff | 0       | 121.5   |
| 8       | < 100 > | 80     | NP-Tensile | 600   | Tersoff | 0       | 123.5   |
| 9       | < 100 > | 90     | NP-Tensile | 600   | Tersoff | 0       | 124.0   |
| 10      | < 100 > | 100    | NP-Tensile | 600   | Tersoff | 0       | 124.8   |
| 2       | < 100 > | 24     | NP-Tensile | 600   | Tersoff | 0       | 111.4   |
| 3       | < 100 > | 36     | NP-Tensile | 600   | Tersoff | 0       | 115.7   |
| 4       | < 100 > | 48     | NP-Tensile | 600   | Tersoff | 0       | 119.0   |
| 5       | < 100 > | 60     | NP-Tensile | 600   | Tersoff | 0       | 120.4   |
| 6       | < 100 > | 72     | NP-Tensile | 600   | Tersoff | 0       | 121.7   |
| 7       | < 100 > | 84     | NP-Tensile | 600   | Tersoff | 0       | 122.5   |
| 8       | < 100 > | 96     | NP-Tensile | 600   | Tersoff | 0       | 124.2   |
| 9       | < 100 > | 108    | NP-Tensile | 600   | Tersoff | 0       | 124.4   |
| 10      | < 100 > | 120    | NP-Tensile | 600   | Tersoff | 0       | 125.1   |
| 2       | < 100 > | 28     | NP-Tensile | 600   | Tersoff | 0       | 109.5   |
| 3       | < 100 > | 42     | NP-Tensile | 600   | Tersoff | 0       | 116.0   |
| 4       | < 100 > | 56     | NP-Tensile | 600   | Tersoff | 0       | 118.5   |
| 5       | < 100 > | 70     | NP-Tensile | 600   | Tersoff | 0       | 119.4   |
| 6       | < 100 > | 84     | NP-Tensile | 600   | Tersoff | 0       | 121.9   |
| 7       | < 100 > | 98     | NP-Tensile | 600   | Tersoff | 0       | 123.0   |
| 8       | < 100 > | 112    | NP-Tensile | 600   | Tersoff | 0       | 124.6   |
| 9       | < 100 > | 126    | NP-Tensile | 600   | Tersoff | 0       | 123.8   |
| 10      | < 100 > | 140    | NP-Tensile | 600   | Tersoff | 0       | 122.4   |
| 2       | < 100 > | 32     | NP-Tensile | 600   | Tersoff | 0       | 110.1   |
| 3       | < 100 > | 48     | NP-Tensile | 600   | Tersoff | 0       | 115.2   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 4       | < 100 > | 64     | NP-Tensile | 600   | Tersoff | 0       | 117.8   |
| 5       | < 100 > | 80     | NP-Tensile | 600   | Tersoff | 0       | 120.5   |
| 6       | < 100 > | 96     | NP-Tensile | 600   | Tersoff | 0       | 122.4   |
| 7       | < 100 > | 112    | NP-Tensile | 600   | Tersoff | 0       | 123.3   |
| 8       | < 100 > | 128    | NP-Tensile | 600   | Tersoff | 0       | 124.8   |
| 9       | < 100 > | 144    | NP-Tensile | 600   | Tersoff | 0       | 122.9   |
| 10      | < 100 > | 160    | NP-Tensile | 600   | Tersoff | 0       | 123.7   |
| 2       | < 100 > | 36     | NP-Tensile | 600   | Tersoff | 0       | 110.7   |
| 3       | < 100 > | 54     | NP-Tensile | 600   | Tersoff | 0       | 115.2   |
| 4       | < 100 > | 72     | NP-Tensile | 600   | Tersoff | 0       | 117.7   |
| 5       | < 100 > | 90     | NP-Tensile | 600   | Tersoff | 0       | 119.7   |
| 6       | < 100 > | 108    | NP-Tensile | 600   | Tersoff | 0       | 122.6   |
| 7       | < 100 > | 126    | NP-Tensile | 600   | Tersoff | 0       | 123.6   |
| 8       | < 100 > | 144    | NP-Tensile | 600   | Tersoff | 0       | 124.8   |
| 9       | < 100 > | 162    | NP-Tensile | 600   | Tersoff | 0       | 121.0   |
| 10      | < 100 > | 180    | NP-Tensile | 600   | Tersoff | 0       | 121.7   |
| 2       | < 100 > | 40     | NP-Tensile | 600   | Tersoff | 0       | 111.3   |
| 3       | < 100 > | 60     | NP-Tensile | 600   | Tersoff | 0       | 115.1   |
| 4       | < 100 > | 80     | NP-Tensile | 600   | Tersoff | 0       | 118.1   |
| 5       | < 100 > | 100    | NP-Tensile | 600   | Tersoff | 0       | 120.9   |
| 6       | < 100 > | 120    | NP-Tensile | 600   | Tersoff | 0       | 123.2   |
| 7       | < 100 > | 140    | NP-Tensile | 600   | Tersoff | 0       | 123.8   |
| 8       | < 100 > | 160    | NP-Tensile | 600   | Tersoff | 0       | 123.3   |
| 9       | < 100 > | 180    | NP-Tensile | 600   | Tersoff | 0       | 123.5   |
| 10      | < 100 > | 200    | NP-Tensile | 600   | Tersoff | 0       | 121.6   |
| 2       | < 100 > | 14     | P-Tensile  | 600   | Tersoff | 0       | 95.6    |
| 3       | < 100 > | 21     | P-Tensile  | 600   | Tersoff | 0       | 95.6    |
| 4       | < 100 > | 28     | P-Tensile  | 600   | Tersoff | 0       | 77.3    |
| 5       | < 100 > | 35     | P-Tensile  | 600   | Tersoff | 0       | 90.2    |
| 6       | < 100 > | 42     | P-Tensile  | 600   | Tersoff | 0       | 86.6    |
| 7       | < 100 > | 49     | P-Tensile  | 600   | Tersoff | 0       | 90.7    |
| 8       | < 100 > | 56     | P-Tensile  | 600   | Tersoff | 0       | 88.3    |
| 9       | < 100 > | 63     | P-Tensile  | 600   | Tersoff | 0       | 90.7    |
| 10      | < 100 > | 70     | P-Tensile  | 600   | Tersoff | 0       | 93.7    |
| 2       | < 100 > | 16     | P-Tensile  | 600   | Tersoff | 0       | 93.4    |
| 3       | < 100 > | 24     | P-Tensile  | 600   | Tersoff | 0       | 87.7    |
| 4       | < 100 > | 32     | P-Tensile  | 600   | Tersoff | 0       | 87.0    |
| 5       | < 100 > | 40     | P-Tensile  | 600   | Tersoff | 0       | 86.3    |
| 6       | < 100 > | 48     | P-Tensile  | 600   | Tersoff | 0       | 90.5    |
| 7       | < 100 > | 56     | P-Tensile  | 600   | Tersoff | 0       | 90.3    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|---------|---------|---------|
| 8       | < 100 > | 64     | P-Tensile | 600   | Tersoff | 0       | 87.7    |
| 9       | < 100 > | 72     | P-Tensile | 600   | Tersoff | 0       | 87.1    |
| 10      | < 100 > | 80     | P-Tensile | 600   | Tersoff | 0       | 89.1    |
| 2       | < 100 > | 18     | P-Tensile | 600   | Tersoff | 0       | 91.5    |
| 3       | < 100 > | 27     | P-Tensile | 600   | Tersoff | 0       | 84.2    |
| 4       | < 100 > | 36     | P-Tensile | 600   | Tersoff | 0       | 91.1    |
| 5       | < 100 > | 45     | P-Tensile | 600   | Tersoff | 0       | 80.0    |
| 6       | < 100 > | 54     | P-Tensile | 600   | Tersoff | 0       | 89.9    |
| 7       | < 100 > | 63     | P-Tensile | 600   | Tersoff | 0       | 90.0    |
| 8       | < 100 > | 72     | P-Tensile | 600   | Tersoff | 0       | 90.9    |
| 9       | < 100 > | 81     | P-Tensile | 600   | Tersoff | 0       | 88.7    |
| 10      | < 100 > | 90     | P-Tensile | 600   | Tersoff | 0       | 89.8    |
| 2       | < 100 > | 20     | P-Tensile | 600   | Tersoff | 0       | 93.2    |
| 3       | < 100 > | 30     | P-Tensile | 600   | Tersoff | 0       | 86.0    |
| 4       | < 100 > | 40     | P-Tensile | 600   | Tersoff | 0       | 90.6    |
| 5       | < 100 > | 50     | P-Tensile | 600   | Tersoff | 0       | 91.7    |
| 6       | < 100 > | 60     | P-Tensile | 600   | Tersoff | 0       | 90.6    |
| 7       | < 100 > | 70     | P-Tensile | 600   | Tersoff | 0       | 88.4    |
| 8       | < 100 > | 80     | P-Tensile | 600   | Tersoff | 0       | 91.0    |
| 9       | < 100 > | 90     | P-Tensile | 600   | Tersoff | 0       | 87.4    |
| 10      | < 100 > | 100    | P-Tensile | 600   | Tersoff | 0       | 88.5    |
| 2       | < 100 > | 24     | P-Tensile | 600   | Tersoff | 0       | 74.4    |
| 3       | < 100 > | 36     | P-Tensile | 600   | Tersoff | 0       | 87.2    |
| 4       | < 100 > | 48     | P-Tensile | 600   | Tersoff | 0       | 95.2    |
| 5       | < 100 > | 60     | P-Tensile | 600   | Tersoff | 0       | 89.7    |
| 6       | < 100 > | 72     | P-Tensile | 600   | Tersoff | 0       | 90.1    |
| 7       | < 100 > | 84     | P-Tensile | 600   | Tersoff | 0       | 83.9    |
| 8       | < 100 > | 96     | P-Tensile | 600   | Tersoff | 0       | 90.8    |
| 9       | < 100 > | 108    | P-Tensile | 600   | Tersoff | 0       | 79.9    |
| 10      | < 100 > | 120    | P-Tensile | 600   | Tersoff | 0       | 88.2    |
| 2       | < 100 > | 28     | P-Tensile | 600   | Tersoff | 0       | 92.1    |
| 3       | < 100 > | 42     | P-Tensile | 600   | Tersoff | 0       | 87.4    |
| 4       | < 100 > | 56     | P-Tensile | 600   | Tersoff | 0       | 86.0    |
| 5       | < 100 > | 70     | P-Tensile | 600   | Tersoff | 0       | 86.6    |
| 6       | < 100 > | 84     | P-Tensile | 600   | Tersoff | 0       | 90.2    |
| 7       | < 100 > | 98     | P-Tensile | 600   | Tersoff | 0       | 89.7    |
| 8       | < 100 > | 112    | P-Tensile | 600   | Tersoff | 0       | 91.0    |
| 9       | < 100 > | 126    | P-Tensile | 600   | Tersoff | 0       | 88.8    |
| 10      | < 100 > | 140    | P-Tensile | 600   | Tersoff | 0       | 89.0    |
| 2       | < 100 > | 32     | P-Tensile | 600   | Tersoff | 0       | 92.8    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 3       | < 100 > | 48     | P-Tensile  | 600   | Tersoff | 0       | 87.4    |
| 4       | < 100 > | 64     | P-Tensile  | 600   | Tersoff | 0       | 90.8    |
| 5       | < 100 > | 80     | P-Tensile  | 600   | Tersoff | 0       | 104.8   |
| 6       | < 100 > | 96     | P-Tensile  | 600   | Tersoff | 0       | 89.7    |
| 7       | < 100 > | 112    | P-Tensile  | 600   | Tersoff | 0       | 87.4    |
| 8       | < 100 > | 128    | P-Tensile  | 600   | Tersoff | 0       | 87.4    |
| 9       | < 100 > | 144    | P-Tensile  | 600   | Tersoff | 0       | 89.0    |
| 10      | < 100 > | 160    | P-Tensile  | 600   | Tersoff | 0       | 89.0    |
| 2       | < 100 > | 36     | P-Tensile  | 600   | Tersoff | 0       | 91.5    |
| 3       | < 100 > | 54     | P-Tensile  | 600   | Tersoff | 0       | 85.2    |
| 4       | < 100 > | 72     | P-Tensile  | 600   | Tersoff | 0       | 90.6    |
| 5       | < 100 > | 90     | P-Tensile  | 600   | Tersoff | 0       | 93.9    |
| 6       | < 100 > | 108    | P-Tensile  | 600   | Tersoff | 0       | 90.4    |
| 7       | < 100 > | 126    | P-Tensile  | 600   | Tersoff | 0       | 84.6    |
| 8       | < 100 > | 144    | P-Tensile  | 600   | Tersoff | 0       | 90.9    |
| 9       | < 100 > | 162    | P-Tensile  | 600   | Tersoff | 0       | 87.5    |
| 10      | < 100 > | 180    | P-Tensile  | 600   | Tersoff | 0       | 89.2    |
| 2       | < 100 > | 40     | P-Tensile  | 600   | Tersoff | 0       | 95.0    |
| 3       | < 100 > | 60     | P-Tensile  | 600   | Tersoff | 0       | 86.9    |
| 4       | < 100 > | 80     | P-Tensile  | 600   | Tersoff | 0       | 78.1    |
| 5       | < 100 > | 100    | P-Tensile  | 600   | Tersoff | 0       | 76.1    |
| 6       | < 100 > | 120    | P-Tensile  | 600   | Tersoff | 0       | 90.1    |
| 7       | < 100 > | 140    | P-Tensile  | 600   | Tersoff | 0       | 86.5    |
| 8       | < 100 > | 160    | P-Tensile  | 600   | Tersoff | 0       | 91.1    |
| 9       | < 100 > | 180    | P-Tensile  | 600   | Tersoff | 0       | 88.7    |
| 10      | < 100 > | 200    | P-Tensile  | 600   | Tersoff | 0       | 89.9    |
| 2       | < 100 > | 14     | NP-Tensile | 600   | SW      | 0       | 87.2    |
| 3       | < 100 > | 21     | NP-Tensile | 600   | SW      | 0       | 101.9   |
| 4       | < 100 > | 28     | NP-Tensile | 600   | SW      | 0       | 113.0   |
| 5       | < 100 > | 35     | NP-Tensile | 600   | SW      | 0       | 118.1   |
| 6       | < 100 > | 42     | NP-Tensile | 600   | SW      | 0       | 122.6   |
| 7       | < 100 > | 49     | NP-Tensile | 600   | SW      | 0       | 124.4   |
| 8       | < 100 > | 56     | NP-Tensile | 600   | SW      | 0       | 127.5   |
| 9       | < 100 > | 63     | NP-Tensile | 600   | SW      | 0       | 129.0   |
| 10      | < 100 > | 70     | NP-Tensile | 600   | SW      | 0       | 130.8   |
| 2       | < 100 > | 16     | NP-Tensile | 600   | SW      | 0       | 89.9    |
| 3       | < 100 > | 24     | NP-Tensile | 600   | SW      | 0       | 105.2   |
| 4       | < 100 > | 32     | NP-Tensile | 600   | SW      | 0       | 114.6   |
| 5       | < 100 > | 40     | NP-Tensile | 600   | SW      | 0       | 117.4   |
| 6       | < 100 > | 48     | NP-Tensile | 600   | SW      | 0       | 122.1   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 7       | < 100 > | 56     | NP-Tensile | 600   | SW  | 0       | 124.6   |
| 8       | < 100 > | 64     | NP-Tensile | 600   | SW  | 0       | 127.2   |
| 9       | < 100 > | 72     | NP-Tensile | 600   | SW  | 0       | 129.3   |
| 10      | < 100 > | 80     | NP-Tensile | 600   | SW  | 0       | 130.7   |
| 2       | < 100 > | 18     | NP-Tensile | 600   | SW  | 0       | 94.6    |
| 3       | < 100 > | 27     | NP-Tensile | 600   | SW  | 0       | 104.2   |
| 4       | < 100 > | 36     | NP-Tensile | 600   | SW  | 0       | 114.1   |
| 5       | < 100 > | 45     | NP-Tensile | 600   | SW  | 0       | 117.3   |
| 6       | < 100 > | 54     | NP-Tensile | 600   | SW  | 0       | 121.7   |
| 7       | < 100 > | 63     | NP-Tensile | 600   | SW  | 0       | 124.3   |
| 8       | < 100 > | 72     | NP-Tensile | 600   | SW  | 0       | 127.4   |
| 9       | < 100 > | 81     | NP-Tensile | 600   | SW  | 0       | 129.0   |
| 10      | < 100 > | 90     | NP-Tensile | 600   | SW  | 0       | 130.6   |
| 2       | < 100 > | 20     | NP-Tensile | 600   | SW  | 0       | 90.3    |
| 3       | < 100 > | 30     | NP-Tensile | 600   | SW  | 0       | 104.1   |
| 4       | < 100 > | 40     | NP-Tensile | 600   | SW  | 0       | 112.6   |
| 5       | < 100 > | 50     | NP-Tensile | 600   | SW  | 0       | 117.1   |
| 6       | < 100 > | 60     | NP-Tensile | 600   | SW  | 0       | 121.7   |
| 7       | < 100 > | 70     | NP-Tensile | 600   | SW  | 0       | 124.6   |
| 8       | < 100 > | 80     | NP-Tensile | 600   | SW  | 0       | 127.4   |
| 9       | < 100 > | 90     | NP-Tensile | 600   | SW  | 0       | 128.9   |
| 10      | < 100 > | 100    | NP-Tensile | 600   | SW  | 0       | 130.7   |
| 2       | < 100 > | 24     | NP-Tensile | 600   | SW  | 0       | 93.9    |
| 3       | < 100 > | 36     | NP-Tensile | 600   | SW  | 0       | 105.0   |
| 4       | < 100 > | 48     | NP-Tensile | 600   | SW  | 0       | 113.4   |
| 5       | < 100 > | 60     | NP-Tensile | 600   | SW  | 0       | 118.1   |
| 6       | < 100 > | 72     | NP-Tensile | 600   | SW  | 0       | 121.7   |
| 7       | < 100 > | 84     | NP-Tensile | 600   | SW  | 0       | 124.4   |
| 8       | < 100 > | 96     | NP-Tensile | 600   | SW  | 0       | 127.1   |
| 9       | < 100 > | 108    | NP-Tensile | 600   | SW  | 0       | 128.9   |
| 10      | < 100 > | 120    | NP-Tensile | 600   | SW  | 0       | 130.5   |
| 2       | < 100 > | 28     | NP-Tensile | 600   | SW  | 0       | 87.9    |
| 3       | < 100 > | 42     | NP-Tensile | 600   | SW  | 0       | 103.4   |
| 4       | < 100 > | 56     | NP-Tensile | 600   | SW  | 0       | 113.4   |
| 5       | < 100 > | 70     | NP-Tensile | 600   | SW  | 0       | 117.3   |
| 6       | < 100 > | 84     | NP-Tensile | 600   | SW  | 0       | 122.1   |
| 7       | < 100 > | 98     | NP-Tensile | 600   | SW  | 0       | 124.5   |
| 8       | < 100 > | 112    | NP-Tensile | 600   | SW  | 0       | 127.0   |
| 9       | < 100 > | 126    | NP-Tensile | 600   | SW  | 0       | 128.7   |
| 10      | < 100 > | 140    | NP-Tensile | 600   | SW  | 0       | 130.4   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 2       | < 100 > | 32     | NP-Tensile | 600   | SW  | 0       | 84.9    |
| 3       | < 100 > | 48     | NP-Tensile | 600   | SW  | 0       | 104.1   |
| 4       | < 100 > | 64     | NP-Tensile | 600   | SW  | 0       | 113.1   |
| 5       | < 100 > | 80     | NP-Tensile | 600   | SW  | 0       | 117.1   |
| 6       | < 100 > | 96     | NP-Tensile | 600   | SW  | 0       | 121.6   |
| 7       | < 100 > | 112    | NP-Tensile | 600   | SW  | 0       | 124.3   |
| 8       | < 100 > | 128    | NP-Tensile | 600   | SW  | 0       | 127.0   |
| 9       | < 100 > | 144    | NP-Tensile | 600   | SW  | 0       | 128.8   |
| 10      | < 100 > | 160    | NP-Tensile | 600   | SW  | 0       | 130.4   |
| 2       | < 100 > | 36     | NP-Tensile | 600   | SW  | 0       | 90.6    |
| 3       | < 100 > | 54     | NP-Tensile | 600   | SW  | 0       | 103.4   |
| 4       | < 100 > | 72     | NP-Tensile | 600   | SW  | 0       | 112.5   |
| 5       | < 100 > | 90     | NP-Tensile | 600   | SW  | 0       | 116.9   |
| 6       | < 100 > | 108    | NP-Tensile | 600   | SW  | 0       | 121.5   |
| 7       | < 100 > | 126    | NP-Tensile | 600   | SW  | 0       | 124.1   |
| 8       | < 100 > | 144    | NP-Tensile | 600   | SW  | 0       | 126.9   |
| 9       | < 100 > | 162    | NP-Tensile | 600   | SW  | 0       | 128.7   |
| 10      | < 100 > | 180    | NP-Tensile | 600   | SW  | 0       | 130.1   |
| 2       | < 100 > | 40     | NP-Tensile | 600   | SW  | 0       | 90.9    |
| 3       | < 100 > | 60     | NP-Tensile | 600   | SW  | 0       | 103.5   |
| 4       | < 100 > | 80     | NP-Tensile | 600   | SW  | 0       | 112.8   |
| 5       | < 100 > | 100    | NP-Tensile | 600   | SW  | 0       | 116.7   |
| 6       | < 100 > | 120    | NP-Tensile | 600   | SW  | 0       | 121.1   |
| 7       | < 100 > | 140    | NP-Tensile | 600   | SW  | 0       | 124.2   |
| 8       | < 100 > | 160    | NP-Tensile | 600   | SW  | 0       | 127.2   |
| 9       | < 100 > | 180    | NP-Tensile | 600   | SW  | 0       | 127.8   |
| 10      | < 100 > | 200    | NP-Tensile | 600   | SW  | 0       | 129.0   |
| 2       | < 100 > | 14     | P-Tensile  | 600   | SW  | 0       | 74.2    |
| 3       | < 100 > | 21     | P-Tensile  | 600   | SW  | 0       | 74.2    |
| 4       | < 100 > | 28     | P-Tensile  | 600   | SW  | 0       | 76.1    |
| 5       | < 100 > | 35     | P-Tensile  | 600   | SW  | 0       | 87.9    |
| 6       | < 100 > | 42     | P-Tensile  | 600   | SW  | 0       | 88.9    |
| 7       | < 100 > | 49     | P-Tensile  | 600   | SW  | 0       | 92.1    |
| 8       | < 100 > | 56     | P-Tensile  | 600   | SW  | 0       | 87.5    |
| 9       | < 100 > | 63     | P-Tensile  | 600   | SW  | 0       | 90.6    |
| 10      | < 100 > | 70     | P-Tensile  | 600   | SW  | 0       | 94.0    |
| 2       | < 100 > | 16     | P-Tensile  | 600   | SW  | 0       | 68.3    |
| 3       | < 100 > | 24     | P-Tensile  | 600   | SW  | 0       | 78.1    |
| 4       | < 100 > | 32     | P-Tensile  | 600   | SW  | 0       | 88.3    |
| 5       | < 100 > | 40     | P-Tensile  | 600   | SW  | 0       | 85.4    |



Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|-----|---------|---------|
| 6       | < 100 > | 48     | P-Tensile | 600   | SW  | 0       | 89.0    |
| 7       | < 100 > | 56     | P-Tensile | 600   | SW  | 0       | 85.9    |
| 8       | < 100 > | 64     | P-Tensile | 600   | SW  | 0       | 91.4    |
| 9       | < 100 > | 72     | P-Tensile | 600   | SW  | 0       | 93.2    |
| 10      | < 100 > | 80     | P-Tensile | 600   | SW  | 0       | 92.4    |
| 2       | < 100 > | 18     | P-Tensile | 600   | SW  | 0       | 76.4    |
| 3       | < 100 > | 27     | P-Tensile | 600   | SW  | 0       | 79.4    |
| 4       | < 100 > | 36     | P-Tensile | 600   | SW  | 0       | 85.0    |
| 5       | < 100 > | 45     | P-Tensile | 600   | SW  | 0       | 86.9    |
| 6       | < 100 > | 54     | P-Tensile | 600   | SW  | 0       | 90.2    |
| 7       | < 100 > | 63     | P-Tensile | 600   | SW  | 0       | 85.5    |
| 8       | < 100 > | 72     | P-Tensile | 600   | SW  | 0       | 90.4    |
| 9       | < 100 > | 81     | P-Tensile | 600   | SW  | 0       | 92.0    |
| 10      | < 100 > | 90     | P-Tensile | 600   | SW  | 0       | 91.6    |
| 2       | < 100 > | 20     | P-Tensile | 600   | SW  | 0       | 72.1    |
| 3       | < 100 > | 30     | P-Tensile | 600   | SW  | 0       | 79.6    |
| 4       | < 100 > | 40     | P-Tensile | 600   | SW  | 0       | 85.8    |
| 5       | < 100 > | 50     | P-Tensile | 600   | SW  | 0       | 83.6    |
| 6       | < 100 > | 60     | P-Tensile | 600   | SW  | 0       | 89.3    |
| 7       | < 100 > | 70     | P-Tensile | 600   | SW  | 0       | 87.6    |
| 8       | < 100 > | 80     | P-Tensile | 600   | SW  | 0       | 90.9    |
| 9       | < 100 > | 90     | P-Tensile | 600   | SW  | 0       | 91.8    |
| 10      | < 100 > | 100    | P-Tensile | 600   | SW  | 0       | 92.8    |
| 2       | < 100 > | 24     | P-Tensile | 600   | SW  | 0       | 78.2    |
| 3       | < 100 > | 36     | P-Tensile | 600   | SW  | 0       | 80.1    |
| 4       | < 100 > | 48     | P-Tensile | 600   | SW  | 0       | 88.7    |
| 5       | < 100 > | 60     | P-Tensile | 600   | SW  | 0       | 86.8    |
| 6       | < 100 > | 72     | P-Tensile | 600   | SW  | 0       | 90.1    |
| 7       | < 100 > | 84     | P-Tensile | 600   | SW  | 0       | 90.1    |
| 8       | < 100 > | 96     | P-Tensile | 600   | SW  | 0       | 91.9    |
| 9       | < 100 > | 108    | P-Tensile | 600   | SW  | 0       | 93.9    |
| 10      | < 100 > | 120    | P-Tensile | 600   | SW  | 0       | 95.0    |
| 2       | < 100 > | 28     | P-Tensile | 600   | SW  | 0       | 74.4    |
| 3       | < 100 > | 42     | P-Tensile | 600   | SW  | 0       | 78.7    |
| 4       | < 100 > | 56     | P-Tensile | 600   | SW  | 0       | 88.1    |
| 5       | < 100 > | 70     | P-Tensile | 600   | SW  | 0       | 84.1    |
| 6       | < 100 > | 84     | P-Tensile | 600   | SW  | 0       | 90.9    |
| 7       | < 100 > | 98     | P-Tensile | 600   | SW  | 0       | 90.2    |
| 8       | < 100 > | 112    | P-Tensile | 600   | SW  | 0       | 91.6    |
| 9       | < 100 > | 126    | P-Tensile | 600   | SW  | 0       | 92.1    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 10      | < 100 > | 140    | P-Tensile  | 600   | SW      | 0       | 95.8    |
| 2       | < 100 > | 32     | P-Tensile  | 600   | SW      | 0       | 75.7    |
| 3       | < 100 > | 48     | P-Tensile  | 600   | SW      | 0       | 80.0    |
| 4       | < 100 > | 64     | P-Tensile  | 600   | SW      | 0       | 87.6    |
| 5       | < 100 > | 80     | P-Tensile  | 600   | SW      | 0       | 84.5    |
| 6       | < 100 > | 96     | P-Tensile  | 600   | SW      | 0       | 90.7    |
| 7       | < 100 > | 112    | P-Tensile  | 600   | SW      | 0       | 87.2    |
| 8       | < 100 > | 128    | P-Tensile  | 600   | SW      | 0       | 90.1    |
| 9       | < 100 > | 144    | P-Tensile  | 600   | SW      | 0       | 93.5    |
| 10      | < 100 > | 160    | P-Tensile  | 600   | SW      | 0       | 94.9    |
| 2       | < 100 > | 36     | P-Tensile  | 600   | SW      | 0       | 76.7    |
| 3       | < 100 > | 54     | P-Tensile  | 600   | SW      | 0       | 79.6    |
| 4       | < 100 > | 72     | P-Tensile  | 600   | SW      | 0       | 86.0    |
| 5       | < 100 > | 90     | P-Tensile  | 600   | SW      | 0       | 85.7    |
| 6       | < 100 > | 108    | P-Tensile  | 600   | SW      | 0       | 92.1    |
| 7       | < 100 > | 126    | P-Tensile  | 600   | SW      | 0       | 91.3    |
| 8       | < 100 > | 144    | P-Tensile  | 600   | SW      | 0       | 90.8    |
| 9       | < 100 > | 162    | P-Tensile  | 600   | SW      | 0       | 83.6    |
| 10      | < 100 > | 180    | P-Tensile  | 600   | SW      | 0       | 96.2    |
| 2       | < 100 > | 40     | P-Tensile  | 600   | SW      | 0       | 67.8    |
| 3       | < 100 > | 60     | P-Tensile  | 600   | SW      | 0       | 78.5    |
| 4       | < 100 > | 80     | P-Tensile  | 600   | SW      | 0       | 86.7    |
| 5       | < 100 > | 100    | P-Tensile  | 600   | SW      | 0       | 86.2    |
| 6       | < 100 > | 120    | P-Tensile  | 600   | SW      | 0       | 90.2    |
| 7       | < 100 > | 140    | P-Tensile  | 600   | SW      | 0       | 88.4    |
| 8       | < 100 > | 160    | P-Tensile  | 600   | SW      | 0       | 91.2    |
| 9       | < 100 > | 180    | P-Tensile  | 600   | SW      | 0       | 90.8    |
| 10      | < 100 > | 200    | P-Tensile  | 600   | SW      | 0       | 96.3    |
| 2       | < 110 > | 14     | NP-Tensile | 600   | Tersoff | 0       | 187.6   |
| 3       | < 110 > | 21     | NP-Tensile | 600   | Tersoff | 0       | 187.4   |
| 4       | < 110 > | 28     | NP-Tensile | 600   | Tersoff | 0       | 176.7   |
| 5       | < 110 > | 35     | NP-Tensile | 600   | Tersoff | 0       | 176.0   |
| 6       | < 110 > | 42     | NP-Tensile | 600   | Tersoff | 0       | 187.3   |
| 7       | < 110 > | 49     | NP-Tensile | 600   | Tersoff | 0       | 186.6   |
| 8       | < 110 > | 56     | NP-Tensile | 600   | Tersoff | 0       | 182.1   |
| 9       | < 110 > | 63     | NP-Tensile | 600   | Tersoff | 0       | 182.7   |
| 10      | < 110 > | 70     | NP-Tensile | 600   | Tersoff | 0       | 187.7   |
| 2       | < 110 > | 16     | NP-Tensile | 600   | Tersoff | 0       | 184.2   |
| 3       | < 110 > | 24     | NP-Tensile | 600   | Tersoff | 0       | 186.6   |
| 4       | < 110 > | 32     | NP-Tensile | 600   | Tersoff | 0       | 176.3   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 5       | < 110 > | 40     | NP-Tensile | 600   | Tersoff | 0       | 175.7   |
| 6       | < 110 > | 48     | NP-Tensile | 600   | Tersoff | 0       | 187.4   |
| 7       | < 110 > | 56     | NP-Tensile | 600   | Tersoff | 0       | 186.7   |
| 8       | < 110 > | 64     | NP-Tensile | 600   | Tersoff | 0       | 182.1   |
| 9       | < 110 > | 72     | NP-Tensile | 600   | Tersoff | 0       | 183.4   |
| 10      | < 110 > | 80     | NP-Tensile | 600   | Tersoff | 0       | 189.8   |
| 2       | < 110 > | 18     | NP-Tensile | 600   | Tersoff | 0       | 187.0   |
| 3       | < 110 > | 27     | NP-Tensile | 600   | Tersoff | 0       | 186.0   |
| 4       | < 110 > | 36     | NP-Tensile | 600   | Tersoff | 0       | 174.3   |
| 5       | < 110 > | 45     | NP-Tensile | 600   | Tersoff | 0       | 175.4   |
| 6       | < 110 > | 54     | NP-Tensile | 600   | Tersoff | 0       | 187.3   |
| 7       | < 110 > | 63     | NP-Tensile | 600   | Tersoff | 0       | 186.5   |
| 8       | < 110 > | 72     | NP-Tensile | 600   | Tersoff | 0       | 182.9   |
| 9       | < 110 > | 81     | NP-Tensile | 600   | Tersoff | 0       | 183.3   |
| 10      | < 110 > | 90     | NP-Tensile | 600   | Tersoff | 0       | 190.3   |
| 2       | < 110 > | 20     | NP-Tensile | 600   | Tersoff | 0       | 189.4   |
| 3       | < 110 > | 30     | NP-Tensile | 600   | Tersoff | 0       | 186.4   |
| 4       | < 110 > | 40     | NP-Tensile | 600   | Tersoff | 0       | 174.7   |
| 5       | < 110 > | 50     | NP-Tensile | 600   | Tersoff | 0       | 174.6   |
| 6       | < 110 > | 60     | NP-Tensile | 600   | Tersoff | 0       | 187.3   |
| 7       | < 110 > | 70     | NP-Tensile | 600   | Tersoff | 0       | 186.9   |
| 8       | < 110 > | 80     | NP-Tensile | 600   | Tersoff | 0       | 183.1   |
| 9       | < 110 > | 90     | NP-Tensile | 600   | Tersoff | 0       | 184.6   |
| 10      | < 110 > | 100    | NP-Tensile | 600   | Tersoff | 0       | 190.9   |
| 2       | < 110 > | 24     | NP-Tensile | 600   | Tersoff | 0       | 183.7   |
| 3       | < 110 > | 36     | NP-Tensile | 600   | Tersoff | 0       | 185.1   |
| 4       | < 110 > | 48     | NP-Tensile | 600   | Tersoff | 0       | 174.0   |
| 5       | < 110 > | 60     | NP-Tensile | 600   | Tersoff | 0       | 173.8   |
| 6       | < 110 > | 72     | NP-Tensile | 600   | Tersoff | 0       | 186.7   |
| 7       | < 110 > | 84     | NP-Tensile | 600   | Tersoff | 0       | 187.0   |
| 8       | < 110 > | 96     | NP-Tensile | 600   | Tersoff | 0       | 183.2   |
| 9       | < 110 > | 108    | NP-Tensile | 600   | Tersoff | 0       | 185.6   |
| 10      | < 110 > | 120    | NP-Tensile | 600   | Tersoff | 0       | 191.6   |
| 2       | < 110 > | 28     | NP-Tensile | 600   | Tersoff | 0       | 183.1   |
| 3       | < 110 > | 42     | NP-Tensile | 600   | Tersoff | 0       | 186.2   |
| 4       | < 110 > | 56     | NP-Tensile | 600   | Tersoff | 0       | 174.1   |
| 5       | < 110 > | 70     | NP-Tensile | 600   | Tersoff | 0       | 179.0   |
| 6       | < 110 > | 84     | NP-Tensile | 600   | Tersoff | 0       | 186.9   |
| 7       | < 110 > | 98     | NP-Tensile | 600   | Tersoff | 0       | 186.6   |
| 8       | < 110 > | 112    | NP-Tensile | 600   | Tersoff | 0       | 184.5   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 9       | < 110 > | 126    | NP-Tensile | 600   | Tersoff | 0       | 186.1   |
| 10      | < 110 > | 140    | NP-Tensile | 600   | Tersoff | 0       | 192.0   |
| 2       | < 110 > | 32     | NP-Tensile | 600   | Tersoff | 0       | 186.7   |
| 3       | < 110 > | 48     | NP-Tensile | 600   | Tersoff | 0       | 185.7   |
| 4       | < 110 > | 64     | NP-Tensile | 600   | Tersoff | 0       | 169.9   |
| 5       | < 110 > | 80     | NP-Tensile | 600   | Tersoff | 0       | 180.0   |
| 6       | < 110 > | 96     | NP-Tensile | 600   | Tersoff | 0       | 186.8   |
| 7       | < 110 > | 112    | NP-Tensile | 600   | Tersoff | 0       | 186.7   |
| 8       | < 110 > | 128    | NP-Tensile | 600   | Tersoff | 0       | 186.0   |
| 9       | < 110 > | 144    | NP-Tensile | 600   | Tersoff | 0       | 180.5   |
| 10      | < 110 > | 160    | NP-Tensile | 600   | Tersoff | 0       | 191.7   |
| 2       | < 110 > | 36     | NP-Tensile | 600   | Tersoff | 0       | 185.3   |
| 3       | < 110 > | 54     | NP-Tensile | 600   | Tersoff | 0       | 187.0   |
| 4       | < 110 > | 72     | NP-Tensile | 600   | Tersoff | 0       | 163.1   |
| 5       | < 110 > | 90     | NP-Tensile | 600   | Tersoff | 0       | 179.2   |
| 6       | < 110 > | 108    | NP-Tensile | 600   | Tersoff | 0       | 186.7   |
| 7       | < 110 > | 126    | NP-Tensile | 600   | Tersoff | 0       | 186.8   |
| 8       | < 110 > | 144    | NP-Tensile | 600   | Tersoff | 0       | 184.9   |
| 9       | < 110 > | 162    | NP-Tensile | 600   | Tersoff | 0       | 187.5   |
| 10      | < 110 > | 180    | NP-Tensile | 600   | Tersoff | 0       | 190.7   |
| 2       | < 110 > | 40     | NP-Tensile | 600   | Tersoff | 0       | 186.5   |
| 3       | < 110 > | 60     | NP-Tensile | 600   | Tersoff | 0       | 186.4   |
| 4       | < 110 > | 80     | NP-Tensile | 600   | Tersoff | 0       | 178.8   |
| 5       | < 110 > | 100    | NP-Tensile | 600   | Tersoff | 0       | 178.6   |
| 6       | < 110 > | 120    | NP-Tensile | 600   | Tersoff | 0       | 186.9   |
| 7       | < 110 > | 140    | NP-Tensile | 600   | Tersoff | 0       | 187.0   |
| 8       | < 110 > | 160    | NP-Tensile | 600   | Tersoff | 0       | 185.4   |
| 9       | < 110 > | 180    | NP-Tensile | 600   | Tersoff | 0       | 187.1   |
| 10      | < 110 > | 200    | NP-Tensile | 600   | Tersoff | 0       | 191.0   |
| 2       | < 110 > | 14     | P-Tensile  | 600   | Tersoff | 0       | 149.7   |
| 3       | < 110 > | 21     | P-Tensile  | 600   | Tersoff | 0       | 152.9   |
| 4       | < 110 > | 28     | P-Tensile  | 600   | Tersoff | 0       | 137.8   |
| 5       | < 110 > | 35     | P-Tensile  | 600   | Tersoff | 0       | 140.2   |
| 6       | < 110 > | 42     | P-Tensile  | 600   | Tersoff | 0       | 134.3   |
| 7       | < 110 > | 49     | P-Tensile  | 600   | Tersoff | 0       | 140.2   |
| 8       | < 110 > | 56     | P-Tensile  | 600   | Tersoff | 0       | 140.7   |
| 9       | < 110 > | 63     | P-Tensile  | 600   | Tersoff | 0       | 128.7   |
| 10      | < 110 > | 70     | P-Tensile  | 600   | Tersoff | 0       | 130.9   |
| 2       | < 110 > | 16     | P-Tensile  | 600   | Tersoff | 0       | 161.4   |
| 3       | < 110 > | 24     | P-Tensile  | 600   | Tersoff | 0       | 140.6   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT                  | L (nm) | BC        | T (K) | POT     | SS (nm) | E (GPa) |
|---------|-----------------------|--------|-----------|-------|---------|---------|---------|
| 4       | $\langle 110 \rangle$ | 32     | P-Tensile | 600   | Tersoff | 0       | 139.1   |
| 5       | $\langle 110 \rangle$ | 40     | P-Tensile | 600   | Tersoff | 0       | 132.5   |
| 6       | $\langle 110 \rangle$ | 48     | P-Tensile | 600   | Tersoff | 0       | 134.6   |
| 7       | $\langle 110 \rangle$ | 56     | P-Tensile | 600   | Tersoff | 0       | 138.9   |
| 8       | $\langle 110 \rangle$ | 64     | P-Tensile | 600   | Tersoff | 0       | 134.3   |
| 9       | $\langle 110 \rangle$ | 72     | P-Tensile | 600   | Tersoff | 0       | 131.2   |
| 10      | $\langle 110 \rangle$ | 80     | P-Tensile | 600   | Tersoff | 0       | 134.9   |
| 2       | $\langle 110 \rangle$ | 18     | P-Tensile | 600   | Tersoff | 0       | 154.8   |
| 3       | $\langle 110 \rangle$ | 27     | P-Tensile | 600   | Tersoff | 0       | 138.1   |
| 4       | $\langle 110 \rangle$ | 36     | P-Tensile | 600   | Tersoff | 0       | 135.9   |
| 5       | $\langle 110 \rangle$ | 45     | P-Tensile | 600   | Tersoff | 0       | 140.7   |
| 6       | $\langle 110 \rangle$ | 54     | P-Tensile | 600   | Tersoff | 0       | 140.9   |
| 7       | $\langle 110 \rangle$ | 63     | P-Tensile | 600   | Tersoff | 0       | 138.5   |
| 8       | $\langle 110 \rangle$ | 72     | P-Tensile | 600   | Tersoff | 0       | 130.0   |
| 9       | $\langle 110 \rangle$ | 81     | P-Tensile | 600   | Tersoff | 0       | 133.4   |
| 10      | $\langle 110 \rangle$ | 90     | P-Tensile | 600   | Tersoff | 0       | 136.8   |
| 2       | $\langle 110 \rangle$ | 20     | P-Tensile | 600   | Tersoff | 0       | 150.8   |
| 3       | $\langle 110 \rangle$ | 30     | P-Tensile | 600   | Tersoff | 0       | 142.3   |
| 4       | $\langle 110 \rangle$ | 40     | P-Tensile | 600   | Tersoff | 0       | 135.0   |
| 5       | $\langle 110 \rangle$ | 50     | P-Tensile | 600   | Tersoff | 0       | 137.9   |
| 6       | $\langle 110 \rangle$ | 60     | P-Tensile | 600   | Tersoff | 0       | 135.9   |
| 7       | $\langle 110 \rangle$ | 70     | P-Tensile | 600   | Tersoff | 0       | 136.5   |
| 8       | $\langle 110 \rangle$ | 80     | P-Tensile | 600   | Tersoff | 0       | 129.9   |
| 9       | $\langle 110 \rangle$ | 90     | P-Tensile | 600   | Tersoff | 0       | 130.9   |
| 10      | $\langle 110 \rangle$ | 100    | P-Tensile | 600   | Tersoff | 0       | 136.7   |
| 2       | $\langle 110 \rangle$ | 24     | P-Tensile | 600   | Tersoff | 0       | 155.4   |
| 3       | $\langle 110 \rangle$ | 36     | P-Tensile | 600   | Tersoff | 0       | 134.4   |
| 4       | $\langle 110 \rangle$ | 48     | P-Tensile | 600   | Tersoff | 0       | 135.5   |
| 5       | $\langle 110 \rangle$ | 60     | P-Tensile | 600   | Tersoff | 0       | 135.9   |
| 6       | $\langle 110 \rangle$ | 72     | P-Tensile | 600   | Tersoff | 0       | 134.4   |
| 7       | $\langle 110 \rangle$ | 84     | P-Tensile | 600   | Tersoff | 0       | 135.7   |
| 8       | $\langle 110 \rangle$ | 96     | P-Tensile | 600   | Tersoff | 0       | 134.6   |
| 9       | $\langle 110 \rangle$ | 108    | P-Tensile | 600   | Tersoff | 0       | 131.1   |
| 10      | $\langle 110 \rangle$ | 120    | P-Tensile | 600   | Tersoff | 0       | 138.9   |
| 2       | $\langle 110 \rangle$ | 28     | P-Tensile | 600   | Tersoff | 0       | 137.6   |
| 3       | $\langle 110 \rangle$ | 42     | P-Tensile | 600   | Tersoff | 0       | 141.5   |
| 4       | $\langle 110 \rangle$ | 56     | P-Tensile | 600   | Tersoff | 0       | 132.9   |
| 5       | $\langle 110 \rangle$ | 70     | P-Tensile | 600   | Tersoff | 0       | 135.4   |
| 6       | $\langle 110 \rangle$ | 84     | P-Tensile | 600   | Tersoff | 0       | 134.8   |
| 7       | $\langle 110 \rangle$ | 98     | P-Tensile | 600   | Tersoff | 0       | 140.5   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 8       | < 110 > | 112    | P-Tensile  | 600   | Tersoff | 0       | 132.4   |
| 9       | < 110 > | 126    | P-Tensile  | 600   | Tersoff | 0       | 135.4   |
| 10      | < 110 > | 140    | P-Tensile  | 600   | Tersoff | 0       | 139.1   |
| 2       | < 110 > | 32     | P-Tensile  | 600   | Tersoff | 0       | 158.4   |
| 3       | < 110 > | 48     | P-Tensile  | 600   | Tersoff | 0       | 142.7   |
| 4       | < 110 > | 64     | P-Tensile  | 600   | Tersoff | 0       | 139.6   |
| 5       | < 110 > | 80     | P-Tensile  | 600   | Tersoff | 0       | 135.6   |
| 6       | < 110 > | 96     | P-Tensile  | 600   | Tersoff | 0       | 140.6   |
| 7       | < 110 > | 112    | P-Tensile  | 600   | Tersoff | 0       | 140.2   |
| 8       | < 110 > | 128    | P-Tensile  | 600   | Tersoff | 0       | 134.3   |
| 9       | < 110 > | 144    | P-Tensile  | 600   | Tersoff | 0       | 134.1   |
| 10      | < 110 > | 160    | P-Tensile  | 600   | Tersoff | 0       | 135.7   |
| 2       | < 110 > | 36     | P-Tensile  | 600   | Tersoff | 0       | 140.2   |
| 3       | < 110 > | 54     | P-Tensile  | 600   | Tersoff | 0       | 129.0   |
| 4       | < 110 > | 72     | P-Tensile  | 600   | Tersoff | 0       | 138.8   |
| 5       | < 110 > | 90     | P-Tensile  | 600   | Tersoff | 0       | 135.5   |
| 6       | < 110 > | 108    | P-Tensile  | 600   | Tersoff | 0       | 139.0   |
| 7       | < 110 > | 126    | P-Tensile  | 600   | Tersoff | 0       | 139.9   |
| 8       | < 110 > | 144    | P-Tensile  | 600   | Tersoff | 0       | 134.1   |
| 9       | < 110 > | 162    | P-Tensile  | 600   | Tersoff | 0       | 135.6   |
| 10      | < 110 > | 180    | P-Tensile  | 600   | Tersoff | 0       | 139.2   |
| 2       | < 110 > | 40     | P-Tensile  | 600   | Tersoff | 0       | 150.9   |
| 3       | < 110 > | 60     | P-Tensile  | 600   | Tersoff | 0       | 140.1   |
| 4       | < 110 > | 80     | P-Tensile  | 600   | Tersoff | 0       | 140.0   |
| 5       | < 110 > | 100    | P-Tensile  | 600   | Tersoff | 0       | 136.3   |
| 6       | < 110 > | 120    | P-Tensile  | 600   | Tersoff | 0       | 131.7   |
| 7       | < 110 > | 140    | P-Tensile  | 600   | Tersoff | 0       | 135.6   |
| 8       | < 110 > | 160    | P-Tensile  | 600   | Tersoff | 0       | 134.6   |
| 9       | < 110 > | 180    | P-Tensile  | 600   | Tersoff | 0       | 135.1   |
| 10      | < 110 > | 200    | P-Tensile  | 600   | Tersoff | 0       | 136.9   |
| 2       | < 110 > | 14     | NP-Tensile | 600   | SW      | 0       | 148.9   |
| 3       | < 110 > | 21     | NP-Tensile | 600   | SW      | 0       | 152.9   |
| 4       | < 110 > | 28     | NP-Tensile | 600   | SW      | 0       | 150.7   |
| 5       | < 110 > | 35     | NP-Tensile | 600   | SW      | 0       | 152.6   |
| 6       | < 110 > | 42     | NP-Tensile | 600   | SW      | 0       | 159.6   |
| 7       | < 110 > | 49     | NP-Tensile | 600   | SW      | 0       | 160.5   |
| 8       | < 110 > | 56     | NP-Tensile | 600   | SW      | 0       | 158.3   |
| 9       | < 110 > | 63     | NP-Tensile | 600   | SW      | 0       | 159.2   |
| 10      | < 110 > | 70     | NP-Tensile | 600   | SW      | 0       | 162.7   |
| 2       | < 110 > | 16     | NP-Tensile | 600   | SW      | 0       | 146.8   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 3       | < 110 > | 24     | NP-Tensile | 600   | SW  | 0       | 151.9   |
| 4       | < 110 > | 32     | NP-Tensile | 600   | SW  | 0       | 151.3   |
| 5       | < 110 > | 40     | NP-Tensile | 600   | SW  | 0       | 152.9   |
| 6       | < 110 > | 48     | NP-Tensile | 600   | SW  | 0       | 159.5   |
| 7       | < 110 > | 56     | NP-Tensile | 600   | SW  | 0       | 160.1   |
| 8       | < 110 > | 64     | NP-Tensile | 600   | SW  | 0       | 158.7   |
| 9       | < 110 > | 72     | NP-Tensile | 600   | SW  | 0       | 159.6   |
| 10      | < 110 > | 80     | NP-Tensile | 600   | SW  | 0       | 162.9   |
| 2       | < 110 > | 18     | NP-Tensile | 600   | SW  | 0       | 147.7   |
| 3       | < 110 > | 27     | NP-Tensile | 600   | SW  | 0       | 151.8   |
| 4       | < 110 > | 36     | NP-Tensile | 600   | SW  | 0       | 150.5   |
| 5       | < 110 > | 45     | NP-Tensile | 600   | SW  | 0       | 152.4   |
| 6       | < 110 > | 54     | NP-Tensile | 600   | SW  | 0       | 159.5   |
| 7       | < 110 > | 63     | NP-Tensile | 600   | SW  | 0       | 160.0   |
| 8       | < 110 > | 72     | NP-Tensile | 600   | SW  | 0       | 158.2   |
| 9       | < 110 > | 81     | NP-Tensile | 600   | SW  | 0       | 159.6   |
| 10      | < 110 > | 90     | NP-Tensile | 600   | SW  | 0       | 162.9   |
| 2       | < 110 > | 20     | NP-Tensile | 600   | SW  | 0       | 149.7   |
| 3       | < 110 > | 30     | NP-Tensile | 600   | SW  | 0       | 154.2   |
| 4       | < 110 > | 40     | NP-Tensile | 600   | SW  | 0       | 150.6   |
| 5       | < 110 > | 50     | NP-Tensile | 600   | SW  | 0       | 152.0   |
| 6       | < 110 > | 60     | NP-Tensile | 600   | SW  | 0       | 159.1   |
| 7       | < 110 > | 70     | NP-Tensile | 600   | SW  | 0       | 160.5   |
| 8       | < 110 > | 80     | NP-Tensile | 600   | SW  | 0       | 158.7   |
| 9       | < 110 > | 90     | NP-Tensile | 600   | SW  | 0       | 159.8   |
| 10      | < 110 > | 100    | NP-Tensile | 600   | SW  | 0       | 162.5   |
| 2       | < 110 > | 24     | NP-Tensile | 600   | SW  | 0       | 152.0   |
| 3       | < 110 > | 36     | NP-Tensile | 600   | SW  | 0       | 152.6   |
| 4       | < 110 > | 48     | NP-Tensile | 600   | SW  | 0       | 149.7   |
| 5       | < 110 > | 60     | NP-Tensile | 600   | SW  | 0       | 152.0   |
| 6       | < 110 > | 72     | NP-Tensile | 600   | SW  | 0       | 159.3   |
| 7       | < 110 > | 84     | NP-Tensile | 600   | SW  | 0       | 160.6   |
| 8       | < 110 > | 96     | NP-Tensile | 600   | SW  | 0       | 158.0   |
| 9       | < 110 > | 108    | NP-Tensile | 600   | SW  | 0       | 159.5   |
| 10      | < 110 > | 120    | NP-Tensile | 600   | SW  | 0       | 162.6   |
| 2       | < 110 > | 28     | NP-Tensile | 600   | SW  | 0       | 151.0   |
| 3       | < 110 > | 42     | NP-Tensile | 600   | SW  | 0       | 153.5   |
| 4       | < 110 > | 56     | NP-Tensile | 600   | SW  | 0       | 149.4   |
| 5       | < 110 > | 70     | NP-Tensile | 600   | SW  | 0       | 152.0   |
| 6       | < 110 > | 84     | NP-Tensile | 600   | SW  | 0       | 159.6   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 7       | < 110 > | 98     | NP-Tensile | 600   | SW  | 0       | 160.5   |
| 8       | < 110 > | 112    | NP-Tensile | 600   | SW  | 0       | 158.1   |
| 9       | < 110 > | 126    | NP-Tensile | 600   | SW  | 0       | 159.2   |
| 10      | < 110 > | 140    | NP-Tensile | 600   | SW  | 0       | 165.8   |
| 2       | < 110 > | 32     | NP-Tensile | 600   | SW  | 0       | 148.0   |
| 3       | < 110 > | 48     | NP-Tensile | 600   | SW  | 0       | 153.0   |
| 4       | < 110 > | 64     | NP-Tensile | 600   | SW  | 0       | 149.7   |
| 5       | < 110 > | 80     | NP-Tensile | 600   | SW  | 0       | 153.4   |
| 6       | < 110 > | 96     | NP-Tensile | 600   | SW  | 0       | 158.9   |
| 7       | < 110 > | 112    | NP-Tensile | 600   | SW  | 0       | 160.3   |
| 8       | < 110 > | 128    | NP-Tensile | 600   | SW  | 0       | 158.2   |
| 9       | < 110 > | 144    | NP-Tensile | 600   | SW  | 0       | 159.4   |
| 10      | < 110 > | 160    | NP-Tensile | 600   | SW  | 0       | 165.7   |
| 2       | < 110 > | 36     | NP-Tensile | 600   | SW  | 0       | 149.2   |
| 3       | < 110 > | 54     | NP-Tensile | 600   | SW  | 0       | 152.8   |
| 4       | < 110 > | 72     | NP-Tensile | 600   | SW  | 0       | 149.6   |
| 5       | < 110 > | 90     | NP-Tensile | 600   | SW  | 0       | 152.5   |
| 6       | < 110 > | 108    | NP-Tensile | 600   | SW  | 0       | 159.1   |
| 7       | < 110 > | 126    | NP-Tensile | 600   | SW  | 0       | 160.1   |
| 8       | < 110 > | 144    | NP-Tensile | 600   | SW  | 0       | 158.1   |
| 9       | < 110 > | 162    | NP-Tensile | 600   | SW  | 0       | 159.2   |
| 10      | < 110 > | 180    | NP-Tensile | 600   | SW  | 0       | 166.9   |
| 2       | < 110 > | 40     | NP-Tensile | 600   | SW  | 0       | 150.6   |
| 3       | < 110 > | 60     | NP-Tensile | 600   | SW  | 0       | 152.6   |
| 4       | < 110 > | 80     | NP-Tensile | 600   | SW  | 0       | 150.5   |
| 5       | < 110 > | 100    | NP-Tensile | 600   | SW  | 0       | 152.5   |
| 6       | < 110 > | 120    | NP-Tensile | 600   | SW  | 0       | 159.0   |
| 7       | < 110 > | 140    | NP-Tensile | 600   | SW  | 0       | 160.2   |
| 8       | < 110 > | 160    | NP-Tensile | 600   | SW  | 0       | 180.0   |
| 9       | < 110 > | 180    | NP-Tensile | 600   | SW  | 0       | 160.6   |
| 10      | < 110 > | 200    | NP-Tensile | 600   | SW  | 0       | 165.1   |
| 2       | < 110 > | 14     | P-Tensile  | 600   | SW  | 0       | 115.3   |
| 3       | < 110 > | 21     | P-Tensile  | 600   | SW  | 0       | 115.3   |
| 4       | < 110 > | 28     | P-Tensile  | 600   | SW  | 0       | 112.5   |
| 5       | < 110 > | 35     | P-Tensile  | 600   | SW  | 0       | 122.1   |
| 6       | < 110 > | 42     | P-Tensile  | 600   | SW  | 0       | 117.8   |
| 7       | < 110 > | 49     | P-Tensile  | 600   | SW  | 0       | 120.8   |
| 8       | < 110 > | 56     | P-Tensile  | 600   | SW  | 0       | 116.1   |
| 9       | < 110 > | 63     | P-Tensile  | 600   | SW  | 0       | 115.2   |
| 10      | < 110 > | 70     | P-Tensile  | 600   | SW  | 0       | 116.1   |



Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|-----|---------|---------|
| 2       | < 110 > | 16     | P-Tensile | 600   | SW  | 0       | 131.9   |
| 3       | < 110 > | 24     | P-Tensile | 600   | SW  | 0       | 118.6   |
| 4       | < 110 > | 32     | P-Tensile | 600   | SW  | 0       | 108.7   |
| 5       | < 110 > | 40     | P-Tensile | 600   | SW  | 0       | 121.5   |
| 6       | < 110 > | 48     | P-Tensile | 600   | SW  | 0       | 114.7   |
| 7       | < 110 > | 56     | P-Tensile | 600   | SW  | 0       | 116.9   |
| 8       | < 110 > | 64     | P-Tensile | 600   | SW  | 0       | 118.6   |
| 9       | < 110 > | 72     | P-Tensile | 600   | SW  | 0       | 119.3   |
| 10      | < 110 > | 80     | P-Tensile | 600   | SW  | 0       | 121.6   |
| 2       | < 110 > | 18     | P-Tensile | 600   | SW  | 0       | 121.0   |
| 3       | < 110 > | 27     | P-Tensile | 600   | SW  | 0       | 106.9   |
| 4       | < 110 > | 36     | P-Tensile | 600   | SW  | 0       | 114.7   |
| 5       | < 110 > | 45     | P-Tensile | 600   | SW  | 0       | 121.4   |
| 6       | < 110 > | 54     | P-Tensile | 600   | SW  | 0       | 117.1   |
| 7       | < 110 > | 63     | P-Tensile | 600   | SW  | 0       | 124.0   |
| 8       | < 110 > | 72     | P-Tensile | 600   | SW  | 0       | 118.0   |
| 9       | < 110 > | 81     | P-Tensile | 600   | SW  | 0       | 119.7   |
| 10      | < 110 > | 90     | P-Tensile | 600   | SW  | 0       | 122.3   |
| 2       | < 110 > | 20     | P-Tensile | 600   | SW  | 0       | 109.5   |
| 3       | < 110 > | 30     | P-Tensile | 600   | SW  | 0       | 114.9   |
| 4       | < 110 > | 40     | P-Tensile | 600   | SW  | 0       | 113.3   |
| 5       | < 110 > | 50     | P-Tensile | 600   | SW  | 0       | 120.9   |
| 6       | < 110 > | 60     | P-Tensile | 600   | SW  | 0       | 119.6   |
| 7       | < 110 > | 70     | P-Tensile | 600   | SW  | 0       | 115.3   |
| 8       | < 110 > | 80     | P-Tensile | 600   | SW  | 0       | 111.9   |
| 9       | < 110 > | 90     | P-Tensile | 600   | SW  | 0       | 119.2   |
| 10      | < 110 > | 100    | P-Tensile | 600   | SW  | 0       | 121.6   |
| 2       | < 110 > | 24     | P-Tensile | 600   | SW  | 0       | 122.4   |
| 3       | < 110 > | 36     | P-Tensile | 600   | SW  | 0       | 117.6   |
| 4       | < 110 > | 48     | P-Tensile | 600   | SW  | 0       | 112.7   |
| 5       | < 110 > | 60     | P-Tensile | 600   | SW  | 0       | 120.9   |
| 6       | < 110 > | 72     | P-Tensile | 600   | SW  | 0       | 116.4   |
| 7       | < 110 > | 84     | P-Tensile | 600   | SW  | 0       | 123.9   |
| 8       | < 110 > | 96     | P-Tensile | 600   | SW  | 0       | 117.7   |
| 9       | < 110 > | 108    | P-Tensile | 600   | SW  | 0       | 116.9   |
| 10      | < 110 > | 120    | P-Tensile | 600   | SW  | 0       | 124.8   |
| 2       | < 110 > | 28     | P-Tensile | 600   | SW  | 0       | 128.2   |
| 3       | < 110 > | 42     | P-Tensile | 600   | SW  | 0       | 112.8   |
| 4       | < 110 > | 56     | P-Tensile | 600   | SW  | 0       | 122.5   |
| 5       | < 110 > | 70     | P-Tensile | 600   | SW  | 0       | 120.3   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 6       | < 110 > | 84     | P-Tensile  | 600   | SW      | 0       | 114.6   |
| 7       | < 110 > | 98     | P-Tensile  | 600   | SW      | 0       | 116.0   |
| 8       | < 110 > | 112    | P-Tensile  | 600   | SW      | 0       | 118.3   |
| 9       | < 110 > | 126    | P-Tensile  | 600   | SW      | 0       | 112.3   |
| 10      | < 110 > | 140    | P-Tensile  | 600   | SW      | 0       | 122.5   |
| 2       | < 110 > | 32     | P-Tensile  | 600   | SW      | 0       | 121.6   |
| 3       | < 110 > | 48     | P-Tensile  | 600   | SW      | 0       | 111.7   |
| 4       | < 110 > | 64     | P-Tensile  | 600   | SW      | 0       | 120.0   |
| 5       | < 110 > | 80     | P-Tensile  | 600   | SW      | 0       | 121.3   |
| 6       | < 110 > | 96     | P-Tensile  | 600   | SW      | 0       | 119.2   |
| 7       | < 110 > | 112    | P-Tensile  | 600   | SW      | 0       | 121.8   |
| 8       | < 110 > | 128    | P-Tensile  | 600   | SW      | 0       | 117.3   |
| 9       | < 110 > | 144    | P-Tensile  | 600   | SW      | 0       | 119.3   |
| 10      | < 110 > | 160    | P-Tensile  | 600   | SW      | 0       | 120.7   |
| 2       | < 110 > | 36     | P-Tensile  | 600   | SW      | 0       | 127.6   |
| 3       | < 110 > | 54     | P-Tensile  | 600   | SW      | 0       | 106.8   |
| 4       | < 110 > | 72     | P-Tensile  | 600   | SW      | 0       | 121.9   |
| 5       | < 110 > | 90     | P-Tensile  | 600   | SW      | 0       | 120.5   |
| 6       | < 110 > | 108    | P-Tensile  | 600   | SW      | 0       | 120.0   |
| 7       | < 110 > | 126    | P-Tensile  | 600   | SW      | 0       | 124.0   |
| 8       | < 110 > | 144    | P-Tensile  | 600   | SW      | 0       | 118.6   |
| 9       | < 110 > | 162    | P-Tensile  | 600   | SW      | 0       | 119.4   |
| 10      | < 110 > | 180    | P-Tensile  | 600   | SW      | 0       | 121.7   |
| 2       | < 110 > | 40     | P-Tensile  | 600   | SW      | 0       | 112.3   |
| 3       | < 110 > | 60     | P-Tensile  | 600   | SW      | 0       | 117.4   |
| 4       | < 110 > | 80     | P-Tensile  | 600   | SW      | 0       | 120.2   |
| 5       | < 110 > | 100    | P-Tensile  | 600   | SW      | 0       | 120.8   |
| 6       | < 110 > | 120    | P-Tensile  | 600   | SW      | 0       | 119.0   |
| 7       | < 110 > | 140    | P-Tensile  | 600   | SW      | 0       | 121.9   |
| 8       | < 110 > | 160    | P-Tensile  | 600   | SW      | 0       | 118.1   |
| 9       | < 110 > | 180    | P-Tensile  | 600   | SW      | 0       | 119.2   |
| 10      | < 110 > | 200    | P-Tensile  | 600   | SW      | 0       | 121.5   |
| 2       | < 111 > | 14     | NP-Tensile | 600   | Tersoff | 0       | 174.6   |
| 3       | < 111 > | 21     | NP-Tensile | 600   | Tersoff | 0       | 188.5   |
| 4       | < 111 > | 28     | NP-Tensile | 600   | Tersoff | 0       | 195.8   |
| 5       | < 111 > | 35     | NP-Tensile | 600   | Tersoff | 0       | 199.0   |
| 6       | < 111 > | 42     | NP-Tensile | 600   | Tersoff | 0       | 201.8   |
| 7       | < 111 > | 49     | NP-Tensile | 600   | Tersoff | 0       | 204.4   |
| 8       | < 111 > | 56     | NP-Tensile | 600   | Tersoff | 0       | 204.7   |
| 9       | < 111 > | 63     | NP-Tensile | 600   | Tersoff | 0       | 206.3   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 10      | < 111 > | 70     | NP-Tensile | 600   | Tersoff | 0       | 207.1   |
| 2       | < 111 > | 16     | NP-Tensile | 600   | Tersoff | 0       | 173.7   |
| 3       | < 111 > | 24     | NP-Tensile | 600   | Tersoff | 0       | 190.0   |
| 4       | < 111 > | 32     | NP-Tensile | 600   | Tersoff | 0       | 194.7   |
| 5       | < 111 > | 40     | NP-Tensile | 600   | Tersoff | 0       | 198.9   |
| 6       | < 111 > | 48     | NP-Tensile | 600   | Tersoff | 0       | 202.3   |
| 7       | < 111 > | 56     | NP-Tensile | 600   | Tersoff | 0       | 203.1   |
| 8       | < 111 > | 64     | NP-Tensile | 600   | Tersoff | 0       | 205.0   |
| 9       | < 111 > | 72     | NP-Tensile | 600   | Tersoff | 0       | 206.3   |
| 10      | < 111 > | 80     | NP-Tensile | 600   | Tersoff | 0       | 210.3   |
| 2       | < 111 > | 18     | NP-Tensile | 600   | Tersoff | 0       | 177.7   |
| 3       | < 111 > | 27     | NP-Tensile | 600   | Tersoff | 0       | 187.8   |
| 4       | < 111 > | 36     | NP-Tensile | 600   | Tersoff | 0       | 194.8   |
| 5       | < 111 > | 45     | NP-Tensile | 600   | Tersoff | 0       | 199.3   |
| 6       | < 111 > | 54     | NP-Tensile | 600   | Tersoff | 0       | 202.7   |
| 7       | < 111 > | 63     | NP-Tensile | 600   | Tersoff | 0       | 203.6   |
| 8       | < 111 > | 72     | NP-Tensile | 600   | Tersoff | 0       | 205.2   |
| 9       | < 111 > | 81     | NP-Tensile | 600   | Tersoff | 0       | 206.4   |
| 10      | < 111 > | 90     | NP-Tensile | 600   | Tersoff | 0       | 211.9   |
| 2       | < 111 > | 20     | NP-Tensile | 600   | Tersoff | 0       | 174.0   |
| 3       | < 111 > | 30     | NP-Tensile | 600   | Tersoff | 0       | 187.1   |
| 4       | < 111 > | 40     | NP-Tensile | 600   | Tersoff | 0       | 194.7   |
| 5       | < 111 > | 50     | NP-Tensile | 600   | Tersoff | 0       | 199.8   |
| 6       | < 111 > | 60     | NP-Tensile | 600   | Tersoff | 0       | 202.0   |
| 7       | < 111 > | 70     | NP-Tensile | 600   | Tersoff | 0       | 203.4   |
| 8       | < 111 > | 80     | NP-Tensile | 600   | Tersoff | 0       | 205.0   |
| 9       | < 111 > | 90     | NP-Tensile | 600   | Tersoff | 0       | 208.4   |
| 10      | < 111 > | 100    | NP-Tensile | 600   | Tersoff | 0       | 214.1   |
| 2       | < 111 > | 24     | NP-Tensile | 600   | Tersoff | 0       | 177.1   |
| 3       | < 111 > | 36     | NP-Tensile | 600   | Tersoff | 0       | 187.7   |
| 4       | < 111 > | 48     | NP-Tensile | 600   | Tersoff | 0       | 195.5   |
| 5       | < 111 > | 60     | NP-Tensile | 600   | Tersoff | 0       | 199.8   |
| 6       | < 111 > | 72     | NP-Tensile | 600   | Tersoff | 0       | 202.1   |
| 7       | < 111 > | 84     | NP-Tensile | 600   | Tersoff | 0       | 203.8   |
| 8       | < 111 > | 96     | NP-Tensile | 600   | Tersoff | 0       | 205.8   |
| 9       | < 111 > | 108    | NP-Tensile | 600   | Tersoff | 0       | 211.8   |
| 10      | < 111 > | 120    | NP-Tensile | 600   | Tersoff | 0       | 215.8   |
| 2       | < 111 > | 28     | NP-Tensile | 600   | Tersoff | 0       | 176.1   |
| 3       | < 111 > | 42     | NP-Tensile | 600   | Tersoff | 0       | 188.5   |
| 4       | < 111 > | 56     | NP-Tensile | 600   | Tersoff | 0       | 194.4   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 5       | < 111 > | 70     | NP-Tensile | 600   | Tersoff | 0       | 199.7   |
| 6       | < 111 > | 84     | NP-Tensile | 600   | Tersoff | 0       | 202.2   |
| 7       | < 111 > | 98     | NP-Tensile | 600   | Tersoff | 0       | 204.4   |
| 8       | < 111 > | 112    | NP-Tensile | 600   | Tersoff | 0       | 211.7   |
| 9       | < 111 > | 126    | NP-Tensile | 600   | Tersoff | 0       | 210.5   |
| 10      | < 111 > | 140    | NP-Tensile | 600   | Tersoff | 0       | 214.9   |
| 2       | < 111 > | 32     | NP-Tensile | 600   | Tersoff | 0       | 176.3   |
| 3       | < 111 > | 48     | NP-Tensile | 600   | Tersoff | 0       | 189.4   |
| 4       | < 111 > | 64     | NP-Tensile | 600   | Tersoff | 0       | 194.9   |
| 5       | < 111 > | 80     | NP-Tensile | 600   | Tersoff | 0       | 200.3   |
| 6       | < 111 > | 96     | NP-Tensile | 600   | Tersoff | 0       | 202.5   |
| 7       | < 111 > | 112    | NP-Tensile | 600   | Tersoff | 0       | 204.3   |
| 8       | < 111 > | 128    | NP-Tensile | 600   | Tersoff | 0       | 207.1   |
| 9       | < 111 > | 144    | NP-Tensile | 600   | Tersoff | 0       | 212.3   |
| 10      | < 111 > | 160    | NP-Tensile | 600   | Tersoff | 0       | 215.4   |
| 2       | < 111 > | 36     | NP-Tensile | 600   | Tersoff | 0       | 176.2   |
| 3       | < 111 > | 54     | NP-Tensile | 600   | Tersoff | 0       | 188.9   |
| 4       | < 111 > | 72     | NP-Tensile | 600   | Tersoff | 0       | 195.2   |
| 5       | < 111 > | 90     | NP-Tensile | 600   | Tersoff | 0       | 200.8   |
| 6       | < 111 > | 108    | NP-Tensile | 600   | Tersoff | 0       | 202.5   |
| 7       | < 111 > | 126    | NP-Tensile | 600   | Tersoff | 0       | 206.3   |
| 8       | < 111 > | 144    | NP-Tensile | 600   | Tersoff | 0       | 209.0   |
| 9       | < 111 > | 162    | NP-Tensile | 600   | Tersoff | 0       | 212.9   |
| 10      | < 111 > | 180    | NP-Tensile | 600   | Tersoff | 0       | 226.6   |
| 2       | < 111 > | 40     | NP-Tensile | 600   | Tersoff | 0       | 176.5   |
| 3       | < 111 > | 60     | NP-Tensile | 600   | Tersoff | 0       | 188.5   |
| 4       | < 111 > | 80     | NP-Tensile | 600   | Tersoff | 0       | 195.2   |
| 5       | < 111 > | 100    | NP-Tensile | 600   | Tersoff | 0       | 201.0   |
| 6       | < 111 > | 120    | NP-Tensile | 600   | Tersoff | 0       | 202.3   |
| 7       | < 111 > | 140    | NP-Tensile | 600   | Tersoff | 0       | 207.7   |
| 8       | < 111 > | 160    | NP-Tensile | 600   | Tersoff | 0       | 212.1   |
| 9       | < 111 > | 180    | NP-Tensile | 600   | Tersoff | 0       | 204.6   |
| 10      | < 111 > | 200    | NP-Tensile | 600   | Tersoff | 0       | 216.3   |
| 2       | < 111 > | 14     | P-Tensile  | 600   | Tersoff | 0       | 115.9   |
| 3       | < 111 > | 21     | P-Tensile  | 600   | Tersoff | 0       | 113.4   |
| 4       | < 111 > | 28     | P-Tensile  | 600   | Tersoff | 0       | 135.0   |
| 5       | < 111 > | 35     | P-Tensile  | 600   | Tersoff | 0       | 145.5   |
| 6       | < 111 > | 42     | P-Tensile  | 600   | Tersoff | 0       | 147.9   |
| 7       | < 111 > | 49     | P-Tensile  | 600   | Tersoff | 0       | 149.7   |
| 8       | < 111 > | 56     | P-Tensile  | 600   | Tersoff | 0       | 149.3   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|---------|---------|---------|
| 9       | < 111 > | 63     | P-Tensile | 600   | Tersoff | 0       | 147.1   |
| 10      | < 111 > | 70     | P-Tensile | 600   | Tersoff | 0       | 151.6   |
| 2       | < 111 > | 16     | P-Tensile | 600   | Tersoff | 0       | 134.6   |
| 3       | < 111 > | 24     | P-Tensile | 600   | Tersoff | 0       | 135.8   |
| 4       | < 111 > | 32     | P-Tensile | 600   | Tersoff | 0       | 144.8   |
| 5       | < 111 > | 40     | P-Tensile | 600   | Tersoff | 0       | 148.9   |
| 6       | < 111 > | 48     | P-Tensile | 600   | Tersoff | 0       | 151.2   |
| 7       | < 111 > | 56     | P-Tensile | 600   | Tersoff | 0       | 91.2    |
| 8       | < 111 > | 64     | P-Tensile | 600   | Tersoff | 0       | 147.9   |
| 9       | < 111 > | 72     | P-Tensile | 600   | Tersoff | 0       | 140.6   |
| 10      | < 111 > | 80     | P-Tensile | 600   | Tersoff | 0       | 153.6   |
| 2       | < 111 > | 18     | P-Tensile | 600   | Tersoff | 0       | 135.9   |
| 3       | < 111 > | 27     | P-Tensile | 600   | Tersoff | 0       | 136.5   |
| 4       | < 111 > | 36     | P-Tensile | 600   | Tersoff | 0       | 145.5   |
| 5       | < 111 > | 45     | P-Tensile | 600   | Tersoff | 0       | 148.0   |
| 6       | < 111 > | 54     | P-Tensile | 600   | Tersoff | 0       | 150.9   |
| 7       | < 111 > | 63     | P-Tensile | 600   | Tersoff | 0       | 151.4   |
| 8       | < 111 > | 72     | P-Tensile | 600   | Tersoff | 0       | 147.5   |
| 9       | < 111 > | 81     | P-Tensile | 600   | Tersoff | 0       | 151.2   |
| 10      | < 111 > | 90     | P-Tensile | 600   | Tersoff | 0       | 154.3   |
| 2       | < 111 > | 20     | P-Tensile | 600   | Tersoff | 0       | 136.8   |
| 3       | < 111 > | 30     | P-Tensile | 600   | Tersoff | 0       | 136.7   |
| 4       | < 111 > | 40     | P-Tensile | 600   | Tersoff | 0       | 146.5   |
| 5       | < 111 > | 50     | P-Tensile | 600   | Tersoff | 0       | 147.6   |
| 6       | < 111 > | 60     | P-Tensile | 600   | Tersoff | 0       | 141.9   |
| 7       | < 111 > | 70     | P-Tensile | 600   | Tersoff | 0       | 151.8   |
| 8       | < 111 > | 80     | P-Tensile | 600   | Tersoff | 0       | 147.8   |
| 9       | < 111 > | 90     | P-Tensile | 600   | Tersoff | 0       | 134.1   |
| 10      | < 111 > | 100    | P-Tensile | 600   | Tersoff | 0       | 152.1   |
| 2       | < 111 > | 24     | P-Tensile | 600   | Tersoff | 0       | 132.3   |
| 3       | < 111 > | 36     | P-Tensile | 600   | Tersoff | 0       | 137.5   |
| 4       | < 111 > | 48     | P-Tensile | 600   | Tersoff | 0       | 145.9   |
| 5       | < 111 > | 60     | P-Tensile | 600   | Tersoff | 0       | 149.8   |
| 6       | < 111 > | 72     | P-Tensile | 600   | Tersoff | 0       | 161.3   |
| 7       | < 111 > | 84     | P-Tensile | 600   | Tersoff | 0       | 155.9   |
| 8       | < 111 > | 96     | P-Tensile | 600   | Tersoff | 0       | 147.5   |
| 9       | < 111 > | 108    | P-Tensile | 600   | Tersoff | 0       | 152.1   |
| 10      | < 111 > | 120    | P-Tensile | 600   | Tersoff | 0       | 157.6   |
| 2       | < 111 > | 28     | P-Tensile | 600   | Tersoff | 0       | 138.2   |
| 3       | < 111 > | 42     | P-Tensile | 600   | Tersoff | 0       | 135.3   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 4       | < 111 > | 56     | P-Tensile  | 600   | Tersoff | 0       | 145.9   |
| 5       | < 111 > | 70     | P-Tensile  | 600   | Tersoff | 0       | 149.3   |
| 6       | < 111 > | 84     | P-Tensile  | 600   | Tersoff | 0       | 151.0   |
| 7       | < 111 > | 98     | P-Tensile  | 600   | Tersoff | 0       | 150.4   |
| 8       | < 111 > | 112    | P-Tensile  | 600   | Tersoff | 0       | 146.9   |
| 9       | < 111 > | 126    | P-Tensile  | 600   | Tersoff | 0       | 151.9   |
| 10      | < 111 > | 140    | P-Tensile  | 600   | Tersoff | 0       | 154.3   |
| 2       | < 111 > | 32     | P-Tensile  | 600   | Tersoff | 0       | 137.9   |
| 3       | < 111 > | 48     | P-Tensile  | 600   | Tersoff | 0       | 135.7   |
| 4       | < 111 > | 64     | P-Tensile  | 600   | Tersoff | 0       | 144.9   |
| 5       | < 111 > | 80     | P-Tensile  | 600   | Tersoff | 0       | 148.3   |
| 6       | < 111 > | 96     | P-Tensile  | 600   | Tersoff | 0       | 150.3   |
| 7       | < 111 > | 112    | P-Tensile  | 600   | Tersoff | 0       | 151.8   |
| 8       | < 111 > | 128    | P-Tensile  | 600   | Tersoff | 0       | 147.0   |
| 9       | < 111 > | 144    | P-Tensile  | 600   | Tersoff | 0       | 151.4   |
| 10      | < 111 > | 160    | P-Tensile  | 600   | Tersoff | 0       | 154.6   |
| 2       | < 111 > | 36     | P-Tensile  | 600   | Tersoff | 0       | 135.4   |
| 3       | < 111 > | 54     | P-Tensile  | 600   | Tersoff | 0       | 136.4   |
| 4       | < 111 > | 72     | P-Tensile  | 600   | Tersoff | 0       | 145.1   |
| 5       | < 111 > | 90     | P-Tensile  | 600   | Tersoff | 0       | 150.2   |
| 6       | < 111 > | 108    | P-Tensile  | 600   | Tersoff | 0       | 150.0   |
| 7       | < 111 > | 126    | P-Tensile  | 600   | Tersoff | 0       | 151.5   |
| 8       | < 111 > | 144    | P-Tensile  | 600   | Tersoff | 0       | 147.3   |
| 9       | < 111 > | 162    | P-Tensile  | 600   | Tersoff | 0       | 151.3   |
| 10      | < 111 > | 180    | P-Tensile  | 600   | Tersoff | 0       | 154.8   |
| 2       | < 111 > | 40     | P-Tensile  | 600   | Tersoff | 0       | 138.9   |
| 3       | < 111 > | 60     | P-Tensile  | 600   | Tersoff | 0       | 135.1   |
| 4       | < 111 > | 80     | P-Tensile  | 600   | Tersoff | 0       | 143.4   |
| 5       | < 111 > | 100    | P-Tensile  | 600   | Tersoff | 0       | 148.6   |
| 6       | < 111 > | 120    | P-Tensile  | 600   | Tersoff | 0       | 142.5   |
| 7       | < 111 > | 140    | P-Tensile  | 600   | Tersoff | 0       | 150.6   |
| 8       | < 111 > | 160    | P-Tensile  | 600   | Tersoff | 0       | 147.7   |
| 9       | < 111 > | 180    | P-Tensile  | 600   | Tersoff | 0       | 151.4   |
| 10      | < 111 > | 200    | P-Tensile  | 600   | Tersoff | 0       | 153.5   |
| 2       | < 111 > | 14     | NP-Tensile | 600   | SW      | 0       | 116.5   |
| 3       | < 111 > | 21     | NP-Tensile | 600   | SW      | 0       | 160.2   |
| 4       | < 111 > | 28     | NP-Tensile | 600   | SW      | 0       | 168.9   |
| 5       | < 111 > | 35     | NP-Tensile | 600   | SW      | 0       | 176.7   |
| 6       | < 111 > | 42     | NP-Tensile | 600   | SW      | 0       | 180.4   |
| 7       | < 111 > | 49     | NP-Tensile | 600   | SW      | 0       | 184.3   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 8       | < 111 > | 56     | NP-Tensile | 600   | SW  | 0       | 186.0   |
| 9       | < 111 > | 63     | NP-Tensile | 600   | SW  | 0       | 188.4   |
| 10      | < 111 > | 70     | NP-Tensile | 600   | SW  | 0       | 189.2   |
| 2       | < 111 > | 16     | NP-Tensile | 600   | SW  | 0       | 121.1   |
| 3       | < 111 > | 24     | NP-Tensile | 600   | SW  | 0       | 155.1   |
| 4       | < 111 > | 32     | NP-Tensile | 600   | SW  | 0       | 169.2   |
| 5       | < 111 > | 40     | NP-Tensile | 600   | SW  | 0       | 176.0   |
| 6       | < 111 > | 48     | NP-Tensile | 600   | SW  | 0       | 180.5   |
| 7       | < 111 > | 56     | NP-Tensile | 600   | SW  | 0       | 184.0   |
| 8       | < 111 > | 64     | NP-Tensile | 600   | SW  | 0       | 186.4   |
| 9       | < 111 > | 72     | NP-Tensile | 600   | SW  | 0       | 187.9   |
| 10      | < 111 > | 80     | NP-Tensile | 600   | SW  | 0       | 188.9   |
| 2       | < 111 > | 18     | NP-Tensile | 600   | SW  | 0       | 127.4   |
| 3       | < 111 > | 27     | NP-Tensile | 600   | SW  | 0       | 155.7   |
| 4       | < 111 > | 36     | NP-Tensile | 600   | SW  | 0       | 169.3   |
| 5       | < 111 > | 45     | NP-Tensile | 600   | SW  | 0       | 178.9   |
| 6       | < 111 > | 54     | NP-Tensile | 600   | SW  | 0       | 182.3   |
| 7       | < 111 > | 63     | NP-Tensile | 600   | SW  | 0       | 184.6   |
| 8       | < 111 > | 72     | NP-Tensile | 600   | SW  | 0       | 186.5   |
| 9       | < 111 > | 81     | NP-Tensile | 600   | SW  | 0       | 187.6   |
| 10      | < 111 > | 90     | NP-Tensile | 600   | SW  | 0       | 188.6   |
| 2       | < 111 > | 20     | NP-Tensile | 600   | SW  | 0       | 124.4   |
| 3       | < 111 > | 30     | NP-Tensile | 600   | SW  | 0       | 156.8   |
| 4       | < 111 > | 40     | NP-Tensile | 600   | SW  | 0       | 169.2   |
| 5       | < 111 > | 50     | NP-Tensile | 600   | SW  | 0       | 177.9   |
| 6       | < 111 > | 60     | NP-Tensile | 600   | SW  | 0       | 181.8   |
| 7       | < 111 > | 70     | NP-Tensile | 600   | SW  | 0       | 184.0   |
| 8       | < 111 > | 80     | NP-Tensile | 600   | SW  | 0       | 185.8   |
| 9       | < 111 > | 90     | NP-Tensile | 600   | SW  | 0       | 187.2   |
| 10      | < 111 > | 100    | NP-Tensile | 600   | SW  | 0       | 188.9   |
| 2       | < 111 > | 24     | NP-Tensile | 600   | SW  | 0       | 119.0   |
| 3       | < 111 > | 36     | NP-Tensile | 600   | SW  | 0       | 155.3   |
| 4       | < 111 > | 48     | NP-Tensile | 600   | SW  | 0       | 169.9   |
| 5       | < 111 > | 60     | NP-Tensile | 600   | SW  | 0       | 178.0   |
| 6       | < 111 > | 72     | NP-Tensile | 600   | SW  | 0       | 181.2   |
| 7       | < 111 > | 84     | NP-Tensile | 600   | SW  | 0       | 183.6   |
| 8       | < 111 > | 96     | NP-Tensile | 600   | SW  | 0       | 186.0   |
| 9       | < 111 > | 108    | NP-Tensile | 600   | SW  | 0       | 187.8   |
| 10      | < 111 > | 120    | NP-Tensile | 600   | SW  | 0       | 189.2   |
| 2       | < 111 > | 28     | NP-Tensile | 600   | SW  | 0       | 125.6   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|-----|---------|---------|
| 3       | < 111 > | 42     | NP-Tensile | 600   | SW  | 0       | 155.0   |
| 4       | < 111 > | 56     | NP-Tensile | 600   | SW  | 0       | 169.4   |
| 5       | < 111 > | 70     | NP-Tensile | 600   | SW  | 0       | 176.9   |
| 6       | < 111 > | 84     | NP-Tensile | 600   | SW  | 0       | 180.7   |
| 7       | < 111 > | 98     | NP-Tensile | 600   | SW  | 0       | 184.1   |
| 8       | < 111 > | 112    | NP-Tensile | 600   | SW  | 0       | 186.1   |
| 9       | < 111 > | 126    | NP-Tensile | 600   | SW  | 0       | 181.8   |
| 10      | < 111 > | 140    | NP-Tensile | 600   | SW  | 0       | 187.2   |
| 2       | < 111 > | 32     | NP-Tensile | 600   | SW  | 0       | 122.3   |
| 3       | < 111 > | 48     | NP-Tensile | 600   | SW  | 0       | 154.4   |
| 4       | < 111 > | 64     | NP-Tensile | 600   | SW  | 0       | 168.9   |
| 5       | < 111 > | 80     | NP-Tensile | 600   | SW  | 0       | 178.2   |
| 6       | < 111 > | 96     | NP-Tensile | 600   | SW  | 0       | 181.0   |
| 7       | < 111 > | 112    | NP-Tensile | 600   | SW  | 0       | 184.1   |
| 8       | < 111 > | 128    | NP-Tensile | 600   | SW  | 0       | 186.4   |
| 9       | < 111 > | 144    | NP-Tensile | 600   | SW  | 0       | 187.8   |
| 10      | < 111 > | 160    | NP-Tensile | 600   | SW  | 0       | 189.2   |
| 2       | < 111 > | 36     | NP-Tensile | 600   | SW  | 0       | 112.2   |
| 3       | < 111 > | 54     | NP-Tensile | 600   | SW  | 0       | 154.0   |
| 4       | < 111 > | 72     | NP-Tensile | 600   | SW  | 0       | 169.1   |
| 5       | < 111 > | 90     | NP-Tensile | 600   | SW  | 0       | 177.3   |
| 6       | < 111 > | 108    | NP-Tensile | 600   | SW  | 0       | 181.2   |
| 7       | < 111 > | 126    | NP-Tensile | 600   | SW  | 0       | 184.3   |
| 8       | < 111 > | 144    | NP-Tensile | 600   | SW  | 0       | 186.2   |
| 9       | < 111 > | 162    | NP-Tensile | 600   | SW  | 0       | 187.7   |
| 10      | < 111 > | 180    | NP-Tensile | 600   | SW  | 0       | 187.5   |
| 2       | < 111 > | 40     | NP-Tensile | 600   | SW  | 0       | 121.7   |
| 3       | < 111 > | 60     | NP-Tensile | 600   | SW  | 0       | 153.6   |
| 4       | < 111 > | 80     | NP-Tensile | 600   | SW  | 0       | 169.0   |
| 5       | < 111 > | 100    | NP-Tensile | 600   | SW  | 0       | 177.0   |
| 6       | < 111 > | 120    | NP-Tensile | 600   | SW  | 0       | 181.0   |
| 7       | < 111 > | 140    | NP-Tensile | 600   | SW  | 0       | 184.0   |
| 8       | < 111 > | 160    | NP-Tensile | 600   | SW  | 0       | 186.6   |
| 9       | < 111 > | 180    | NP-Tensile | 600   | SW  | 0       | 188.3   |
| 10      | < 111 > | 200    | NP-Tensile | 600   | SW  | 0       | 188.3   |
| 2       | < 111 > | 14     | P-Tensile  | 600   | SW  | 0       | 90.6    |
| 3       | < 111 > | 21     | P-Tensile  | 600   | SW  | 0       | 90.6    |
| 4       | < 111 > | 28     | P-Tensile  | 600   | SW  | 0       | 84.0    |
| 5       | < 111 > | 35     | P-Tensile  | 600   | SW  | 0       | 119.2   |
| 6       | < 111 > | 42     | P-Tensile  | 600   | SW  | 0       | 126.9   |



Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|-----|---------|---------|
| 7       | < 111 > | 49     | P-Tensile | 600   | SW  | 0       | 127.1   |
| 8       | < 111 > | 56     | P-Tensile | 600   | SW  | 0       | 132.3   |
| 9       | < 111 > | 63     | P-Tensile | 600   | SW  | 0       | 131.2   |
| 10      | < 111 > | 70     | P-Tensile | 600   | SW  | 0       | 135.6   |
| 2       | < 111 > | 16     | P-Tensile | 600   | SW  | 0       | 114.7   |
| 3       | < 111 > | 24     | P-Tensile | 600   | SW  | 0       | 111.4   |
| 4       | < 111 > | 32     | P-Tensile | 600   | SW  | 0       | 122.6   |
| 5       | < 111 > | 40     | P-Tensile | 600   | SW  | 0       | 128.4   |
| 6       | < 111 > | 48     | P-Tensile | 600   | SW  | 0       | 129.7   |
| 7       | < 111 > | 56     | P-Tensile | 600   | SW  | 0       | 130.2   |
| 8       | < 111 > | 64     | P-Tensile | 600   | SW  | 0       | 133.9   |
| 9       | < 111 > | 72     | P-Tensile | 600   | SW  | 0       | 133.7   |
| 10      | < 111 > | 80     | P-Tensile | 600   | SW  | 0       | 137.6   |
| 2       | < 111 > | 18     | P-Tensile | 600   | SW  | 0       | 100.2   |
| 3       | < 111 > | 27     | P-Tensile | 600   | SW  | 0       | 110.7   |
| 4       | < 111 > | 36     | P-Tensile | 600   | SW  | 0       | 124.7   |
| 5       | < 111 > | 45     | P-Tensile | 600   | SW  | 0       | 127.3   |
| 6       | < 111 > | 54     | P-Tensile | 600   | SW  | 0       | 127.7   |
| 7       | < 111 > | 63     | P-Tensile | 600   | SW  | 0       | 131.9   |
| 8       | < 111 > | 72     | P-Tensile | 600   | SW  | 0       | 130.1   |
| 9       | < 111 > | 81     | P-Tensile | 600   | SW  | 0       | 134.7   |
| 10      | < 111 > | 90     | P-Tensile | 600   | SW  | 0       | 137.1   |
| 2       | < 111 > | 20     | P-Tensile | 600   | SW  | 0       | 106.1   |
| 3       | < 111 > | 30     | P-Tensile | 600   | SW  | 0       | 108.1   |
| 4       | < 111 > | 40     | P-Tensile | 600   | SW  | 0       | 126.6   |
| 5       | < 111 > | 50     | P-Tensile | 600   | SW  | 0       | 127.7   |
| 6       | < 111 > | 60     | P-Tensile | 600   | SW  | 0       | 129.9   |
| 7       | < 111 > | 70     | P-Tensile | 600   | SW  | 0       | 130.8   |
| 8       | < 111 > | 80     | P-Tensile | 600   | SW  | 0       | 131.9   |
| 9       | < 111 > | 90     | P-Tensile | 600   | SW  | 0       | 133.7   |
| 10      | < 111 > | 100    | P-Tensile | 600   | SW  | 0       | 136.4   |
| 2       | < 111 > | 24     | P-Tensile | 600   | SW  | 0       | 102.6   |
| 3       | < 111 > | 36     | P-Tensile | 600   | SW  | 0       | 112.8   |
| 4       | < 111 > | 48     | P-Tensile | 600   | SW  | 0       | 123.8   |
| 5       | < 111 > | 60     | P-Tensile | 600   | SW  | 0       | 129.2   |
| 6       | < 111 > | 72     | P-Tensile | 600   | SW  | 0       | 130.6   |
| 7       | < 111 > | 84     | P-Tensile | 600   | SW  | 0       | 130.9   |
| 8       | < 111 > | 96     | P-Tensile | 600   | SW  | 0       | 134.4   |
| 9       | < 111 > | 108    | P-Tensile | 600   | SW  | 0       | 136.4   |
| 10      | < 111 > | 120    | P-Tensile | 600   | SW  | 0       | 138.2   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 2       | < 111 > | 28     | P-Tensile  | 600   | SW      | 0       | 107.1   |
| 3       | < 111 > | 42     | P-Tensile  | 600   | SW      | 0       | 109.9   |
| 4       | < 111 > | 56     | P-Tensile  | 600   | SW      | 0       | 126.8   |
| 5       | < 111 > | 70     | P-Tensile  | 600   | SW      | 0       | 130.9   |
| 6       | < 111 > | 84     | P-Tensile  | 600   | SW      | 0       | 131.5   |
| 7       | < 111 > | 98     | P-Tensile  | 600   | SW      | 0       | 132.3   |
| 8       | < 111 > | 112    | P-Tensile  | 600   | SW      | 0       | 132.4   |
| 9       | < 111 > | 126    | P-Tensile  | 600   | SW      | 0       | 134.6   |
| 10      | < 111 > | 140    | P-Tensile  | 600   | SW      | 0       | 137.1   |
| 2       | < 111 > | 32     | P-Tensile  | 600   | SW      | 0       | 106.7   |
| 3       | < 111 > | 48     | P-Tensile  | 600   | SW      | 0       | 113.7   |
| 4       | < 111 > | 64     | P-Tensile  | 600   | SW      | 0       | 125.0   |
| 5       | < 111 > | 80     | P-Tensile  | 600   | SW      | 0       | 130.8   |
| 6       | < 111 > | 96     | P-Tensile  | 600   | SW      | 0       | 130.0   |
| 7       | < 111 > | 112    | P-Tensile  | 600   | SW      | 0       | 132.2   |
| 8       | < 111 > | 128    | P-Tensile  | 600   | SW      | 0       | 133.9   |
| 9       | < 111 > | 144    | P-Tensile  | 600   | SW      | 0       | 134.8   |
| 10      | < 111 > | 160    | P-Tensile  | 600   | SW      | 0       | 137.1   |
| 2       | < 111 > | 36     | P-Tensile  | 600   | SW      | 0       | 106.5   |
| 3       | < 111 > | 54     | P-Tensile  | 600   | SW      | 0       | 113.5   |
| 4       | < 111 > | 72     | P-Tensile  | 600   | SW      | 0       | 127.1   |
| 5       | < 111 > | 90     | P-Tensile  | 600   | SW      | 0       | 130.6   |
| 6       | < 111 > | 108    | P-Tensile  | 600   | SW      | 0       | 130.5   |
| 7       | < 111 > | 126    | P-Tensile  | 600   | SW      | 0       | 131.8   |
| 8       | < 111 > | 144    | P-Tensile  | 600   | SW      | 0       | 132.2   |
| 9       | < 111 > | 162    | P-Tensile  | 600   | SW      | 0       | 134.3   |
| 10      | < 111 > | 180    | P-Tensile  | 600   | SW      | 0       | 137.5   |
| 2       | < 111 > | 40     | P-Tensile  | 600   | SW      | 0       | 106.3   |
| 3       | < 111 > | 60     | P-Tensile  | 600   | SW      | 0       | 109.7   |
| 4       | < 111 > | 80     | P-Tensile  | 600   | SW      | 0       | 121.9   |
| 5       | < 111 > | 100    | P-Tensile  | 600   | SW      | 0       | 130.9   |
| 6       | < 111 > | 120    | P-Tensile  | 600   | SW      | 0       | 128.9   |
| 7       | < 111 > | 140    | P-Tensile  | 600   | SW      | 0       | 129.5   |
| 8       | < 111 > | 160    | P-Tensile  | 600   | SW      | 0       | 132.0   |
| 9       | < 111 > | 180    | P-Tensile  | 600   | SW      | 0       | 134.7   |
| 10      | < 111 > | 200    | P-Tensile  | 600   | SW      | 0       | 137.3   |
| 5       | < 100 > | 100    | NP-Tensile | 10    | Tersoff | 5       | 82.7    |
| 5       | < 110 > | 100    | NP-Tensile | 10    | Tersoff | 5       | 130.5   |
| 5       | < 100 > | 35     | P-Tensile  | 10    | Tersoff | 5       | 63.8    |
| 5       | < 100 > | 50     | P-Tensile  | 10    | Tersoff | 5       | 63.6    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|---------|---------|---------|
| 5       | < 100 > | 75     | P-Tensile | 10    | Tersoff | 5       | 63.5    |
| 5       | < 100 > | 100    | P-Tensile | 10    | Tersoff | 5       | 63.4    |
| 5       | < 100 > | 125    | P-Tensile | 10    | Tersoff | 5       | 63.3    |
| 5       | < 100 > | 150    | P-Tensile | 10    | Tersoff | 5       | 63.3    |
| 5       | < 100 > | 175    | P-Tensile | 10    | Tersoff | 5       | 63.3    |
| 5       | < 100 > | 200    | P-Tensile | 10    | Tersoff | 5       | 63.5    |
| 6       | < 100 > | 42     | P-Tensile | 10    | Tersoff | 10      | 58.1    |
| 6       | < 100 > | 60     | P-Tensile | 10    | Tersoff | 10      | 58.5    |
| 6       | < 100 > | 90     | P-Tensile | 10    | Tersoff | 10      | 54.4    |
| 6       | < 100 > | 120    | P-Tensile | 10    | Tersoff | 10      | 54.7    |
| 6       | < 100 > | 150    | P-Tensile | 10    | Tersoff | 10      | 54.7    |
| 6       | < 100 > | 180    | P-Tensile | 10    | Tersoff | 10      | 54.6    |
| 6       | < 100 > | 210    | P-Tensile | 10    | Tersoff | 10      | 54.4    |
| 6       | < 100 > | 240    | P-Tensile | 10    | Tersoff | 10      | 54.6    |
| 8       | < 100 > | 56     | P-Tensile | 10    | Tersoff | 5       | 72.9    |
| 8       | < 100 > | 80     | P-Tensile | 10    | Tersoff | 5       | 72.7    |
| 8       | < 100 > | 120    | P-Tensile | 10    | Tersoff | 5       | 72.3    |
| 8       | < 100 > | 160    | P-Tensile | 10    | Tersoff | 5       | 72.8    |
| 8       | < 100 > | 200    | P-Tensile | 10    | Tersoff | 5       | 72.9    |
| 8       | < 100 > | 240    | P-Tensile | 10    | Tersoff | 5       | 72.5    |
| 8       | < 100 > | 280    | P-Tensile | 10    | Tersoff | 5       | 72.6    |
| 8       | < 100 > | 320    | P-Tensile | 10    | Tersoff | 5       | 72.6    |
| 9       | < 100 > | 63     | P-Tensile | 10    | Tersoff | 10      | 66.2    |
| 9       | < 100 > | 90     | P-Tensile | 10    | Tersoff | 10      | 65.8    |
| 9       | < 100 > | 135    | P-Tensile | 10    | Tersoff | 10      | 65.5    |
| 9       | < 100 > | 180    | P-Tensile | 10    | Tersoff | 10      | 65.8    |
| 9       | < 100 > | 225    | P-Tensile | 10    | Tersoff | 10      | 65.7    |
| 9       | < 100 > | 270    | P-Tensile | 10    | Tersoff | 10      | 65.8    |
| 9       | < 100 > | 31.5   | P-Tensile | 10    | Tersoff | 10      | 65.7    |
| 9       | < 100 > | 360    | P-Tensile | 10    | Tersoff | 10      | 65.8    |
| 5       | < 110 > | 35     | P-Tensile | 10    | Tersoff | 5       | 102.2   |
| 5       | < 110 > | 50     | P-Tensile | 10    | Tersoff | 5       | 101.7   |
| 5       | < 110 > | 75     | P-Tensile | 10    | Tersoff | 5       | 101.7   |
| 5       | < 110 > | 100    | P-Tensile | 10    | Tersoff | 5       | 101.6   |
| 5       | < 110 > | 125    | P-Tensile | 10    | Tersoff | 5       | 101.7   |
| 5       | < 110 > | 150    | P-Tensile | 10    | Tersoff | 5       | 101.8   |
| 5       | < 110 > | 175    | P-Tensile | 10    | Tersoff | 5       | 101.9   |
| 5       | < 110 > | 200    | P-Tensile | 10    | Tersoff | 5       | 101.2   |
| 6       | < 110 > | 42     | P-Tensile | 10    | Tersoff | 10      | 83.6    |
| 6       | < 110 > | 60     | P-Tensile | 10    | Tersoff | 10      | 84.1    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|---------|---------|---------|
| 6       | < 110 > | 90     | P-Tensile | 10    | Tersoff | 10      | 80.5    |
| 6       | < 110 > | 120    | P-Tensile | 10    | Tersoff | 10      | 80.5    |
| 6       | < 110 > | 150    | P-Tensile | 10    | Tersoff | 10      | 80.4    |
| 6       | < 110 > | 180    | P-Tensile | 10    | Tersoff | 10      | 80.7    |
| 6       | < 110 > | 210    | P-Tensile | 10    | Tersoff | 10      | 80.6    |
| 6       | < 110 > | 240    | P-Tensile | 10    | Tersoff | 10      | 80.4    |
| 8       | < 110 > | 56     | P-Tensile | 10    | Tersoff | 5       | 116.7   |
| 8       | < 110 > | 80     | P-Tensile | 10    | Tersoff | 5       | 116.8   |
| 8       | < 110 > | 120    | P-Tensile | 10    | Tersoff | 5       | 116.5   |
| 8       | < 110 > | 160    | P-Tensile | 10    | Tersoff | 5       | 116.8   |
| 8       | < 110 > | 200    | P-Tensile | 10    | Tersoff | 5       | 116.8   |
| 8       | < 110 > | 240    | P-Tensile | 10    | Tersoff | 5       | 116.6   |
| 8       | < 110 > | 280    | P-Tensile | 10    | Tersoff | 5       | 116.6   |
| 8       | < 110 > | 320    | P-Tensile | 10    | Tersoff | 5       | 116.6   |
| 9       | < 110 > | 63     | P-Tensile | 10    | Tersoff | 10      | 97.6    |
| 9       | < 110 > | 90     | P-Tensile | 10    | Tersoff | 10      | 96.8    |
| 9       | < 110 > | 135    | P-Tensile | 10    | Tersoff | 10      | 97.0    |
| 9       | < 110 > | 180    | P-Tensile | 10    | Tersoff | 10      | 96.9    |
| 9       | < 110 > | 225    | P-Tensile | 10    | Tersoff | 10      | 96.9    |
| 9       | < 110 > | 270    | P-Tensile | 10    | Tersoff | 10      | 96.9    |
| 9       | < 110 > | 31.5   | P-Tensile | 10    | Tersoff | 10      | 96.9    |
| 9       | < 110 > | 360    | P-Tensile | 10    | Tersoff | 10      | 96.9    |
| 5       | < 100 > | 35     | P-Tensile | 10    | SW      | 5       | 75.5    |
| 5       | < 100 > | 50     | P-Tensile | 10    | SW      | 5       | 73.6    |
| 5       | < 100 > | 75     | P-Tensile | 10    | SW      | 5       | 73.0    |
| 5       | < 100 > | 100    | P-Tensile | 10    | SW      | 5       | 73.2    |
| 5       | < 100 > | 125    | P-Tensile | 10    | SW      | 5       | 73.4    |
| 5       | < 100 > | 150    | P-Tensile | 10    | SW      | 5       | 73.7    |
| 5       | < 100 > | 175    | P-Tensile | 10    | SW      | 5       | 73.3    |
| 5       | < 100 > | 200    | P-Tensile | 10    | SW      | 5       | 73.2    |
| 6       | < 100 > | 42     | P-Tensile | 10    | SW      | 10      | 78.9    |
| 6       | < 100 > | 60     | P-Tensile | 10    | SW      | 10      | 80.6    |
| 6       | < 100 > | 90     | P-Tensile | 10    | SW      | 10      | 72.2    |
| 6       | < 100 > | 120    | P-Tensile | 10    | SW      | 10      | 72.8    |
| 6       | < 100 > | 150    | P-Tensile | 10    | SW      | 10      | 72.4    |
| 6       | < 100 > | 180    | P-Tensile | 10    | SW      | 10      | 72.6    |
| 6       | < 100 > | 210    | P-Tensile | 10    | SW      | 10      | 72.5    |
| 6       | < 100 > | 240    | P-Tensile | 10    | SW      | 10      | 72.5    |
| 8       | < 100 > | 56     | P-Tensile | 10    | SW      | 5       | 73.5    |
| 8       | < 100 > | 80     | P-Tensile | 10    | SW      | 5       | 72.8    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC        | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|-----------|-------|-----|---------|---------|
| 8       | < 100 > | 120    | P-Tensile | 10    | SW  | 5       | 73.2    |
| 8       | < 100 > | 160    | P-Tensile | 10    | SW  | 5       | 73.2    |
| 8       | < 100 > | 200    | P-Tensile | 10    | SW  | 5       | 72.9    |
| 8       | < 100 > | 240    | P-Tensile | 10    | SW  | 5       | 73.1    |
| 8       | < 100 > | 280    | P-Tensile | 10    | SW  | 5       | 73.2    |
| 8       | < 100 > | 320    | P-Tensile | 10    | SW  | 5       | 73.2    |
| 9       | < 100 > | 63     | P-Tensile | 10    | SW  | 10      | 81.5    |
| 9       | < 100 > | 90     | P-Tensile | 10    | SW  | 10      | 81.5    |
| 9       | < 100 > | 135    | P-Tensile | 10    | SW  | 10      | 81.4    |
| 9       | < 100 > | 180    | P-Tensile | 10    | SW  | 10      | 81.3    |
| 9       | < 100 > | 225    | P-Tensile | 10    | SW  | 10      | 81.3    |
| 9       | < 100 > | 270    | P-Tensile | 10    | SW  | 10      | 81.5    |
| 9       | < 100 > | 31.5   | P-Tensile | 10    | SW  | 10      | 81.1    |
| 9       | < 100 > | 360    | P-Tensile | 10    | SW  | 10      | 81.2    |
| 5       | < 110 > | 35     | P-Tensile | 10    | SW  | 5       | 92.1    |
| 5       | < 110 > | 50     | P-Tensile | 10    | SW  | 5       | 92.0    |
| 5       | < 110 > | 75     | P-Tensile | 10    | SW  | 5       | 91.8    |
| 5       | < 110 > | 100    | P-Tensile | 10    | SW  | 5       | 91.7    |
| 5       | < 110 > | 125    | P-Tensile | 10    | SW  | 5       | 91.6    |
| 5       | < 110 > | 150    | P-Tensile | 10    | SW  | 5       | 91.4    |
| 5       | < 110 > | 175    | P-Tensile | 10    | SW  | 5       | 91.6    |
| 5       | < 110 > | 200    | P-Tensile | 10    | SW  | 5       | 91.5    |
| 6       | < 110 > | 42     | P-Tensile | 10    | SW  | 10      | 93.5    |
| 6       | < 110 > | 60     | P-Tensile | 10    | SW  | 10      | 94.5    |
| 6       | < 110 > | 90     | P-Tensile | 10    | SW  | 10      | 86.8    |
| 6       | < 110 > | 120    | P-Tensile | 10    | SW  | 10      | 86.9    |
| 6       | < 110 > | 150    | P-Tensile | 10    | SW  | 10      | 86.9    |
| 6       | < 110 > | 180    | P-Tensile | 10    | SW  | 10      | 87.2    |
| 6       | < 110 > | 210    | P-Tensile | 10    | SW  | 10      | 87.2    |
| 6       | < 110 > | 240    | P-Tensile | 10    | SW  | 10      | 87.2    |
| 8       | < 110 > | 56     | P-Tensile | 10    | SW  | 5       | 106.3   |
| 8       | < 110 > | 80     | P-Tensile | 10    | SW  | 5       | 106.3   |
| 8       | < 110 > | 120    | P-Tensile | 10    | SW  | 5       | 106.0   |
| 8       | < 110 > | 160    | P-Tensile | 10    | SW  | 5       | 106.2   |
| 8       | < 110 > | 200    | P-Tensile | 10    | SW  | 5       | 106.0   |
| 8       | < 110 > | 240    | P-Tensile | 10    | SW  | 5       | 106.1   |
| 8       | < 110 > | 280    | P-Tensile | 10    | SW  | 5       | 106.1   |
| 8       | < 110 > | 320    | P-Tensile | 10    | SW  | 5       | 106.0   |
| 9       | < 110 > | 63     | P-Tensile | 10    | SW  | 10      | 98.6    |
| 9       | < 110 > | 90     | P-Tensile | 10    | SW  | 10      | 98.4    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 9       | < 110 > | 135    | P-Tensile  | 10    | SW      | 10      | 98.6    |
| 9       | < 110 > | 180    | P-Tensile  | 10    | SW      | 10      | 98.3    |
| 9       | < 110 > | 225    | P-Tensile  | 10    | SW      | 10      | 98.2    |
| 9       | < 110 > | 270    | P-Tensile  | 10    | SW      | 10      | 98.4    |
| 9       | < 110 > | 31.5   | P-Tensile  | 10    | SW      | 10      | 98.0    |
| 9       | < 110 > | 360    | P-Tensile  | 10    | SW      | 10      | 98.1    |
| 4.5     | < 100 > | 90     | P-Tensile  | 10    | Tersoff | 2.5     | 71.1    |
| 5       | < 100 > | 100    | P-Tensile  | 10    | Tersoff | 5       | 63.8    |
| 5.5     | < 100 > | 110    | P-Tensile  | 10    | Tersoff | 7.5     | 55.8    |
| 6       | < 100 > | 120    | P-Tensile  | 10    | Tersoff | 10      | 54.8    |
| 4.5     | < 110 > | 90     | P-Tensile  | 10    | Tersoff | 2.5     | 118.4   |
| 5       | < 110 > | 100    | P-Tensile  | 10    | Tersoff | 5       | 102.1   |
| 5.5     | < 110 > | 110    | P-Tensile  | 10    | Tersoff | 7.5     | 86.0    |
| 6       | < 110 > | 120    | P-Tensile  | 10    | Tersoff | 10      | 80.5    |
| 4.5     | < 100 > | 90     | P-Tensile  | 10    | SW      | 2.5     | 80.5    |
| 5       | < 100 > | 100    | P-Tensile  | 10    | SW      | 5       | 73.7    |
| 5.5     | < 100 > | 110    | P-Tensile  | 10    | SW      | 7.5     | 69.2    |
| 6       | < 100 > | 120    | P-Tensile  | 10    | SW      | 10      | 72.6    |
| 4.5     | < 110 > | 90     | P-Tensile  | 10    | SW      | 2.5     | 103.4   |
| 5       | < 110 > | 100    | P-Tensile  | 10    | SW      | 5       | 92.0    |
| 5.5     | < 110 > | 110    | P-Tensile  | 10    | SW      | 7.5     | 85.4    |
| 6       | < 110 > | 120    | P-Tensile  | 10    | SW      | 10      | 84.2    |
| 4       | < 100 > | 28     | NP-Tensile | 10    | Tersoff | 5       | 88.5    |
| 4       | < 100 > | 40     | NP-Tensile | 10    | Tersoff | 5       | 77.4    |
| 4       | < 100 > | 48     | NP-Tensile | 10    | Tersoff | 5       | 73.8    |
| 4       | < 100 > | 60     | NP-Tensile | 10    | Tersoff | 5       | 73.6    |
| 4       | < 100 > | 80     | NP-Tensile | 10    | Tersoff | 5       | 73.5    |
| 4       | < 100 > | 100    | NP-Tensile | 10    | Tersoff | 5       | 73.8    |
| 6       | < 100 > | 42     | NP-Tensile | 10    | Tersoff | 5       | 103.2   |
| 6       | < 100 > | 60     | NP-Tensile | 10    | Tersoff | 5       | 90.9    |
| 6       | < 100 > | 72     | NP-Tensile | 10    | Tersoff | 5       | 87.8    |
| 6       | < 100 > | 90     | NP-Tensile | 10    | Tersoff | 5       | 87.9    |
| 6       | < 100 > | 120    | NP-Tensile | 10    | Tersoff | 5       | 87.7    |
| 6       | < 100 > | 150    | NP-Tensile | 10    | Tersoff | 5       | 87.8    |
| 8       | < 100 > | 56     | NP-Tensile | 10    | Tersoff | 5       | 95.7    |
| 8       | < 100 > | 80     | NP-Tensile | 10    | Tersoff | 5       | 95.7    |
| 8       | < 100 > | 96     | NP-Tensile | 10    | Tersoff | 5       | 96.0    |
| 8       | < 100 > | 120    | NP-Tensile | 10    | Tersoff | 5       | 95.9    |
| 8       | < 100 > | 160    | NP-Tensile | 10    | Tersoff | 5       | 95.5    |
| 8       | < 100 > | 200    | NP-Tensile | 10    | Tersoff | 5       | 95.3    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 4       | < 110 > | 28     | NP-Tensile | 10    | Tersoff | 5       | 108.8   |
| 4       | < 110 > | 40     | NP-Tensile | 10    | Tersoff | 5       | 95.7    |
| 4       | < 110 > | 48     | NP-Tensile | 10    | Tersoff | 5       | 91.6    |
| 4       | < 110 > | 60     | NP-Tensile | 10    | Tersoff | 5       | 92.3    |
| 4       | < 110 > | 80     | NP-Tensile | 10    | Tersoff | 5       | 92.0    |
| 4       | < 110 > | 100    | NP-Tensile | 10    | Tersoff | 5       | 92.3    |
| 6       | < 110 > | 42     | NP-Tensile | 10    | Tersoff | 5       | 127.2   |
| 6       | < 110 > | 60     | NP-Tensile | 10    | Tersoff | 5       | 112.9   |
| 6       | < 110 > | 72     | NP-Tensile | 10    | Tersoff | 5       | 107.4   |
| 6       | < 110 > | 90     | NP-Tensile | 10    | Tersoff | 5       | 108.8   |
| 6       | < 110 > | 120    | NP-Tensile | 10    | Tersoff | 5       | 107.8   |
| 6       | < 110 > | 150    | NP-Tensile | 10    | Tersoff | 5       | 107.9   |
| 8       | < 110 > | 56     | NP-Tensile | 10    | Tersoff | 5       | 119.1   |
| 8       | < 110 > | 80     | NP-Tensile | 10    | Tersoff | 5       | 118.8   |
| 8       | < 110 > | 96     | NP-Tensile | 10    | Tersoff | 5       | 118.5   |
| 8       | < 110 > | 120    | NP-Tensile | 10    | Tersoff | 5       | 118.6   |
| 8       | < 110 > | 160    | NP-Tensile | 10    | Tersoff | 5       | 118.3   |
| 8       | < 110 > | 200    | NP-Tensile | 10    | Tersoff | 5       | 118.4   |
| 4       | < 111 > | 28     | NP-Tensile | 10    | Tersoff | 5       | 113.6   |
| 4       | < 111 > | 40     | NP-Tensile | 10    | Tersoff | 5       | 99.7    |
| 4       | < 111 > | 48     | NP-Tensile | 10    | Tersoff | 5       | 97.4    |
| 4       | < 111 > | 60     | NP-Tensile | 10    | Tersoff | 5       | 97.1    |
| 4       | < 111 > | 80     | NP-Tensile | 10    | Tersoff | 5       | 96.6    |
| 4       | < 111 > | 100    | NP-Tensile | 10    | Tersoff | 5       | 97.0    |
| 6       | < 111 > | 42     | NP-Tensile | 10    | Tersoff | 5       | 138.3   |
| 6       | < 111 > | 60     | NP-Tensile | 10    | Tersoff | 5       | 122.0   |
| 6       | < 111 > | 72     | NP-Tensile | 10    | Tersoff | 5       | 117.3   |
| 6       | < 111 > | 90     | NP-Tensile | 10    | Tersoff | 5       | 116.8   |
| 6       | < 111 > | 120    | NP-Tensile | 10    | Tersoff | 5       | 117.1   |
| 6       | < 111 > | 150    | NP-Tensile | 10    | Tersoff | 5       | 117.0   |
| 8       | < 111 > | 56     | NP-Tensile | 10    | Tersoff | 5       | 130.2   |
| 8       | < 111 > | 80     | NP-Tensile | 10    | Tersoff | 5       | 129.8   |
| 8       | < 111 > | 96     | NP-Tensile | 10    | Tersoff | 5       | 129.8   |
| 8       | < 111 > | 120    | NP-Tensile | 10    | Tersoff | 5       | 129.8   |
| 8       | < 111 > | 160    | NP-Tensile | 10    | Tersoff | 5       | 129.4   |
| 8       | < 111 > | 200    | NP-Tensile | 10    | Tersoff | 5       | 129.5   |
| 4       | < 100 > | 40     | NP-Tensile | 10    | Tersoff | 5       | 77.4    |
| 4       | < 100 > | 40     | NP-Tensile | 300   | Tersoff | 5       | 74.4    |
| 4       | < 100 > | 40     | NP-Tensile | 600   | Tersoff | 5       | 70.3    |
| 4       | < 100 > | 40     | NP-Tensile | 900   | Tersoff | 5       | 61.5    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 4       | < 100 > | 40     | NP-Tensile | 1200  | Tersoff | 5       | 57.5    |
| 6       | < 100 > | 60     | NP-Tensile | 10    | Tersoff | 5       | 90.9    |
| 6       | < 100 > | 60     | NP-Tensile | 300   | Tersoff | 5       | 85.8    |
| 6       | < 100 > | 60     | NP-Tensile | 600   | Tersoff | 5       | 81.1    |
| 6       | < 100 > | 60     | NP-Tensile | 900   | Tersoff | 5       | 71.1    |
| 6       | < 100 > | 60     | NP-Tensile | 1200  | Tersoff | 5       | 55.0    |
| 8       | < 100 > | 80     | NP-Tensile | 10    | Tersoff | 5       | 95.7    |
| 8       | < 100 > | 80     | NP-Tensile | 300   | Tersoff | 5       | 92.6    |
| 8       | < 100 > | 80     | NP-Tensile | 600   | Tersoff | 5       | 87.9    |
| 8       | < 100 > | 80     | NP-Tensile | 900   | Tersoff | 5       | 80.7    |
| 8       | < 100 > | 80     | NP-Tensile | 1200  | Tersoff | 5       | 72.6    |
| 4       | < 110 > | 40     | NP-Tensile | 10    | Tersoff | 5       | 95.7    |
| 4       | < 110 > | 40     | NP-Tensile | 300   | Tersoff | 5       | 91.4    |
| 4       | < 110 > | 40     | NP-Tensile | 600   | Tersoff | 5       | 85.1    |
| 4       | < 110 > | 40     | NP-Tensile | 900   | Tersoff | 5       | 77.7    |
| 4       | < 110 > | 40     | NP-Tensile | 1200  | Tersoff | 5       | 65.9    |
| 6       | < 110 > | 60     | NP-Tensile | 10    | Tersoff | 5       | 112.9   |
| 6       | < 110 > | 60     | NP-Tensile | 300   | Tersoff | 5       | 105.8   |
| 6       | < 110 > | 60     | NP-Tensile | 600   | Tersoff | 5       | 101.2   |
| 6       | < 110 > | 60     | NP-Tensile | 900   | Tersoff | 5       | 91.6    |
| 6       | < 110 > | 60     | NP-Tensile | 1200  | Tersoff | 5       | 71.5    |
| 8       | < 110 > | 80     | NP-Tensile | 10    | Tersoff | 5       | 118.8   |
| 8       | < 110 > | 80     | NP-Tensile | 300   | Tersoff | 5       | 115.3   |
| 8       | < 110 > | 80     | NP-Tensile | 600   | Tersoff | 5       | 111.3   |
| 8       | < 110 > | 80     | NP-Tensile | 900   | Tersoff | 5       | 102.1   |
| 8       | < 110 > | 80     | NP-Tensile | 1200  | Tersoff | 5       | 92.8    |
| 4       | < 111 > | 40     | NP-Tensile | 10    | Tersoff | 5       | 99.7    |
| 4       | < 111 > | 40     | NP-Tensile | 300   | Tersoff | 5       | 96.5    |
| 4       | < 111 > | 40     | NP-Tensile | 600   | Tersoff | 5       | 89.3    |
| 4       | < 111 > | 40     | NP-Tensile | 900   | Tersoff | 5       | 75.5    |
| 4       | < 111 > | 40     | NP-Tensile | 1200  | Tersoff | 5       | 67.3    |
| 6       | < 111 > | 60     | NP-Tensile | 10    | Tersoff | 5       | 122.0   |
| 6       | < 111 > | 60     | NP-Tensile | 300   | Tersoff | 5       | 115.1   |
| 6       | < 111 > | 60     | NP-Tensile | 600   | Tersoff | 5       | 109.3   |
| 6       | < 111 > | 60     | NP-Tensile | 900   | Tersoff | 5       | 97.2    |
| 6       | < 111 > | 60     | NP-Tensile | 1200  | Tersoff | 5       | 67.5    |
| 8       | < 111 > | 80     | NP-Tensile | 10    | Tersoff | 5       | 129.8   |
| 8       | < 111 > | 80     | NP-Tensile | 300   | Tersoff | 5       | 126.9   |
| 8       | < 111 > | 80     | NP-Tensile | 600   | Tersoff | 5       | 122.7   |
| 8       | < 111 > | 80     | NP-Tensile | 900   | Tersoff | 5       | 109.0   |



Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|------------|-------|---------|---------|---------|
| 8       | < 111 > | 80     | NP-Tensile | 1200  | Tersoff | 5       | 99.7    |
| 4       | < 100 > | 40     | NP-Tensile | 300   | Tersoff | 5       | 66.9    |
| 5       | < 100 > | 50     | NP-Tensile | 300   | Tersoff | 5       | 72.5    |
| 6       | < 100 > | 60     | NP-Tensile | 300   | Tersoff | 5       | 76.7    |
| 7       | < 100 > | 70     | NP-Tensile | 300   | Tersoff | 5       | 80.6    |
| 8       | < 100 > | 80     | NP-Tensile | 300   | Tersoff | 5       | 81.4    |
| 4       | < 100 > | 40     | NP-Tensile | 300   | Tersoff | 10      | 54.8    |
| 5       | < 100 > | 50     | NP-Tensile | 300   | Tersoff | 10      | 58.9    |
| 6       | < 100 > | 60     | NP-Tensile | 300   | Tersoff | 10      | 65.6    |
| 7       | < 100 > | 70     | NP-Tensile | 300   | Tersoff | 10      | 69.9    |
| 8       | < 100 > | 80     | NP-Tensile | 300   | Tersoff | 10      | 72.9    |
| 4       | < 100 > | 40     | NP-Tensile | 300   | SW      | 5       | 73.5    |
| 5       | < 100 > | 50     | NP-Tensile | 300   | SW      | 5       | 80.4    |
| 6       | < 100 > | 60     | NP-Tensile | 300   | SW      | 5       | 84.1    |
| 7       | < 100 > | 70     | NP-Tensile | 300   | SW      | 5       | 89.1    |
| 8       | < 100 > | 80     | NP-Tensile | 300   | SW      | 5       | 92.3    |
| 4       | < 100 > | 40     | NP-Tensile | 300   | SW      | 10      | 70.0    |
| 5       | < 100 > | 50     | NP-Tensile | 300   | SW      | 10      | 75.1    |
| 6       | < 100 > | 60     | NP-Tensile | 300   | SW      | 10      | 83.6    |
| 7       | < 100 > | 70     | NP-Tensile | 300   | SW      | 10      | 87.0    |
| 8       | < 100 > | 80     | NP-Tensile | 300   | SW      | 10      | 89.9    |
| 4       | < 110 > | 40     | NP-Tensile | 300   | Tersoff | 5       | 98.3    |
| 5       | < 110 > | 50     | NP-Tensile | 300   | Tersoff | 5       | 109.3   |
| 6       | < 110 > | 60     | NP-Tensile | 300   | Tersoff | 5       | 117.0   |
| 7       | < 110 > | 70     | NP-Tensile | 300   | Tersoff | 5       | 123.4   |
| 8       | < 110 > | 80     | NP-Tensile | 300   | Tersoff | 5       | 126.4   |
| 4       | < 110 > | 40     | NP-Tensile | 300   | Tersoff | 10      | 69.1    |
| 5       | < 110 > | 50     | NP-Tensile | 300   | Tersoff | 10      | 79.7    |
| 6       | < 110 > | 60     | NP-Tensile | 300   | Tersoff | 10      | 89.8    |
| 7       | < 110 > | 70     | NP-Tensile | 300   | Tersoff | 10      | 98.4    |
| 8       | < 110 > | 80     | NP-Tensile | 300   | Tersoff | 10      | 104.6   |
| 4       | < 110 > | 40     | NP-Tensile | 300   | SW      | 5       | 89.7    |
| 5       | < 110 > | 50     | NP-Tensile | 300   | SW      | 5       | 98.6    |
| 6       | < 110 > | 60     | NP-Tensile | 300   | SW      | 5       | 105.6   |
| 7       | < 110 > | 70     | NP-Tensile | 300   | SW      | 5       | 111.2   |
| 8       | < 110 > | 80     | NP-Tensile | 300   | SW      | 5       | 115.5   |
| 4       | < 110 > | 40     | NP-Tensile | 300   | SW      | 10      | 76.0    |
| 5       | < 110 > | 50     | NP-Tensile | 300   | SW      | 10      | 85.3    |
| 6       | < 110 > | 60     | NP-Tensile | 300   | SW      | 10      | 95.2    |
| 7       | < 110 > | 70     | NP-Tensile | 300   | SW      | 10      | 100.8   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT                  | L (nm) | BC         | T (K) | POT     | SS (nm) | E (GPa) |
|---------|-----------------------|--------|------------|-------|---------|---------|---------|
| 8       | $\langle 110 \rangle$ | 80     | NP-Tensile | 300   | SW      | 10      | 105.0   |
| 4       | $\langle 111 \rangle$ | 40     | NP-Tensile | 300   | Tersoff | 5       | 109.5   |
| 5       | $\langle 111 \rangle$ | 50     | NP-Tensile | 300   | Tersoff | 5       | 122.6   |
| 6       | $\langle 111 \rangle$ | 60     | NP-Tensile | 300   | Tersoff | 5       | 133.4   |
| 7       | $\langle 111 \rangle$ | 70     | NP-Tensile | 300   | Tersoff | 5       | 141.1   |
| 8       | $\langle 111 \rangle$ | 80     | NP-Tensile | 300   | Tersoff | 5       | 145.2   |
| 4       | $\langle 111 \rangle$ | 40     | NP-Tensile | 300   | Tersoff | 10      | 71.1    |
| 5       | $\langle 111 \rangle$ | 50     | NP-Tensile | 300   | Tersoff | 10      | 84.3    |
| 6       | $\langle 111 \rangle$ | 60     | NP-Tensile | 300   | Tersoff | 10      | 98.3    |
| 7       | $\langle 111 \rangle$ | 70     | NP-Tensile | 300   | Tersoff | 10      | 109.5   |
| 8       | $\langle 111 \rangle$ | 80     | NP-Tensile | 300   | Tersoff | 10      | 118.0   |
| 4       | $\langle 111 \rangle$ | 40     | NP-Tensile | 300   | SW      | 5       | 94.5    |
| 5       | $\langle 111 \rangle$ | 50     | NP-Tensile | 300   | SW      | 5       | 106.3   |
| 6       | $\langle 111 \rangle$ | 60     | NP-Tensile | 300   | SW      | 5       | 114.3   |
| 7       | $\langle 111 \rangle$ | 70     | NP-Tensile | 300   | SW      | 5       | 121.2   |
| 8       | $\langle 111 \rangle$ | 80     | NP-Tensile | 300   | SW      | 5       | 125.9   |
| 4       | $\langle 111 \rangle$ | 40     | NP-Tensile | 300   | SW      | 10      | 79.0    |
| 5       | $\langle 111 \rangle$ | 50     | NP-Tensile | 300   | SW      | 10      | 88.3    |
| 6       | $\langle 111 \rangle$ | 60     | NP-Tensile | 300   | SW      | 10      | 98.5    |
| 7       | $\langle 111 \rangle$ | 70     | NP-Tensile | 300   | SW      | 10      | 106.7   |
| 8       | $\langle 111 \rangle$ | 80     | NP-Tensile | 300   | SW      | 10      | 112.3   |
| 2       | $\langle 110 \rangle$ | 14     | Bending    | 10    | Tersoff | 0       | 230.0   |
| 3       | $\langle 110 \rangle$ | 21     | Bending    | 10    | Tersoff | 0       | 145.0   |
| 4       | $\langle 110 \rangle$ | 28     | Bending    | 10    | Tersoff | 0       | 136.0   |
| 5       | $\langle 110 \rangle$ | 35     | Bending    | 10    | Tersoff | 0       | 125.0   |
| 2       | $\langle 110 \rangle$ | 16     | Bending    | 10    | Tersoff | 0       | 210.0   |
| 3       | $\langle 110 \rangle$ | 24     | Bending    | 10    | Tersoff | 0       | 141.0   |
| 4       | $\langle 110 \rangle$ | 32     | Bending    | 10    | Tersoff | 0       | 134.0   |
| 5       | $\langle 110 \rangle$ | 40     | Bending    | 10    | Tersoff | 0       | 130.0   |
| 2       | $\langle 110 \rangle$ | 18     | Bending    | 10    | Tersoff | 0       | 200.0   |
| 3       | $\langle 110 \rangle$ | 27     | Bending    | 10    | Tersoff | 0       | 140.0   |
| 4       | $\langle 110 \rangle$ | 36     | Bending    | 10    | Tersoff | 0       | 133.0   |
| 5       | $\langle 110 \rangle$ | 45     | Bending    | 10    | Tersoff | 0       | 129.0   |
| 2       | $\langle 110 \rangle$ | 20     | Bending    | 10    | Tersoff | 0       | 190.0   |
| 3       | $\langle 110 \rangle$ | 30     | Bending    | 10    | Tersoff | 0       | 170.0   |
| 4       | $\langle 110 \rangle$ | 40     | Bending    | 10    | Tersoff | 0       | 150.0   |
| 5       | $\langle 110 \rangle$ | 50     | Bending    | 10    | Tersoff | 0       | 153.0   |
| 2       | $\langle 110 \rangle$ | 24     | Bending    | 10    | Tersoff | 0       | 193.0   |
| 3       | $\langle 110 \rangle$ | 36     | Bending    | 10    | Tersoff | 0       | 163.0   |
| 4       | $\langle 110 \rangle$ | 48     | Bending    | 10    | Tersoff | 0       | 148.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|---------|---------|---------|
| 5       | < 110 > | 60     | Bending | 10    | Tersoff | 0       | 149.0   |
| 2       | < 110 > | 28     | Bending | 10    | Tersoff | 0       | 190.0   |
| 3       | < 110 > | 42     | Bending | 10    | Tersoff | 0       | 160.0   |
| 4       | < 110 > | 56     | Bending | 10    | Tersoff | 0       | 160.0   |
| 5       | < 110 > | 70     | Bending | 10    | Tersoff | 0       | 170.0   |
| 2       | < 110 > | 32     | Bending | 10    | Tersoff | 0       | 170.0   |
| 3       | < 110 > | 48     | Bending | 10    | Tersoff | 0       | 160.0   |
| 4       | < 110 > | 64     | Bending | 10    | Tersoff | 0       | 155.0   |
| 5       | < 110 > | 80     | Bending | 10    | Tersoff | 0       | 175.0   |
| 2       | < 110 > | 36     | Bending | 10    | Tersoff | 0       | 180.0   |
| 3       | < 110 > | 54     | Bending | 10    | Tersoff | 0       | 170.0   |
| 4       | < 110 > | 72     | Bending | 10    | Tersoff | 0       | 180.0   |
| 5       | < 110 > | 90     | Bending | 10    | Tersoff | 0       | 180.0   |
| 2       | < 110 > | 40     | Bending | 10    | Tersoff | 0       | 180.0   |
| 3       | < 110 > | 60     | Bending | 10    | Tersoff | 0       | 180.0   |
| 4       | < 110 > | 80     | Bending | 10    | Tersoff | 0       | 179.0   |
| 5       | < 110 > | 100    | Bending | 10    | Tersoff | 0       | 180.0   |
| 2       | < 110 > | 14     | Bending | 10    | SW      | 0       | 200.0   |
| 3       | < 110 > | 21     | Bending | 10    | SW      | 0       | 190.0   |
| 4       | < 110 > | 28     | Bending | 10    | SW      | 0       | 180.0   |
| 5       | < 110 > | 35     | Bending | 10    | SW      | 0       | 160.0   |
| 2       | < 110 > | 16     | Bending | 10    | SW      | 0       | 205.0   |
| 3       | < 110 > | 24     | Bending | 10    | SW      | 0       | 200.0   |
| 4       | < 110 > | 32     | Bending | 10    | SW      | 0       | 190.0   |
| 5       | < 110 > | 40     | Bending | 10    | SW      | 0       | 180.0   |
| 2       | < 110 > | 18     | Bending | 10    | SW      | 0       | 195.0   |
| 3       | < 110 > | 27     | Bending | 10    | SW      | 0       | 190.0   |
| 4       | < 110 > | 36     | Bending | 10    | SW      | 0       | 175.0   |
| 5       | < 110 > | 45     | Bending | 10    | SW      | 0       | 165.0   |
| 2       | < 110 > | 20     | Bending | 10    | SW      | 0       | 189.0   |
| 3       | < 110 > | 30     | Bending | 10    | SW      | 0       | 185.0   |
| 4       | < 110 > | 40     | Bending | 10    | SW      | 0       | 180.0   |
| 5       | < 110 > | 50     | Bending | 10    | SW      | 0       | 175.0   |
| 2       | < 110 > | 24     | Bending | 10    | SW      | 0       | 185.0   |
| 3       | < 110 > | 36     | Bending | 10    | SW      | 0       | 175.0   |
| 4       | < 110 > | 48     | Bending | 10    | SW      | 0       | 160.0   |
| 5       | < 110 > | 60     | Bending | 10    | SW      | 0       | 155.0   |
| 2       | < 110 > | 28     | Bending | 10    | SW      | 0       | 189.0   |
| 3       | < 110 > | 42     | Bending | 10    | SW      | 0       | 180.0   |
| 4       | < 110 > | 56     | Bending | 10    | SW      | 0       | 170.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|---------|---------|---------|
| 5       | < 110 > | 70     | Bending | 10    | SW      | 0       | 165.0   |
| 2       | < 110 > | 32     | Bending | 10    | SW      | 0       | 185.0   |
| 3       | < 110 > | 48     | Bending | 10    | SW      | 0       | 180.0   |
| 4       | < 110 > | 64     | Bending | 10    | SW      | 0       | 173.0   |
| 5       | < 110 > | 80     | Bending | 10    | SW      | 0       | 163.0   |
| 2       | < 110 > | 36     | Bending | 10    | SW      | 0       | 189.0   |
| 3       | < 110 > | 54     | Bending | 10    | SW      | 0       | 180.0   |
| 4       | < 110 > | 72     | Bending | 10    | SW      | 0       | 178.0   |
| 5       | < 110 > | 90     | Bending | 10    | SW      | 0       | 178.0   |
| 2       | < 110 > | 40     | Bending | 10    | SW      | 0       | 190.0   |
| 3       | < 110 > | 60     | Bending | 10    | SW      | 0       | 185.0   |
| 4       | < 110 > | 80     | Bending | 10    | SW      | 0       | 180.0   |
| 5       | < 110 > | 100    | Bending | 10    | SW      | 0       | 180.0   |
| 2       | < 110 > | 14     | Bending | 300   | Tersoff | 0       | 200.0   |
| 3       | < 110 > | 21     | Bending | 300   | Tersoff | 0       | 150.0   |
| 4       | < 110 > | 28     | Bending | 300   | Tersoff | 0       | 130.0   |
| 5       | < 110 > | 35     | Bending | 300   | Tersoff | 0       | 110.0   |
| 2       | < 110 > | 16     | Bending | 300   | Tersoff | 0       | 190.0   |
| 3       | < 110 > | 24     | Bending | 300   | Tersoff | 0       | 170.0   |
| 4       | < 110 > | 32     | Bending | 300   | Tersoff | 0       | 140.0   |
| 5       | < 110 > | 40     | Bending | 300   | Tersoff | 0       | 140.0   |
| 2       | < 110 > | 18     | Bending | 300   | Tersoff | 0       | 185.0   |
| 3       | < 110 > | 27     | Bending | 300   | Tersoff | 0       | 140.0   |
| 4       | < 110 > | 36     | Bending | 300   | Tersoff | 0       | 120.0   |
| 5       | < 110 > | 45     | Bending | 300   | Tersoff | 0       | 118.0   |
| 2       | < 110 > | 20     | Bending | 300   | Tersoff | 0       | 190.0   |
| 3       | < 110 > | 30     | Bending | 300   | Tersoff | 0       | 165.0   |
| 4       | < 110 > | 40     | Bending | 300   | Tersoff | 0       | 150.0   |
| 5       | < 110 > | 50     | Bending | 300   | Tersoff | 0       | 130.0   |
| 2       | < 110 > | 24     | Bending | 300   | Tersoff | 0       | 191.0   |
| 3       | < 110 > | 36     | Bending | 300   | Tersoff | 0       | 160.0   |
| 4       | < 110 > | 48     | Bending | 300   | Tersoff | 0       | 140.0   |
| 5       | < 110 > | 60     | Bending | 300   | Tersoff | 0       | 130.0   |
| 2       | < 110 > | 28     | Bending | 300   | Tersoff | 0       | 195.0   |
| 3       | < 110 > | 42     | Bending | 300   | Tersoff | 0       | 190.0   |
| 4       | < 110 > | 56     | Bending | 300   | Tersoff | 0       | 185.0   |
| 5       | < 110 > | 70     | Bending | 300   | Tersoff | 0       | 170.0   |
| 2       | < 110 > | 32     | Bending | 300   | Tersoff | 0       | 190.0   |
| 3       | < 110 > | 48     | Bending | 300   | Tersoff | 0       | 190.0   |
| 4       | < 110 > | 64     | Bending | 300   | Tersoff | 0       | 180.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|---------|---------|---------|
| 5       | < 110 > | 80     | Bending | 300   | Tersoff | 0       | 175.0   |
| 2       | < 110 > | 36     | Bending | 300   | Tersoff | 0       | 190.0   |
| 3       | < 110 > | 54     | Bending | 300   | Tersoff | 0       | 170.0   |
| 4       | < 110 > | 72     | Bending | 300   | Tersoff | 0       | 180.0   |
| 5       | < 110 > | 90     | Bending | 300   | Tersoff | 0       | 175.0   |
| 2       | < 110 > | 40     | Bending | 300   | Tersoff | 0       | 180.0   |
| 3       | < 110 > | 60     | Bending | 300   | Tersoff | 0       | 170.0   |
| 4       | < 110 > | 80     | Bending | 300   | Tersoff | 0       | 165.0   |
| 5       | < 110 > | 100    | Bending | 300   | Tersoff | 0       | 160.0   |
| 2       | < 110 > | 14     | Bending | 300   | SW      | 0       | 190.0   |
| 3       | < 110 > | 21     | Bending | 300   | SW      | 0       | 150.0   |
| 4       | < 110 > | 28     | Bending | 300   | SW      | 0       | 140.0   |
| 5       | < 110 > | 35     | Bending | 300   | SW      | 0       | 130.0   |
| 2       | < 110 > | 16     | Bending | 300   | SW      | 0       | 165.0   |
| 3       | < 110 > | 24     | Bending | 300   | SW      | 0       | 110.0   |
| 4       | < 110 > | 32     | Bending | 300   | SW      | 0       | 100.0   |
| 5       | < 110 > | 40     | Bending | 300   | SW      | 0       | 90.0    |
| 2       | < 110 > | 18     | Bending | 300   | SW      | 0       | 180.0   |
| 3       | < 110 > | 27     | Bending | 300   | SW      | 0       | 165.0   |
| 4       | < 110 > | 36     | Bending | 300   | SW      | 0       | 130.0   |
| 5       | < 110 > | 45     | Bending | 300   | SW      | 0       | 120.0   |
| 2       | < 110 > | 20     | Bending | 300   | SW      | 0       | 182.0   |
| 3       | < 110 > | 30     | Bending | 300   | SW      | 0       | 170.0   |
| 4       | < 110 > | 40     | Bending | 300   | SW      | 0       | 165.0   |
| 5       | < 110 > | 50     | Bending | 300   | SW      | 0       | 164.0   |
| 2       | < 110 > | 24     | Bending | 300   | SW      | 0       | 180.0   |
| 3       | < 110 > | 36     | Bending | 300   | SW      | 0       | 164.0   |
| 4       | < 110 > | 48     | Bending | 300   | SW      | 0       | 160.0   |
| 5       | < 110 > | 60     | Bending | 300   | SW      | 0       | 170.0   |
| 2       | < 110 > | 28     | Bending | 300   | SW      | 0       | 183.0   |
| 3       | < 110 > | 42     | Bending | 300   | SW      | 0       | 180.0   |
| 4       | < 110 > | 56     | Bending | 300   | SW      | 0       | 182.0   |
| 5       | < 110 > | 70     | Bending | 300   | SW      | 0       | 184.0   |
| 2       | < 110 > | 32     | Bending | 300   | SW      | 0       | 190.0   |
| 3       | < 110 > | 48     | Bending | 300   | SW      | 0       | 189.0   |
| 4       | < 110 > | 64     | Bending | 300   | SW      | 0       | 188.0   |
| 5       | < 110 > | 80     | Bending | 300   | SW      | 0       | 185.0   |
| 2       | < 110 > | 36     | Bending | 300   | SW      | 0       | 195.0   |
| 3       | < 110 > | 54     | Bending | 300   | SW      | 0       | 194.0   |
| 4       | < 110 > | 72     | Bending | 300   | SW      | 0       | 200.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|---------|---------|---------|
| 5       | < 110 > | 90     | Bending | 300   | SW      | 0       | 195.0   |
| 2       | < 110 > | 40     | Bending | 300   | SW      | 0       | 205.0   |
| 3       | < 110 > | 60     | Bending | 300   | SW      | 0       | 210.0   |
| 4       | < 110 > | 80     | Bending | 300   | SW      | 0       | 215.0   |
| 5       | < 110 > | 100    | Bending | 300   | SW      | 0       | 215.0   |
| 2       | < 110 > | 14     | Bending | 600   | Tersoff | 0       | 120.0   |
| 3       | < 110 > | 21     | Bending | 600   | Tersoff | 0       | 110.0   |
| 4       | < 110 > | 28     | Bending | 600   | Tersoff | 0       | 100.0   |
| 5       | < 110 > | 35     | Bending | 600   | Tersoff | 0       | 100.0   |
| 2       | < 110 > | 16     | Bending | 600   | Tersoff | 0       | 100.0   |
| 3       | < 110 > | 24     | Bending | 600   | Tersoff | 0       | 85.0    |
| 4       | < 110 > | 32     | Bending | 600   | Tersoff | 0       | 87.0    |
| 5       | < 110 > | 40     | Bending | 600   | Tersoff | 0       | 90.0    |
| 2       | < 110 > | 18     | Bending | 600   | Tersoff | 0       | 83.0    |
| 3       | < 110 > | 27     | Bending | 600   | Tersoff | 0       | 87.0    |
| 4       | < 110 > | 36     | Bending | 600   | Tersoff | 0       | 87.0    |
| 5       | < 110 > | 45     | Bending | 600   | Tersoff | 0       | 88.0    |
| 2       | < 110 > | 20     | Bending | 600   | Tersoff | 0       | 81.0    |
| 3       | < 110 > | 30     | Bending | 600   | Tersoff | 0       | 78.0    |
| 4       | < 110 > | 40     | Bending | 600   | Tersoff | 0       | 80.0    |
| 5       | < 110 > | 50     | Bending | 600   | Tersoff | 0       | 69.0    |
| 2       | < 110 > | 24     | Bending | 600   | Tersoff | 0       | 82.0    |
| 3       | < 110 > | 36     | Bending | 600   | Tersoff | 0       | 83.0    |
| 4       | < 110 > | 48     | Bending | 600   | Tersoff | 0       | 86.0    |
| 5       | < 110 > | 60     | Bending | 600   | Tersoff | 0       | 86.0    |
| 2       | < 110 > | 28     | Bending | 600   | Tersoff | 0       | 95.0    |
| 3       | < 110 > | 42     | Bending | 600   | Tersoff | 0       | 86.0    |
| 4       | < 110 > | 56     | Bending | 600   | Tersoff | 0       | 80.0    |
| 5       | < 110 > | 70     | Bending | 600   | Tersoff | 0       | 95.0    |
| 2       | < 110 > | 32     | Bending | 600   | Tersoff | 0       | 90.0    |
| 3       | < 110 > | 48     | Bending | 600   | Tersoff | 0       | 75.0    |
| 4       | < 110 > | 64     | Bending | 600   | Tersoff | 0       | 80.0    |
| 5       | < 110 > | 80     | Bending | 600   | Tersoff | 0       | 85.0    |
| 2       | < 110 > | 36     | Bending | 600   | Tersoff | 0       | 90.0    |
| 3       | < 110 > | 54     | Bending | 600   | Tersoff | 0       | 70.0    |
| 4       | < 110 > | 72     | Bending | 600   | Tersoff | 0       | 80.0    |
| 5       | < 110 > | 90     | Bending | 600   | Tersoff | 0       | 90.0    |
| 2       | < 110 > | 40     | Bending | 600   | Tersoff | 0       | 70.0    |
| 3       | < 110 > | 60     | Bending | 600   | Tersoff | 0       | 75.0    |
| 4       | < 110 > | 80     | Bending | 600   | Tersoff | 0       | 75.0    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|---------|---------|---------|
| 5       | < 110 > | 100    | Bending | 600   | Tersoff | 0       | 80.0    |
| 2       | < 110 > | 14     | Bending | 600   | SW      | 0       | 170.0   |
| 3       | < 110 > | 21     | Bending | 600   | SW      | 0       | 160.0   |
| 4       | < 110 > | 28     | Bending | 600   | SW      | 0       | 150.0   |
| 5       | < 110 > | 35     | Bending | 600   | SW      | 0       | 140.0   |
| 2       | < 110 > | 16     | Bending | 600   | SW      | 0       | 190.0   |
| 3       | < 110 > | 24     | Bending | 600   | SW      | 0       | 185.0   |
| 4       | < 110 > | 32     | Bending | 600   | SW      | 0       | 180.0   |
| 5       | < 110 > | 40     | Bending | 600   | SW      | 0       | 175.0   |
| 2       | < 110 > | 18     | Bending | 600   | SW      | 0       | 190.0   |
| 3       | < 110 > | 27     | Bending | 600   | SW      | 0       | 190.0   |
| 4       | < 110 > | 36     | Bending | 600   | SW      | 0       | 180.0   |
| 5       | < 110 > | 45     | Bending | 600   | SW      | 0       | 175.0   |
| 2       | < 110 > | 20     | Bending | 600   | SW      | 0       | 190.0   |
| 3       | < 110 > | 30     | Bending | 600   | SW      | 0       | 190.0   |
| 4       | < 110 > | 40     | Bending | 600   | SW      | 0       | 180.0   |
| 5       | < 110 > | 50     | Bending | 600   | SW      | 0       | 180.0   |
| 2       | < 110 > | 24     | Bending | 600   | SW      | 0       | 190.0   |
| 3       | < 110 > | 36     | Bending | 600   | SW      | 0       | 190.0   |
| 4       | < 110 > | 48     | Bending | 600   | SW      | 0       | 188.0   |
| 5       | < 110 > | 60     | Bending | 600   | SW      | 0       | 188.0   |
| 2       | < 110 > | 28     | Bending | 600   | SW      | 0       | 193.0   |
| 3       | < 110 > | 42     | Bending | 600   | SW      | 0       | 190.0   |
| 4       | < 110 > | 56     | Bending | 600   | SW      | 0       | 191.0   |
| 5       | < 110 > | 70     | Bending | 600   | SW      | 0       | 192.0   |
| 2       | < 110 > | 32     | Bending | 600   | SW      | 0       | 190.0   |
| 3       | < 110 > | 48     | Bending | 600   | SW      | 0       | 190.0   |
| 4       | < 110 > | 64     | Bending | 600   | SW      | 0       | 188.0   |
| 5       | < 110 > | 80     | Bending | 600   | SW      | 0       | 192.0   |
| 2       | < 110 > | 36     | Bending | 600   | SW      | 0       | 195.0   |
| 3       | < 110 > | 54     | Bending | 600   | SW      | 0       | 192.0   |
| 4       | < 110 > | 72     | Bending | 600   | SW      | 0       | 194.0   |
| 5       | < 110 > | 90     | Bending | 600   | SW      | 0       | 195.0   |
| 2       | < 110 > | 40     | Bending | 600   | SW      | 0       | 192.0   |
| 3       | < 110 > | 60     | Bending | 600   | SW      | 0       | 192.0   |
| 4       | < 110 > | 80     | Bending | 600   | SW      | 0       | 193.0   |
| 5       | < 110 > | 100    | Bending | 600   | SW      | 0       | 194.0   |
| 2       | < 100 > | 14     | Bending | 10    | Tersoff | 0       | 170.0   |
| 3       | < 100 > | 21     | Bending | 10    | Tersoff | 0       | 110.0   |
| 4       | < 100 > | 28     | Bending | 10    | Tersoff | 0       | 90.0    |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|---------|---------|---------|
| 5       | < 100 > | 35     | Bending | 10    | Tersoff | 0       | 83.0    |
| 2       | < 100 > | 16     | Bending | 10    | Tersoff | 0       | 160.0   |
| 3       | < 100 > | 24     | Bending | 10    | Tersoff | 0       | 105.0   |
| 4       | < 100 > | 32     | Bending | 10    | Tersoff | 0       | 100.0   |
| 5       | < 100 > | 40     | Bending | 10    | Tersoff | 0       | 90.0    |
| 2       | < 100 > | 18     | Bending | 10    | Tersoff | 0       | 150.0   |
| 3       | < 100 > | 27     | Bending | 10    | Tersoff | 0       | 105.0   |
| 4       | < 100 > | 36     | Bending | 10    | Tersoff | 0       | 95.0    |
| 5       | < 100 > | 45     | Bending | 10    | Tersoff | 0       | 87.0    |
| 2       | < 100 > | 20     | Bending | 10    | Tersoff | 0       | 137.0   |
| 3       | < 100 > | 30     | Bending | 10    | Tersoff | 0       | 103.0   |
| 4       | < 100 > | 40     | Bending | 10    | Tersoff | 0       | 95.0    |
| 5       | < 100 > | 50     | Bending | 10    | Tersoff | 0       | 93.0    |
| 2       | < 100 > | 24     | Bending | 10    | Tersoff | 0       | 143.0   |
| 3       | < 100 > | 36     | Bending | 10    | Tersoff | 0       | 103.0   |
| 4       | < 100 > | 48     | Bending | 10    | Tersoff | 0       | 98.0    |
| 5       | < 100 > | 60     | Bending | 10    | Tersoff | 0       | 97.0    |
| 2       | < 100 > | 28     | Bending | 10    | Tersoff | 0       | 146.0   |
| 3       | < 100 > | 42     | Bending | 10    | Tersoff | 0       | 107.0   |
| 4       | < 100 > | 56     | Bending | 10    | Tersoff | 0       | 104.0   |
| 5       | < 100 > | 70     | Bending | 10    | Tersoff | 0       | 98.0    |
| 2       | < 100 > | 32     | Bending | 10    | Tersoff | 0       | 140.0   |
| 3       | < 100 > | 48     | Bending | 10    | Tersoff | 0       | 126.0   |
| 4       | < 100 > | 64     | Bending | 10    | Tersoff | 0       | 116.0   |
| 5       | < 100 > | 80     | Bending | 10    | Tersoff | 0       | 106.0   |
| 2       | < 100 > | 36     | Bending | 10    | Tersoff | 0       | 137.0   |
| 3       | < 100 > | 54     | Bending | 10    | Tersoff | 0       | 107.0   |
| 4       | < 100 > | 72     | Bending | 10    | Tersoff | 0       | 105.0   |
| 5       | < 100 > | 90     | Bending | 10    | Tersoff | 0       | 104.0   |
| 2       | < 100 > | 40     | Bending | 10    | Tersoff | 0       | 156.0   |
| 3       | < 100 > | 60     | Bending | 10    | Tersoff | 0       | 133.0   |
| 4       | < 100 > | 80     | Bending | 10    | Tersoff | 0       | 126.0   |
| 5       | < 100 > | 100    | Bending | 10    | Tersoff | 0       | 110.0   |
| 2       | < 100 > | 14     | Bending | 10    | SW      | 0       | 136.0   |
| 3       | < 100 > | 21     | Bending | 10    | SW      | 0       | 134.0   |
| 4       | < 100 > | 28     | Bending | 10    | SW      | 0       | 133.0   |
| 5       | < 100 > | 35     | Bending | 10    | SW      | 0       | 130.0   |
| 2       | < 100 > | 16     | Bending | 10    | SW      | 0       | 137.0   |
| 3       | < 100 > | 24     | Bending | 10    | SW      | 0       | 135.0   |
| 4       | < 100 > | 32     | Bending | 10    | SW      | 0       | 134.0   |



Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|---------|---------|---------|
| 5       | < 100 > | 40     | Bending | 10    | SW      | 0       | 133.0   |
| 2       | < 100 > | 18     | Bending | 10    | SW      | 0       | 138.0   |
| 3       | < 100 > | 27     | Bending | 10    | SW      | 0       | 136.0   |
| 4       | < 100 > | 36     | Bending | 10    | SW      | 0       | 135.0   |
| 5       | < 100 > | 45     | Bending | 10    | SW      | 0       | 134.0   |
| 2       | < 100 > | 20     | Bending | 10    | SW      | 0       | 138.0   |
| 3       | < 100 > | 30     | Bending | 10    | SW      | 0       | 136.0   |
| 4       | < 100 > | 40     | Bending | 10    | SW      | 0       | 135.0   |
| 5       | < 100 > | 50     | Bending | 10    | SW      | 0       | 134.0   |
| 2       | < 100 > | 24     | Bending | 10    | SW      | 0       | 134.0   |
| 3       | < 100 > | 36     | Bending | 10    | SW      | 0       | 125.0   |
| 4       | < 100 > | 48     | Bending | 10    | SW      | 0       | 124.0   |
| 5       | < 100 > | 60     | Bending | 10    | SW      | 0       | 121.0   |
| 2       | < 100 > | 28     | Bending | 10    | SW      | 0       | 135.0   |
| 3       | < 100 > | 42     | Bending | 10    | SW      | 0       | 133.0   |
| 4       | < 100 > | 56     | Bending | 10    | SW      | 0       | 132.0   |
| 5       | < 100 > | 70     | Bending | 10    | SW      | 0       | 133.0   |
| 2       | < 100 > | 32     | Bending | 10    | SW      | 0       | 135.0   |
| 3       | < 100 > | 48     | Bending | 10    | SW      | 0       | 134.0   |
| 4       | < 100 > | 64     | Bending | 10    | SW      | 0       | 134.0   |
| 5       | < 100 > | 80     | Bending | 10    | SW      | 0       | 133.0   |
| 2       | < 100 > | 36     | Bending | 10    | SW      | 0       | 135.0   |
| 3       | < 100 > | 54     | Bending | 10    | SW      | 0       | 135.0   |
| 4       | < 100 > | 72     | Bending | 10    | SW      | 0       | 136.0   |
| 5       | < 100 > | 90     | Bending | 10    | SW      | 0       | 137.0   |
| 2       | < 100 > | 40     | Bending | 10    | SW      | 0       | 138.0   |
| 3       | < 100 > | 60     | Bending | 10    | SW      | 0       | 137.0   |
| 4       | < 100 > | 80     | Bending | 10    | SW      | 0       | 134.0   |
| 5       | < 100 > | 100    | Bending | 10    | SW      | 0       | 130.0   |
| 2       | < 100 > | 14     | Bending | 300   | Tersoff | 0       | 150.0   |
| 3       | < 100 > | 21     | Bending | 300   | Tersoff | 0       | 110.0   |
| 4       | < 100 > | 28     | Bending | 300   | Tersoff | 0       | 105.0   |
| 5       | < 100 > | 35     | Bending | 300   | Tersoff | 0       | 90.0    |
| 2       | < 100 > | 16     | Bending | 300   | Tersoff | 0       | 130.0   |
| 3       | < 100 > | 24     | Bending | 300   | Tersoff | 0       | 115.0   |
| 4       | < 100 > | 32     | Bending | 300   | Tersoff | 0       | 110.0   |
| 5       | < 100 > | 40     | Bending | 300   | Tersoff | 0       | 95.0    |
| 2       | < 100 > | 18     | Bending | 300   | Tersoff | 0       | 125.0   |
| 3       | < 100 > | 27     | Bending | 300   | Tersoff | 0       | 115.0   |
| 4       | < 100 > | 36     | Bending | 300   | Tersoff | 0       | 110.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|---------|---------|---------|
| 5       | < 100 > | 45     | Bending | 300   | Tersoff | 0       | 105.0   |
| 2       | < 100 > | 20     | Bending | 300   | Tersoff | 0       | 137.0   |
| 3       | < 100 > | 30     | Bending | 300   | Tersoff | 0       | 125.0   |
| 4       | < 100 > | 40     | Bending | 300   | Tersoff | 0       | 120.0   |
| 5       | < 100 > | 50     | Bending | 300   | Tersoff | 0       | 110.0   |
| 2       | < 100 > | 24     | Bending | 300   | Tersoff | 0       | 145.0   |
| 3       | < 100 > | 36     | Bending | 300   | Tersoff | 0       | 135.0   |
| 4       | < 100 > | 48     | Bending | 300   | Tersoff | 0       | 125.0   |
| 5       | < 100 > | 60     | Bending | 300   | Tersoff | 0       | 115.0   |
| 2       | < 100 > | 28     | Bending | 300   | Tersoff | 0       | 150.0   |
| 3       | < 100 > | 42     | Bending | 300   | Tersoff | 0       | 140.0   |
| 4       | < 100 > | 56     | Bending | 300   | Tersoff | 0       | 133.0   |
| 5       | < 100 > | 70     | Bending | 300   | Tersoff | 0       | 132.0   |
| 2       | < 100 > | 32     | Bending | 300   | Tersoff | 0       | 145.0   |
| 3       | < 100 > | 48     | Bending | 300   | Tersoff | 0       | 135.0   |
| 4       | < 100 > | 64     | Bending | 300   | Tersoff | 0       | 125.0   |
| 5       | < 100 > | 80     | Bending | 300   | Tersoff | 0       | 115.0   |
| 2       | < 100 > | 36     | Bending | 300   | Tersoff | 0       | 142.0   |
| 3       | < 100 > | 54     | Bending | 300   | Tersoff | 0       | 132.0   |
| 4       | < 100 > | 72     | Bending | 300   | Tersoff | 0       | 121.0   |
| 5       | < 100 > | 90     | Bending | 300   | Tersoff | 0       | 111.0   |
| 2       | < 100 > | 40     | Bending | 300   | Tersoff | 0       | 150.0   |
| 3       | < 100 > | 60     | Bending | 300   | Tersoff | 0       | 142.0   |
| 4       | < 100 > | 80     | Bending | 300   | Tersoff | 0       | 140.0   |
| 5       | < 100 > | 100    | Bending | 300   | Tersoff | 0       | 138.0   |
| 2       | < 100 > | 14     | Bending | 300   | SW      | 0       | 140.0   |
| 3       | < 100 > | 21     | Bending | 300   | SW      | 0       | 135.0   |
| 4       | < 100 > | 28     | Bending | 300   | SW      | 0       | 133.0   |
| 5       | < 100 > | 35     | Bending | 300   | SW      | 0       | 131.0   |
| 2       | < 100 > | 16     | Bending | 300   | SW      | 0       | 155.0   |
| 3       | < 100 > | 24     | Bending | 300   | SW      | 0       | 152.0   |
| 4       | < 100 > | 32     | Bending | 300   | SW      | 0       | 151.0   |
| 5       | < 100 > | 40     | Bending | 300   | SW      | 0       | 149.0   |
| 2       | < 100 > | 18     | Bending | 300   | SW      | 0       | 160.0   |
| 3       | < 100 > | 27     | Bending | 300   | SW      | 0       | 155.0   |
| 4       | < 100 > | 36     | Bending | 300   | SW      | 0       | 154.0   |
| 5       | < 100 > | 45     | Bending | 300   | SW      | 0       | 153.0   |
| 2       | < 100 > | 20     | Bending | 300   | SW      | 0       | 168.0   |
| 3       | < 100 > | 30     | Bending | 300   | SW      | 0       | 164.0   |
| 4       | < 100 > | 40     | Bending | 300   | SW      | 0       | 162.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|---------|---------|---------|
| 5       | < 100 > | 50     | Bending | 300   | SW      | 0       | 160.0   |
| 2       | < 100 > | 24     | Bending | 300   | SW      | 0       | 165.0   |
| 3       | < 100 > | 36     | Bending | 300   | SW      | 0       | 163.0   |
| 4       | < 100 > | 48     | Bending | 300   | SW      | 0       | 162.0   |
| 5       | < 100 > | 60     | Bending | 300   | SW      | 0       | 163.0   |
| 2       | < 100 > | 28     | Bending | 300   | SW      | 0       | 165.0   |
| 3       | < 100 > | 42     | Bending | 300   | SW      | 0       | 165.0   |
| 4       | < 100 > | 56     | Bending | 300   | SW      | 0       | 163.0   |
| 5       | < 100 > | 70     | Bending | 300   | SW      | 0       | 163.0   |
| 2       | < 100 > | 32     | Bending | 300   | SW      | 0       | 162.0   |
| 3       | < 100 > | 48     | Bending | 300   | SW      | 0       | 168.0   |
| 4       | < 100 > | 64     | Bending | 300   | SW      | 0       | 164.0   |
| 5       | < 100 > | 80     | Bending | 300   | SW      | 0       | 163.0   |
| 2       | < 100 > | 36     | Bending | 300   | SW      | 0       | 165.0   |
| 3       | < 100 > | 54     | Bending | 300   | SW      | 0       | 164.0   |
| 4       | < 100 > | 72     | Bending | 300   | SW      | 0       | 164.0   |
| 5       | < 100 > | 90     | Bending | 300   | SW      | 0       | 163.0   |
| 2       | < 100 > | 40     | Bending | 300   | SW      | 0       | 165.0   |
| 3       | < 100 > | 60     | Bending | 300   | SW      | 0       | 163.0   |
| 4       | < 100 > | 80     | Bending | 300   | SW      | 0       | 163.0   |
| 5       | < 100 > | 100    | Bending | 300   | SW      | 0       | 162.0   |
| 2       | < 100 > | 14     | Bending | 600   | Tersoff | 0       | 145.0   |
| 3       | < 100 > | 21     | Bending | 600   | Tersoff | 0       | 125.0   |
| 4       | < 100 > | 28     | Bending | 600   | Tersoff | 0       | 105.0   |
| 5       | < 100 > | 35     | Bending | 600   | Tersoff | 0       | 104.0   |
| 2       | < 100 > | 16     | Bending | 600   | Tersoff | 0       | 115.0   |
| 3       | < 100 > | 24     | Bending | 600   | Tersoff | 0       | 110.0   |
| 4       | < 100 > | 32     | Bending | 600   | Tersoff | 0       | 105.0   |
| 5       | < 100 > | 40     | Bending | 600   | Tersoff | 0       | 100.0   |
| 2       | < 100 > | 18     | Bending | 600   | Tersoff | 0       | 108.0   |
| 3       | < 100 > | 27     | Bending | 600   | Tersoff | 0       | 106.0   |
| 4       | < 100 > | 36     | Bending | 600   | Tersoff | 0       | 100.0   |
| 5       | < 100 > | 45     | Bending | 600   | Tersoff | 0       | 95.0    |
| 2       | < 100 > | 20     | Bending | 600   | Tersoff | 0       | 130.0   |
| 3       | < 100 > | 30     | Bending | 600   | Tersoff | 0       | 125.0   |
| 4       | < 100 > | 40     | Bending | 600   | Tersoff | 0       | 123.0   |
| 5       | < 100 > | 50     | Bending | 600   | Tersoff | 0       | 120.0   |
| 2       | < 100 > | 24     | Bending | 600   | Tersoff | 0       | 140.0   |
| 3       | < 100 > | 36     | Bending | 600   | Tersoff | 0       | 136.0   |
| 4       | < 100 > | 48     | Bending | 600   | Tersoff | 0       | 135.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|---------|---------|---------|
| 5       | < 100 > | 60     | Bending | 600   | Tersoff | 0       | 130.0   |
| 2       | < 100 > | 28     | Bending | 600   | Tersoff | 0       | 146.0   |
| 3       | < 100 > | 42     | Bending | 600   | Tersoff | 0       | 144.0   |
| 4       | < 100 > | 56     | Bending | 600   | Tersoff | 0       | 140.0   |
| 5       | < 100 > | 70     | Bending | 600   | Tersoff | 0       | 138.0   |
| 2       | < 100 > | 32     | Bending | 600   | Tersoff | 0       | 145.0   |
| 3       | < 100 > | 48     | Bending | 600   | Tersoff | 0       | 144.0   |
| 4       | < 100 > | 64     | Bending | 600   | Tersoff | 0       | 142.0   |
| 5       | < 100 > | 80     | Bending | 600   | Tersoff | 0       | 140.0   |
| 2       | < 100 > | 36     | Bending | 600   | Tersoff | 0       | 146.0   |
| 3       | < 100 > | 54     | Bending | 600   | Tersoff | 0       | 145.0   |
| 4       | < 100 > | 72     | Bending | 600   | Tersoff | 0       | 139.0   |
| 5       | < 100 > | 90     | Bending | 600   | Tersoff | 0       | 145.0   |
| 2       | < 100 > | 40     | Bending | 600   | Tersoff | 0       | 155.0   |
| 3       | < 100 > | 60     | Bending | 600   | Tersoff | 0       | 154.0   |
| 4       | < 100 > | 80     | Bending | 600   | Tersoff | 0       | 152.0   |
| 5       | < 100 > | 100    | Bending | 600   | Tersoff | 0       | 150.0   |
| 2       | < 100 > | 14     | Bending | 600   | SW      | 0       | 143.0   |
| 3       | < 100 > | 21     | Bending | 600   | SW      | 0       | 141.0   |
| 4       | < 100 > | 28     | Bending | 600   | SW      | 0       | 140.0   |
| 5       | < 100 > | 35     | Bending | 600   | SW      | 0       | 134.0   |
| 2       | < 100 > | 16     | Bending | 600   | SW      | 0       | 150.0   |
| 3       | < 100 > | 24     | Bending | 600   | SW      | 0       | 145.0   |
| 4       | < 100 > | 32     | Bending | 600   | SW      | 0       | 144.0   |
| 5       | < 100 > | 40     | Bending | 600   | SW      | 0       | 141.0   |
| 2       | < 100 > | 18     | Bending | 600   | SW      | 0       | 154.0   |
| 3       | < 100 > | 27     | Bending | 600   | SW      | 0       | 151.0   |
| 4       | < 100 > | 36     | Bending | 600   | SW      | 0       | 150.0   |
| 5       | < 100 > | 45     | Bending | 600   | SW      | 0       | 150.0   |
| 2       | < 100 > | 20     | Bending | 600   | SW      | 0       | 160.0   |
| 3       | < 100 > | 30     | Bending | 600   | SW      | 0       | 159.0   |
| 4       | < 100 > | 40     | Bending | 600   | SW      | 0       | 156.0   |
| 5       | < 100 > | 50     | Bending | 600   | SW      | 0       | 155.0   |
| 2       | < 100 > | 24     | Bending | 600   | SW      | 0       | 165.0   |
| 3       | < 100 > | 36     | Bending | 600   | SW      | 0       | 162.0   |
| 4       | < 100 > | 48     | Bending | 600   | SW      | 0       | 160.0   |
| 5       | < 100 > | 60     | Bending | 600   | SW      | 0       | 158.0   |
| 2       | < 100 > | 28     | Bending | 600   | SW      | 0       | 168.0   |
| 3       | < 100 > | 42     | Bending | 600   | SW      | 0       | 166.0   |
| 4       | < 100 > | 56     | Bending | 600   | SW      | 0       | 166.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|---------|---------|---------|
| 5       | < 100 > | 70     | Bending | 600   | SW      | 0       | 167.0   |
| 2       | < 100 > | 32     | Bending | 600   | SW      | 0       | 170.0   |
| 3       | < 100 > | 48     | Bending | 600   | SW      | 0       | 168.0   |
| 4       | < 100 > | 64     | Bending | 600   | SW      | 0       | 168.0   |
| 5       | < 100 > | 80     | Bending | 600   | SW      | 0       | 167.0   |
| 2       | < 100 > | 36     | Bending | 600   | SW      | 0       | 172.0   |
| 3       | < 100 > | 54     | Bending | 600   | SW      | 0       | 170.0   |
| 4       | < 100 > | 72     | Bending | 600   | SW      | 0       | 171.0   |
| 5       | < 100 > | 90     | Bending | 600   | SW      | 0       | 170.0   |
| 2       | < 100 > | 40     | Bending | 600   | SW      | 0       | 175.0   |
| 3       | < 100 > | 60     | Bending | 600   | SW      | 0       | 170.0   |
| 4       | < 100 > | 80     | Bending | 600   | SW      | 0       | 171.0   |
| 5       | < 100 > | 100    | Bending | 600   | SW      | 0       | 171.0   |
| 2       | < 111 > | 14     | Bending | 10    | Tersoff | 0       | 192.0   |
| 3       | < 111 > | 21     | Bending | 10    | Tersoff | 0       | 178.0   |
| 4       | < 111 > | 28     | Bending | 10    | Tersoff | 0       | 155.0   |
| 5       | < 111 > | 35     | Bending | 10    | Tersoff | 0       | 134.0   |
| 2       | < 111 > | 16     | Bending | 10    | Tersoff | 0       | 185.0   |
| 3       | < 111 > | 24     | Bending | 10    | Tersoff | 0       | 181.0   |
| 4       | < 111 > | 32     | Bending | 10    | Tersoff | 0       | 175.0   |
| 5       | < 111 > | 40     | Bending | 10    | Tersoff | 0       | 165.0   |
| 2       | < 111 > | 18     | Bending | 10    | Tersoff | 0       | 175.0   |
| 3       | < 111 > | 27     | Bending | 10    | Tersoff | 0       | 168.0   |
| 4       | < 111 > | 36     | Bending | 10    | Tersoff | 0       | 164.0   |
| 5       | < 111 > | 45     | Bending | 10    | Tersoff | 0       | 160.0   |
| 2       | < 111 > | 20     | Bending | 10    | Tersoff | 0       | 172.0   |
| 3       | < 111 > | 30     | Bending | 10    | Tersoff | 0       | 170.0   |
| 4       | < 111 > | 40     | Bending | 10    | Tersoff | 0       | 169.0   |
| 5       | < 111 > | 50     | Bending | 10    | Tersoff | 0       | 166.0   |
| 2       | < 111 > | 24     | Bending | 10    | Tersoff | 0       | 170.0   |
| 3       | < 111 > | 36     | Bending | 10    | Tersoff | 0       | 169.0   |
| 4       | < 111 > | 48     | Bending | 10    | Tersoff | 0       | 167.0   |
| 5       | < 111 > | 60     | Bending | 10    | Tersoff | 0       | 166.0   |
| 2       | < 111 > | 28     | Bending | 10    | Tersoff | 0       | 173.0   |
| 3       | < 111 > | 42     | Bending | 10    | Tersoff | 0       | 170.0   |
| 4       | < 111 > | 56     | Bending | 10    | Tersoff | 0       | 169.0   |
| 5       | < 111 > | 70     | Bending | 10    | Tersoff | 0       | 171.0   |
| 2       | < 111 > | 32     | Bending | 10    | Tersoff | 0       | 170.0   |
| 3       | < 111 > | 48     | Bending | 10    | Tersoff | 0       | 169.0   |
| 4       | < 111 > | 64     | Bending | 10    | Tersoff | 0       | 171.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|---------|---------|---------|
| 5       | < 111 > | 80     | Bending | 10    | Tersoff | 0       | 171.0   |
| 2       | < 111 > | 36     | Bending | 10    | Tersoff | 0       | 174.0   |
| 3       | < 111 > | 54     | Bending | 10    | Tersoff | 0       | 171.0   |
| 4       | < 111 > | 72     | Bending | 10    | Tersoff | 0       | 170.0   |
| 5       | < 111 > | 90     | Bending | 10    | Tersoff | 0       | 170.0   |
| 2       | < 111 > | 40     | Bending | 10    | Tersoff | 0       | 180.0   |
| 3       | < 111 > | 60     | Bending | 10    | Tersoff | 0       | 175.0   |
| 4       | < 111 > | 80     | Bending | 10    | Tersoff | 0       | 174.0   |
| 5       | < 111 > | 100    | Bending | 10    | Tersoff | 0       | 171.0   |
| 2       | < 111 > | 14     | Bending | 10    | SW      | 0       | 188.0   |
| 3       | < 111 > | 21     | Bending | 10    | SW      | 0       | 171.0   |
| 4       | < 111 > | 28     | Bending | 10    | SW      | 0       | 160.0   |
| 5       | < 111 > | 35     | Bending | 10    | SW      | 0       | 150.0   |
| 2       | < 111 > | 16     | Bending | 10    | SW      | 0       | 191.0   |
| 3       | < 111 > | 24     | Bending | 10    | SW      | 0       | 181.0   |
| 4       | < 111 > | 32     | Bending | 10    | SW      | 0       | 176.0   |
| 5       | < 111 > | 40     | Bending | 10    | SW      | 0       | 171.0   |
| 2       | < 111 > | 18     | Bending | 10    | SW      | 0       | 192.0   |
| 3       | < 111 > | 27     | Bending | 10    | SW      | 0       | 188.0   |
| 4       | < 111 > | 36     | Bending | 10    | SW      | 0       | 180.0   |
| 5       | < 111 > | 45     | Bending | 10    | SW      | 0       | 179.0   |
| 2       | < 111 > | 20     | Bending | 10    | SW      | 0       | 193.0   |
| 3       | < 111 > | 30     | Bending | 10    | SW      | 0       | 189.0   |
| 4       | < 111 > | 40     | Bending | 10    | SW      | 0       | 190.0   |
| 5       | < 111 > | 50     | Bending | 10    | SW      | 0       | 188.0   |
| 2       | < 111 > | 24     | Bending | 10    | SW      | 0       | 192.0   |
| 3       | < 111 > | 36     | Bending | 10    | SW      | 0       | 190.0   |
| 4       | < 111 > | 48     | Bending | 10    | SW      | 0       | 189.0   |
| 5       | < 111 > | 60     | Bending | 10    | SW      | 0       | 188.0   |
| 2       | < 111 > | 28     | Bending | 10    | SW      | 0       | 194.0   |
| 3       | < 111 > | 42     | Bending | 10    | SW      | 0       | 190.0   |
| 4       | < 111 > | 56     | Bending | 10    | SW      | 0       | 191.0   |
| 5       | < 111 > | 70     | Bending | 10    | SW      | 0       | 192.0   |
| 2       | < 111 > | 32     | Bending | 10    | SW      | 0       | 192.0   |
| 3       | < 111 > | 48     | Bending | 10    | SW      | 0       | 192.0   |
| 4       | < 111 > | 64     | Bending | 10    | SW      | 0       | 190.0   |
| 5       | < 111 > | 80     | Bending | 10    | SW      | 0       | 185.0   |
| 2       | < 111 > | 36     | Bending | 10    | SW      | 0       | 195.0   |
| 3       | < 111 > | 54     | Bending | 10    | SW      | 0       | 189.0   |
| 4       | < 111 > | 72     | Bending | 10    | SW      | 0       | 190.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|---------|---------|---------|
| 5       | < 111 > | 90     | Bending | 10    | SW      | 0       | 190.0   |
| 2       | < 111 > | 40     | Bending | 10    | SW      | 0       | 191.0   |
| 3       | < 111 > | 60     | Bending | 10    | SW      | 0       | 190.0   |
| 4       | < 111 > | 80     | Bending | 10    | SW      | 0       | 187.0   |
| 5       | < 111 > | 100    | Bending | 10    | SW      | 0       | 187.0   |
| 2       | < 111 > | 14     | Bending | 300   | Tersoff | 0       | 190.0   |
| 3       | < 111 > | 21     | Bending | 300   | Tersoff | 0       | 145.0   |
| 4       | < 111 > | 28     | Bending | 300   | Tersoff | 0       | 135.0   |
| 5       | < 111 > | 35     | Bending | 300   | Tersoff | 0       | 136.0   |
| 2       | < 111 > | 16     | Bending | 300   | Tersoff | 0       | 183.0   |
| 3       | < 111 > | 24     | Bending | 300   | Tersoff | 0       | 170.0   |
| 4       | < 111 > | 32     | Bending | 300   | Tersoff | 0       | 151.0   |
| 5       | < 111 > | 40     | Bending | 300   | Tersoff | 0       | 128.0   |
| 2       | < 111 > | 18     | Bending | 300   | Tersoff | 0       | 171.0   |
| 3       | < 111 > | 27     | Bending | 300   | Tersoff | 0       | 150.0   |
| 4       | < 111 > | 36     | Bending | 300   | Tersoff | 0       | 147.0   |
| 5       | < 111 > | 45     | Bending | 300   | Tersoff | 0       | 132.0   |
| 2       | < 111 > | 20     | Bending | 300   | Tersoff | 0       | 155.0   |
| 3       | < 111 > | 30     | Bending | 300   | Tersoff | 0       | 130.0   |
| 4       | < 111 > | 40     | Bending | 300   | Tersoff | 0       | 129.0   |
| 5       | < 111 > | 50     | Bending | 300   | Tersoff | 0       | 133.0   |
| 2       | < 111 > | 24     | Bending | 300   | Tersoff | 0       | 173.0   |
| 3       | < 111 > | 36     | Bending | 300   | Tersoff | 0       | 165.0   |
| 4       | < 111 > | 48     | Bending | 300   | Tersoff | 0       | 158.0   |
| 5       | < 111 > | 60     | Bending | 300   | Tersoff | 0       | 153.0   |
| 2       | < 111 > | 28     | Bending | 300   | Tersoff | 0       | 155.0   |
| 3       | < 111 > | 42     | Bending | 300   | Tersoff | 0       | 153.0   |
| 4       | < 111 > | 56     | Bending | 300   | Tersoff | 0       | 156.0   |
| 5       | < 111 > | 70     | Bending | 300   | Tersoff | 0       | 155.0   |
| 2       | < 111 > | 32     | Bending | 300   | Tersoff | 0       | 156.0   |
| 3       | < 111 > | 48     | Bending | 300   | Tersoff | 0       | 172.0   |
| 4       | < 111 > | 64     | Bending | 300   | Tersoff | 0       | 170.0   |
| 5       | < 111 > | 80     | Bending | 300   | Tersoff | 0       | 171.0   |
| 2       | < 111 > | 36     | Bending | 300   | Tersoff | 0       | 172.0   |
| 3       | < 111 > | 54     | Bending | 300   | Tersoff | 0       | 173.0   |
| 4       | < 111 > | 72     | Bending | 300   | Tersoff | 0       | 170.0   |
| 5       | < 111 > | 90     | Bending | 300   | Tersoff | 0       | 174.0   |
| 2       | < 111 > | 40     | Bending | 300   | Tersoff | 0       | 181.0   |
| 3       | < 111 > | 60     | Bending | 300   | Tersoff | 0       | 176.0   |
| 4       | < 111 > | 80     | Bending | 300   | Tersoff | 0       | 173.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|---------|---------|---------|
| 5       | < 111 > | 100    | Bending | 300   | Tersoff | 0       | 173.0   |
| 2       | < 111 > | 14     | Bending | 300   | SW      | 0       | 182.0   |
| 3       | < 111 > | 21     | Bending | 300   | SW      | 0       | 160.0   |
| 4       | < 111 > | 28     | Bending | 300   | SW      | 0       | 145.0   |
| 5       | < 111 > | 35     | Bending | 300   | SW      | 0       | 135.0   |
| 2       | < 111 > | 16     | Bending | 300   | SW      | 0       | 195.0   |
| 3       | < 111 > | 24     | Bending | 300   | SW      | 0       | 184.0   |
| 4       | < 111 > | 32     | Bending | 300   | SW      | 0       | 170.0   |
| 5       | < 111 > | 40     | Bending | 300   | SW      | 0       | 165.0   |
| 2       | < 111 > | 18     | Bending | 300   | SW      | 0       | 195.0   |
| 3       | < 111 > | 27     | Bending | 300   | SW      | 0       | 185.0   |
| 4       | < 111 > | 36     | Bending | 300   | SW      | 0       | 175.0   |
| 5       | < 111 > | 45     | Bending | 300   | SW      | 0       | 172.0   |
| 2       | < 111 > | 20     | Bending | 300   | SW      | 0       | 198.0   |
| 3       | < 111 > | 30     | Bending | 300   | SW      | 0       | 184.0   |
| 4       | < 111 > | 40     | Bending | 300   | SW      | 0       | 181.0   |
| 5       | < 111 > | 50     | Bending | 300   | SW      | 0       | 180.0   |
| 2       | < 111 > | 24     | Bending | 300   | SW      | 0       | 205.0   |
| 3       | < 111 > | 36     | Bending | 300   | SW      | 0       | 185.0   |
| 4       | < 111 > | 48     | Bending | 300   | SW      | 0       | 176.0   |
| 5       | < 111 > | 60     | Bending | 300   | SW      | 0       | 178.0   |
| 2       | < 111 > | 28     | Bending | 300   | SW      | 0       | 211.0   |
| 3       | < 111 > | 42     | Bending | 300   | SW      | 0       | 186.0   |
| 4       | < 111 > | 56     | Bending | 300   | SW      | 0       | 176.0   |
| 5       | < 111 > | 70     | Bending | 300   | SW      | 0       | 175.0   |
| 2       | < 111 > | 32     | Bending | 300   | SW      | 0       | 210.0   |
| 3       | < 111 > | 48     | Bending | 300   | SW      | 0       | 189.0   |
| 4       | < 111 > | 64     | Bending | 300   | SW      | 0       | 184.0   |
| 5       | < 111 > | 80     | Bending | 300   | SW      | 0       | 183.0   |
| 2       | < 111 > | 36     | Bending | 300   | SW      | 0       | 208.0   |
| 3       | < 111 > | 54     | Bending | 300   | SW      | 0       | 203.0   |
| 4       | < 111 > | 72     | Bending | 300   | SW      | 0       | 200.0   |
| 5       | < 111 > | 90     | Bending | 300   | SW      | 0       | 195.0   |
| 2       | < 111 > | 40     | Bending | 300   | SW      | 0       | 195.0   |
| 3       | < 111 > | 60     | Bending | 300   | SW      | 0       | 196.0   |
| 4       | < 111 > | 80     | Bending | 300   | SW      | 0       | 197.0   |
| 5       | < 111 > | 100    | Bending | 300   | SW      | 0       | 197.0   |
| 2       | < 111 > | 14     | Bending | 600   | Tersoff | 0       | 170.0   |
| 3       | < 111 > | 21     | Bending | 600   | Tersoff | 0       | 140.0   |
| 4       | < 111 > | 28     | Bending | 600   | Tersoff | 0       | 100.0   |



Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT     | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|---------|---------|---------|
| 5       | < 111 > | 35     | Bending | 600   | Tersoff | 0       | 91.0    |
| 2       | < 111 > | 16     | Bending | 600   | Tersoff | 0       | 165.0   |
| 3       | < 111 > | 24     | Bending | 600   | Tersoff | 0       | 150.0   |
| 4       | < 111 > | 32     | Bending | 600   | Tersoff | 0       | 145.0   |
| 5       | < 111 > | 40     | Bending | 600   | Tersoff | 0       | 144.0   |
| 2       | < 111 > | 18     | Bending | 600   | Tersoff | 0       | 160.0   |
| 3       | < 111 > | 27     | Bending | 600   | Tersoff | 0       | 145.0   |
| 4       | < 111 > | 36     | Bending | 600   | Tersoff | 0       | 125.0   |
| 5       | < 111 > | 45     | Bending | 600   | Tersoff | 0       | 118.0   |
| 2       | < 111 > | 20     | Bending | 600   | Tersoff | 0       | 165.0   |
| 3       | < 111 > | 30     | Bending | 600   | Tersoff | 0       | 160.0   |
| 4       | < 111 > | 40     | Bending | 600   | Tersoff | 0       | 155.0   |
| 5       | < 111 > | 50     | Bending | 600   | Tersoff | 0       | 148.0   |
| 2       | < 111 > | 24     | Bending | 600   | Tersoff | 0       | 181.0   |
| 3       | < 111 > | 36     | Bending | 600   | Tersoff | 0       | 178.0   |
| 4       | < 111 > | 48     | Bending | 600   | Tersoff | 0       | 171.0   |
| 5       | < 111 > | 60     | Bending | 600   | Tersoff | 0       | 165.0   |
| 2       | < 111 > | 28     | Bending | 600   | Tersoff | 0       | 180.0   |
| 3       | < 111 > | 42     | Bending | 600   | Tersoff | 0       | 179.0   |
| 4       | < 111 > | 56     | Bending | 600   | Tersoff | 0       | 164.0   |
| 5       | < 111 > | 70     | Bending | 600   | Tersoff | 0       | 163.0   |
| 2       | < 111 > | 32     | Bending | 600   | Tersoff | 0       | 184.0   |
| 3       | < 111 > | 48     | Bending | 600   | Tersoff | 0       | 182.0   |
| 4       | < 111 > | 64     | Bending | 600   | Tersoff | 0       | 175.0   |
| 5       | < 111 > | 80     | Bending | 600   | Tersoff | 0       | 173.0   |
| 2       | < 111 > | 36     | Bending | 600   | Tersoff | 0       | 183.0   |
| 3       | < 111 > | 54     | Bending | 600   | Tersoff | 0       | 183.0   |
| 4       | < 111 > | 72     | Bending | 600   | Tersoff | 0       | 178.0   |
| 5       | < 111 > | 90     | Bending | 600   | Tersoff | 0       | 177.0   |
| 2       | < 111 > | 40     | Bending | 600   | Tersoff | 0       | 181.0   |
| 3       | < 111 > | 60     | Bending | 600   | Tersoff | 0       | 182.0   |
| 4       | < 111 > | 80     | Bending | 600   | Tersoff | 0       | 178.0   |
| 5       | < 111 > | 100    | Bending | 600   | Tersoff | 0       | 179.0   |
| 2       | < 111 > | 14     | Bending | 600   | SW      | 0       | 201.0   |
| 3       | < 111 > | 21     | Bending | 600   | SW      | 0       | 188.0   |
| 4       | < 111 > | 28     | Bending | 600   | SW      | 0       | 167.0   |
| 5       | < 111 > | 35     | Bending | 600   | SW      | 0       | 168.0   |
| 2       | < 111 > | 16     | Bending | 600   | SW      | 0       | 215.0   |
| 3       | < 111 > | 24     | Bending | 600   | SW      | 0       | 201.0   |
| 4       | < 111 > | 32     | Bending | 600   | SW      | 0       | 189.0   |

Table A.1: Molecular dynamics database used for machine learning.

| CD (nm) | ORNT    | L (nm) | BC      | T (K) | POT | SS (nm) | E (GPa) |
|---------|---------|--------|---------|-------|-----|---------|---------|
| 5       | < 111 > | 40     | Bending | 600   | SW  | 0       | 181.0   |
| 2       | < 111 > | 18     | Bending | 600   | SW  | 0       | 199.0   |
| 3       | < 111 > | 27     | Bending | 600   | SW  | 0       | 190.0   |
| 4       | < 111 > | 36     | Bending | 600   | SW  | 0       | 185.0   |
| 5       | < 111 > | 45     | Bending | 600   | SW  | 0       | 183.0   |
| 2       | < 111 > | 20     | Bending | 600   | SW  | 0       | 184.0   |
| 3       | < 111 > | 30     | Bending | 600   | SW  | 0       | 181.0   |
| 4       | < 111 > | 40     | Bending | 600   | SW  | 0       | 182.0   |
| 5       | < 111 > | 50     | Bending | 600   | SW  | 0       | 183.0   |
| 2       | < 111 > | 24     | Bending | 600   | SW  | 0       | 193.0   |
| 3       | < 111 > | 36     | Bending | 600   | SW  | 0       | 196.0   |
| 4       | < 111 > | 48     | Bending | 600   | SW  | 0       | 193.0   |
| 5       | < 111 > | 60     | Bending | 600   | SW  | 0       | 193.0   |
| 2       | < 111 > | 28     | Bending | 600   | SW  | 0       | 190.0   |
| 3       | < 111 > | 42     | Bending | 600   | SW  | 0       | 183.0   |
| 4       | < 111 > | 56     | Bending | 600   | SW  | 0       | 180.0   |
| 5       | < 111 > | 70     | Bending | 600   | SW  | 0       | 179.0   |
| 2       | < 111 > | 32     | Bending | 600   | SW  | 0       | 192.0   |
| 3       | < 111 > | 48     | Bending | 600   | SW  | 0       | 188.0   |
| 4       | < 111 > | 64     | Bending | 600   | SW  | 0       | 182.0   |
| 5       | < 111 > | 80     | Bending | 600   | SW  | 0       | 182.0   |
| 2       | < 111 > | 36     | Bending | 600   | SW  | 0       | 193.0   |
| 3       | < 111 > | 54     | Bending | 600   | SW  | 0       | 191.0   |
| 4       | < 111 > | 72     | Bending | 600   | SW  | 0       | 192.0   |
| 5       | < 111 > | 90     | Bending | 600   | SW  | 0       | 193.0   |
| 2       | < 111 > | 40     | Bending | 600   | SW  | 0       | 215.0   |
| 3       | < 111 > | 60     | Bending | 600   | SW  | 0       | 218.0   |
| 4       | < 111 > | 80     | Bending | 600   | SW  | 0       | 221.0   |
| 5       | < 111 > | 100    | Bending | 600   | SW  | 0       | 219.0   |