

A New Composite Resonator Architecture based on Coupled Vertical NW Arrays

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Yasin KILINÇ

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Yasin KILINÇ

and have found that it is complete and satisfactory in all respects,
and that any and all revisions required by the final
examining committee have been made.

Committee Members:

B. Erdem Alaca, Ph.D. (Advisor)

Yusuf Leblebici, Prof.

Demircan Canadinç, Ph.D.

Arda D. Yalçinkaya, Ph.D.

Alphan Sennaroğlu, Ph.D.

Date: _____



ABSTRACT

A new composite resonator architecture is developed at the nanoscale by stacking nanowires (NWs) perpendicular to the surface of a substrate and coupling the NWs in the resulting vertical array mechanically by means of a membrane-type coupling element called coupling membrane (CM). Employment of CMs corresponds to a significant expansion to rather limited mechanical coupling toolkit at the nanoscale due to connections even between non-adjacent resonators. Electromechanical characterization of resonators is performed using electrostatic actuation and piezoresistive readout to ensure the best integration possibility with on-chip electronics in the future. Electrical measurements are performed not only for coupled vertical NW arrays but also for single clamped-clamped NWs to examine effects of mechanical coupling and multiple resonators in an array on frequency spectrum characteristics. Coupled NW arrays consisting of 8 NWs designed based on finite element modeling (FEM) modal analysis simulations are fabricated using the developed top-down fabrication flow from the 1 μm thick device layer of a silicon-on-insulator (SOI) wafer. Effects of resonator and coupling element on frequency spectrum response are studied separately by changing the lengths of NW and CM systematically. Two piezoresistive frequency downmixing techniques of the two-source/ 1ω and two-source/ 2ω schemes are compared in terms of detected signal amplitudes and their dependence on gate voltages. In general, frequency spectrum measurements provide mechanical modes up to 130 MHz in high vacuum. Electromechanical characterization of piezoresistive single Si NW samples fabricated in the 10 μm thick device layer of a SOI substrate is demonstrated for the first time in the literature. Detected mechanical modes from 18 MHz to 101 MHz for single NW samples are successfully associated to the first flexural in-plane and out-of-plane modes using FEM simulations thanks to the determination of an actual NW cross section by TEM measurements. Moreover, NW array measurements result in multiple mechanical modes both dispersed in a wide frequency range and in close proximity such that being reminiscent of typical spectrum response of a bandpass filter. However, inevitable nonuniformity of NWs in an array and absence of accurate spatial measurements complicate implementation of FEM simulations in the NW array case. Thus, FEM simulations are conducted to investigate more fundamental issues such as proving existence of mechanical coupling between NWs in a stack by distinguishing collective array modes from an individual NW resonance. To this end, experimental resonance frequency shifts of single NW and NW array samples with respect to electrode voltages are compared between each other and with FEM results. These comparisons between simulations and measurements reveal similar and distinct characteristics simultaneously for different spectrum modes.

ÖZETÇE

Alttaş yüzeyine dik olarak nanotellerin istiflenmesi ve meydana gelen dikey dizideki nanotellerin kuplaj membranı olarak adlandırılan membran tipi bağlama elemanları ile mekanik olarak bağlanması ile nano ölçeğinde yeni bir kompozit çınlaç mimarisi geliştirilmiştir. Kuplaj membranı kullanımı birbirleriyle komşu olmayan çınlaçların bile bağlanması sebebiyle nano ölçeğinde kısıtlı olan mekanik kuplaj araç takımı için önemli bir genişlemeye karşılık gelmektedir. Yonga üzerindeki elektronik devrelerle gelecekteki en iyi bütünleşme olasılığını güvenceye almak için çınlaçların elektromekanik karakterizasyonu elektrostatik tahrik ve piezoresistif okuma kullanarak yapılmıştır. Mekanik bağlamanın ve çoklu çınlaçların tel dizisinin frekans spektrum karakteristikleri üzerindeki etkilerini sınamak için elektriksel ölçümler sadece bağlı nanotel dizileri için değil iki ucu sabitlenmiş tekli nanoteller için de gerçekleştirilmiştir. Tasarımı sonlu eleman modal analiz simülasyonlarına dayanan, 8 nanotelden oluşan bağlı nanotel dizileri geliştirilen tepeden inme üretim şeması kullanılarak 1 μm cihaz katmanına sahip yalıtkan üstü silisyum alttaştan üretilmiştir. Çınlaç ve bağlama elemanının frekans spektrumu cevabı üzerine etkileri nanotel ve kuplaj membranı uzunluklarını sistematik olarak değiştirerek çalışılmıştır. Kullanılan piezoresistif frekans indirgeme teknikleri olan iki-kaynak/ 1ω ve iki-kaynak/ 2ω şemaları ölçülen sinyal genlikleri ve sinyalin elektrot voltajına bağlılığı bakımından karşılaştırılmıştır. Genel olarak frekans spektrum ölçümleri yüksek vakumda 130 MHz'e kadar mekanik modlar sağlamıştır. 10 μm cihaz katmanı kalınlığına sahip yalıtkan üstü silisyum alttaştan üretilen piezoresistif tekli silisyum nanotellerin elektromekanik karakterizasyonları literatürde ilk kez gösterilmiştir. Tekli nanotel numuneleri için 18 MHz'den 101 MHz'e kadar saptanan mekanik modlar geçirmeli elektron mikroskobu ölçümleri ile gerçek nanotel kesitinin belirlenmesi sayesinde yapılan sonlu eleman simülasyonları sonucunda ilk eğilme düzlem içi ve düzlem dışı modlarına başarıyla ilişkilendirilmiştir. Ek olarak, nanotel dizisi için spektrum ölçümleri hem geniş bir frekans aralığında dağılan hem de bir bant-geçirgen elektromekanik filtrenin tipik spektrum cevabını hatırlatacak şekilde çok yakın bir şekilde yerleşen çoklu mekanik modlara yol açmıştır. Buna karşılık, dizi içerisinde bulunan nanoteller arasındaki kaçınılmaz boyutsal benzeşmezlikler ve hassas boyutsal ölçümler eksikliği nanotel dizisi için sonlu eleman simülasyonlarının gerçekleştirilmesini karmaşıktırmaktadır. Bu sebeple sonlu eleman simülasyonları, müşterek dizi modlarının tekli nanotel rezonanslarından ayırarak dizi içerisindeki mekanik bağın varlığını kanıtlamak gibi daha temel konuları araştırmak için yapılmıştır. Bu maksatla, tekli nanotel ve nanotel dizilerinin elektrot voltajına bağlı olarak çınlama frekansındaki deneysel kaymalar birbirleriyle ve simülasyon sonuçları ile karşılaştırılmıştır. Ölçümler ve simülasyonlar arasındaki bu karşılaştırmalar farklı spektrum modları için benzer ve farklı karakteristikleri ortaya çıkarmıştır.

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NOMENCLATURE

BOX	Buried oxide
BW	Electromechanical filter bandwidth
CM	Coupling membrane
DRIE	Deep reactive ion etching
FEM	Finite element modeling
f_0	Electromechanical filter center frequency
MEMS	Microelectromechanical System
NEMS	Nanoelectromechanical System
NW	Nanowire
Q	Quality factor
SOI	Silicon-on-insulator
$\lambda/4$	Quarter-wavelength

Chapter 1: Introduction to electromechanical resonators and filters

Exact beginning of time can be traced back to the creation of the universe *i.e.* the big bang. From early on, humans observed the cyclic nature of various worldly phenomena such as daily sunrise and sunset, subsequent change of seasons, regular flooding of rivers. They perceived all of these events as if connected with some invisible chain called time. Thus, they have begun their long journey to first estimate and then control of recurring events *i.e.* subduing the world by determining and quantifying time. However, it is not surprising to see that they were more interested in relative rather than absolute time measurements with their crude equipment such as sundial.

Importance of accurate timekeeping was exploded in “modern times” with quantification and optimization of every aspect of life such as worker working efficiency. Growing synchronization requirements stemming from global communication demands convert the world little larger than a village. A typical timekeeping device has two fundamental components namely a frequency reference and a counter. An ideal frequency reference device *i.e.* an oscillator provides oscillatory output with a given time period to detect the passage of a certain time interval. A counter is employed to measure the number of intervals precisely.

Introduction of digital electronics in the 20th century enables to separate the two components of a timekeeper and study them separately. A frequency reference now forming an indispensable subpart of almost all electronic systems is used to regulate rudimentary system functions in addition to determine elapsed time period. Billions of frequency reference devices are now fabricated annually in the form of radio and digital systems such as computers, mobile phones, televisions, wearables, global positioning systems (GPS) etc.

Any kind of system demonstrating some resonance behavior can be employed as a frequency reference such as pendulum, beam, tuning fork, guitar string and resistor-inductor-capacitance (RLC) circuit. Strong dependence of oscillator characteristics such as resonance frequency, quality factor (Q), frequency stability and aging on the type of employed resonator requires that selection of a proper resonator in order to meet specific design criteria is an essential part of a frequency reference design. Oscillator technologies differ fundamentally due to use of different types of resonators.

Traditionally, crystal and all-electronic oscillators were employed for frequency reference applications. A simple RC- or LC-based resonance circuit can provide a frequency reference for all-electronic oscillators. Microelectronics compatibility and batch manufacturability of all-

electronic oscillators make them especially suited for applications where shock immunity, device size and cost are main priorities. Low frequency stability and high power consumption associated with low resonator Q are among the fundamental challenges of all-electronic oscillators. Low frequency stability of all-electronic oscillators can be compensated with on-chip temperature compensation at the expense of further system complexity and an increase in already high power consumption.

On the other hand, electromechanical crystal oscillators such as surface acoustic wave (SAW), film bulk acoustic wave (FBAR) and quartz tuning fork are based on piezoelectric materials that readily convert mechanical energy as a vibration signal into electrical energy as a voltage or current signal or vice versa. This signal conversion between mechanical and electrical domains back and forth is used to engineer an oscillator output signal having desired frequency spectrum characteristics. Quartz provides best performance in terms of frequency stability and low power dissipation at the highest cost for high-precision frequency applications. Thus, intense research and development efforts have been made for the quartz technology starting with the first demonstration in 1922 [1]. Challenges associated with the quartz technology are two-fold. First, relatively large sizes of Quartz oscillators together with their little capability for further miniaturization present a formidable obstacle to reduce unit cost in contrast to contemporary oscillator miniaturization trends following Moore's Law. Second, incompatibilities with common Si-based microsystems or complementary-metal-oxide-semiconductor (CMOS) electronics necessitate extra board-level integration with additional electronics at the expense of overall size, cost, power consumption and noise level increases.

The bottleneck of crystal oscillators related to miniaturization and CMOS integration is addressed with the introduction of microelectromechanical systems (MEMS) oscillators. MEMS oscillators are based on a miniature resonating mass made of usually silicon or similar materials. Miniaturization process from macroscopic to microscopic resonators dating back to 1960s was accelerated with novel design concepts and new processing techniques together with the expansion of the set of MEMS materials.

The first MEMS resonator fabricated as a microcantilever was employed as a frequency selector in conjunction with integration circuits [2]. Though initial MEMS resonators offered considerable size reductions, they suffered from low resonator Q s, reliability issues and temperature instabilities. However, these issues were overcome over time with novel hermetic sealing and on-chip digital tuning technologies leading to resonator Q s more than 100 000 in vacuum [3] and resonance frequency temperature coefficients much less than -10 ppm/ $^{\circ}\text{C}$ [4].

Although MEMS resonators have long been studied for a variety of geometries [3, 5], transduction techniques [6, 7], materials [7-9] and resonator excitation modes [3, 10] etc. In order to reach

resonance frequencies higher than those provided by comb-drive based architecture, flexural resonators having various geometries such as double-clamped [11] or free-free beam [12] or disc [13], ring [14], tuning fork [15] and square plate resonators [16] etc. were investigated thoroughly. Some of the examined MEMS resonator configurations are shown in Fig. 1.1.

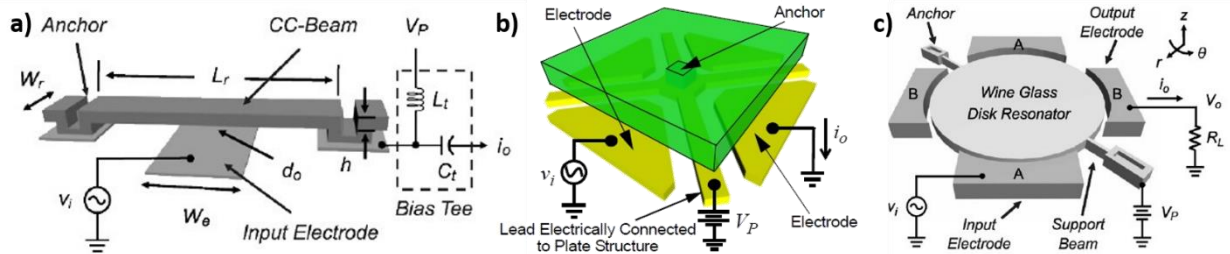


Figure 1. 1: MEMS resonators in the shape of a clamped-clamped beam (a) [17], a plate (b) [18] or a disc (c) [17] together with capacitive transduction schemes.

Resonators based on MEMS are utilized widely in on-chip, high Q and low insertion loss oscillators [19-22]. Thus, MEMS oscillators having performance characteristics on par with some crystal oscillators enjoy a fast-growing commercial application portfolio when considered additional miniaturization and a high level of integration advantages. MEMS oscillators are already engaged in head-on competition with 32 kHz crystal counterparts in the timing market with less than 1 μ A power consumption and ± 5 ppm frequency stability for mobile and wearable electronics [23]. For example, a 524-kHz Si double tuning fork design featuring ± 100 ppm frequency stability and approximately 100- μ A power consumption can provide oscillation frequencies up to 26 MHz [24].

As the size of a resonator shrinks, involved minuscule displacements even at resonance and significantly increased motional impedance cause detection of motion-dependent readout signals increasingly difficult. In oscillator applications with capacitive readout, reduction of motional impedances can be achieved by various ways such as reduction of electrode-to-resonator gap [25], raising DC potential applied to the resonator itself or employment of multiple resonators. Arraying resonators in a stack is preferred over other mentioned solutions since superimposing the currents stemming from motion of individual resonators decreases overall motional impedance proportional to number of employed resonators without introduction of nonlinearity [16, 26, 27].

Further miniaturization of MEMS resonators presents nanoelectromechanical system (NEMS) resonators as the next stage of evolution with operation frequencies in extreme UHF and microwave bands. Although impedance reduction solutions such as resonator arraying suggested for MEMS-based architectures can be exploited to inspire further progress for NEMS resonators, scaling induced challenges emphasized at the nanoscale such as adsorption-desorption noise, low dynamic range [28], temperature fluctuation noise and insufficient power handling become even more severe for NEMS resonators.

Dependence of the resonance frequency of a resonator on its dimensions simply makes impossible to fabricate identical resonators in an array having a common resonance frequency. Hence, slightly different resonators in an array result in a different individual resonant frequency for each resonator having detrimental effect on signal amplitude gains at a common in-phase signal frequency [18]. Thus, it is imperative to use some kind of coupling through mechanical or electrical means to compensate small resonance frequency deviations of resonators in an array. In this way, use of resonators in a parallel configuration rather than a single resonator structure to increase the magnitude of an output signal proportional to resonator number can be ensured by mechanical coupling by providing in-phase resonances for even considerable different resonators in the array.

Another issue related to the use of multiple resonators in a parallel array is the increase of overall resonator real estate in the plane of a substrate proportional to number of resonators in an array reported for MEMS resonator arrays in the literature [27]. Moreover, the use of mechanical coupling in a resonator array is shown to enhance resonator fabrication precision by decreasing device-to-device resonance frequency deviations [29].

The use of coupling in coupled resonant systems represents a variety of advantages. These include providing improvements in device properties such as increased sensitivity to perturbations [30], enabling completely new functionalities such as signal filtering [31] and mixing [32] and more control on resonator properties such as motional resistance and reproducibility [33] etc. Sensitivity improvements are even accentuated by switching from micro to nano structures [34].

One of the most promising applications of MEMS resonators is in electrical signal filtering. MEMS electromechanical filters are used in multi-band, multi-mode wireless applications such as wireless receivers as RF channel select filter banks [31, 35]. Starting from one of the first MEMS filters with a filter center frequency (f_0) of 300-340 kHz and Q of 590-800 consisting of three mechanically-coupled resonators with a comb-drive-based architecture [36, 37], much research efforts in this field has been channeled to increase filter resonance frequency and Q simultaneously.

Although the most common excited mode for any individual resonator in a filter is the first out-of-plane flexural mode in the literature, any resonance mode can be accentuated by proper selection of transduction mechanism, electrode placement and signal phasing [38]. MEMS filters comprised of resonators having different excited modes of flexural [25], extensional [10], wine-glass [39] or whispering gallery [3] modes were also studied.

Mechanical coupling between sequential resonators can be delivered either by employing various mechanical elements such as unusual U- [40] and V- [41] shaped coupling beams or altering

resonator anchor characteristics by undercutting ledges of suspended arrays [42, 43], the latter being the only reported mechanical coupling technique at the nanoscale.

Fig. 1.2.a presents the most common series out-of-plane flexural second-order electromechanical filter in the literature together with input/output electrodes and corresponding filter mode shapes. It consists of two clamped-clamped beam resonators. The resonators are coupled mechanically through a flexural-mode coupling beam at a specific point along the resonator length.

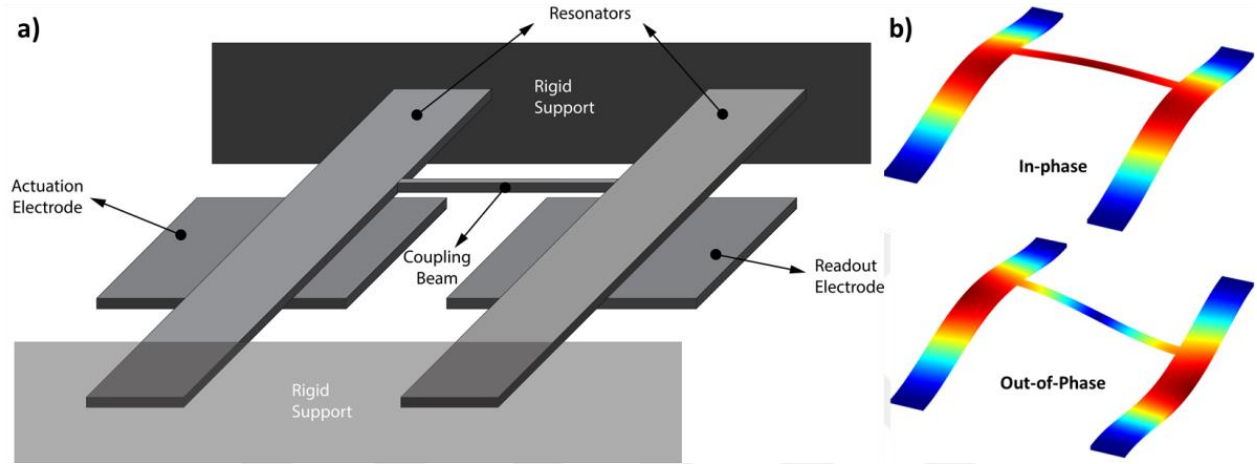


Figure 1. 2: (a) Second-order out-of-plane electromechanical filter together with electrodes (b) Associated in-phase and out-of-phase filter mode shapes

An electromechanical filter is effectively a signal engineering device being composed of mechanical (acoustic) resonators and coupling elements. At a filter input port, an electrical input signal is converted to a mechanical signal to be engineered in the mechanical domain. Then, the processed mechanical signal is converted back to another electrical signal at a filter output port. Electrostatic transduction between a resonator and an actuation electrode induces mechanical vibrations. Connecting resonator pairs with a network of coupling beams results in filter modes proportional to the number of resonators in a filter. Lowest frequency array mode consisting of resonators vibrating in the same direction together is called the in-phase mode. Besides, each resonator moves in the opposite direction of neighboring resonators in case of the out-of-phase mode. These modes correspond to distinct peaks in the associated filter frequency spectrum. The in-phase and out-of-phase modes are shown in Fig. 1.2.b for the out-of-plane flexural second-order electromechanical filter of Fig. 1.2.a.

Multiple resonators coupled mechanically with certain coupling elements can be stacked to form parallel resonator architecture. As mentioned previously, parallel stacking of resonators of various types such as beams, plates or discs is employed to enhance robustness of MEMS and NEMS. Moreover, parallel resonator stacks can be combined through different coupling elements in a series fashion to form an electromechanical filter similar to single resonators. These so-called composite structures are used to enhance and tune frequency spectrum characteristics such as

signal-to-noise ratio, phase noise, filter shape factor and bandpass ripple. Figure 1.3 exemplifies some of the parallel and series resonator stacks investigated in the literature.

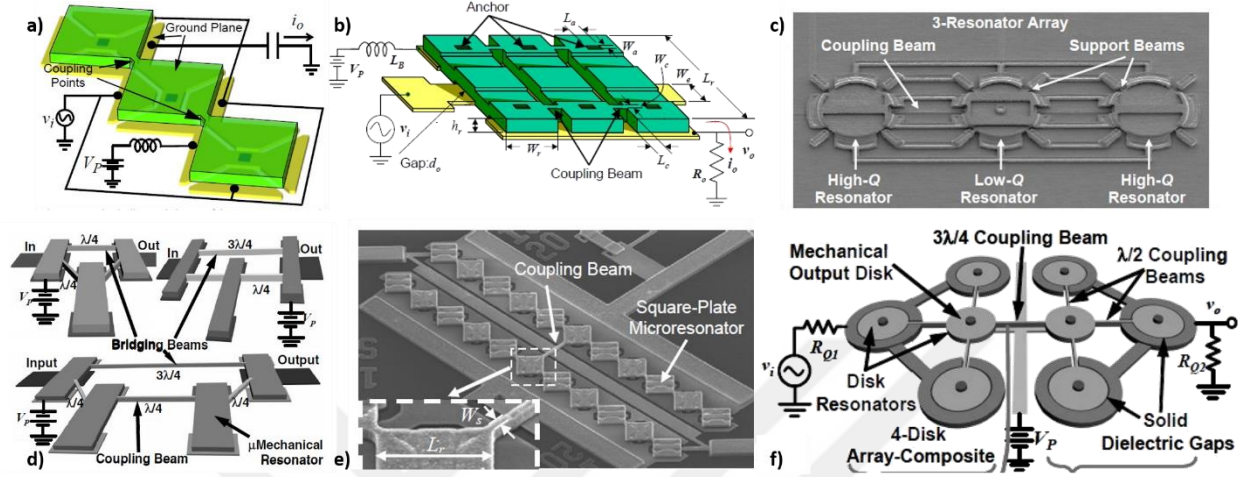


Figure 1. 3: In addition to individual resonators in (d) [44], mechanical coupling of several parallel resonator arrays consisting of plates (a) [18], free-free beams (b) [45] and discs (c) [46] results in composite electromechanical filters (e [27], f [47])

Fig. 1.4a-b compares frequency spectrum responses from an oscillator and electromechanical filter using parallel and series MEMS resonator stacks. Effect of various MEMS filter design parameters such as number of resonators, coupling beam dimensions and schemes, coupling location, anchor properties on frequency spectrum characteristics such as phase noise, filter Q , passband ripple, dynamic range and insertion loss is investigated rigorously to engineer filter signal output accordingly. Moreover, numerous oscillators and electromechanical filters consisting of MEMS parallel and series resonator stacks can be fabricated on a single die to address certain frequency bands for various applications specifically as shown in Fig. 1.4.c [48].

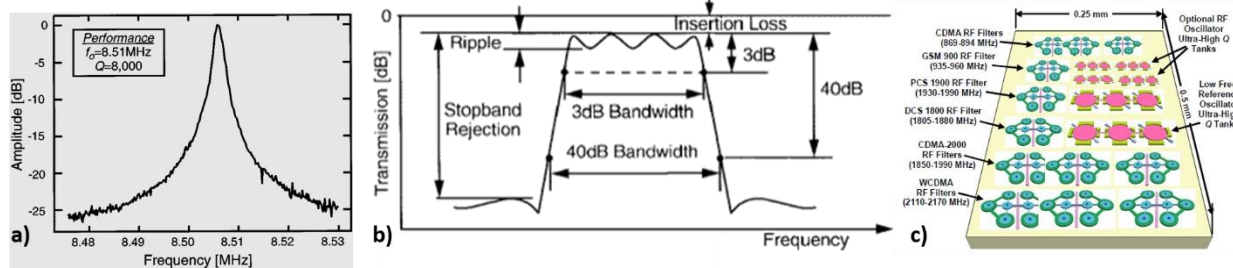


Figure 1.4: Parallel and series MEMS resonators stacks yielding distinct spectrum responses in (a) [25] and in (b) [49] respectively can be fabricated on a chip to address particular frequency bands specifically (c) [48].

Similar to early macroscopic electromechanical filters, MEMS filters are designed by equivalent circuit modeling methodologies to get a desired filtering behavior. Once the equivalent circuit of an electromechanical filter is obtained, integration of a filter with the rest of mechanical/electrical components in a system in the electrical domain and further processing of an output signal by subsequent electronic stages are possible.

Electromechanical modeling of a single MEMS/NEMS resonator is based on well-established analytical techniques [10, 25, 50]. Although the idea of mechanical coupling and the associated introduction of collective modes are interesting, the addition of a coupling beam into the overall picture necessitates a proper coupling beam design for a successful device implementation. When the coupling beam mass is on the same order of the resonator mass as in the case of micro/nanoscale filters, this mass has to be taken into consideration, complicating further coupling beam design [25]. Moreover, analytical methods used to model MEMS/NEMS resonators cannot be borrowed to model coupling and support beams directly.

In the literature, an analytical approach known as quarter-wavelength ($\lambda/4$) modeling is employed to design coupling beams and support beams [38, 49]. The $\lambda/4$ model imposes certain coupling beam lengths for a given resonator geometry to maximize Q . Moreover, analytical solutions are only available for a limited number of coupling beam designs having specific boundary conditions. Furthermore, the $\lambda/4$ model loses its accuracy to predict the lumped parameters of a coupling beam, when the coupling beam's width becomes comparable to that of attached resonators. These inaccuracies lead to significant deviations between designed and realized filter spectrum characteristics. Instead, a numerical filter modeling methodology can be developed to have filter spectrum properties as a function of coupling dimensions directly from modal analyses using finite element modeling. Thus, any mechanical coupling modeling methodology should reflect the specific coupling beam configuration at hand.

Further miniaturization of established MEMS filters in the literature down to the nanoscale is a straightforward way to increase their operation frequencies. However, considering cases where utilization of very compliant *i.e.* very thin coupling beams is required even for microscale systems, direct scaling of existing mechanically-coupled MEMS filter structures into the nanoscale seems impractical. Moreover, scaling-induced limitations emphasized at the nanoscale such as insufficient power handling may enforce employment of multiple sensors. Resonator coupling represents more than frequency selective on-chip components. For example, amplification in sensor sensitivity to perturbations can be achieved as a result of coupling [30]. Thus, delivering desired level of mechanical coupling at the nanoscale is highly crucial.

Furthermore, the conventional coupling beam of Fig. 1.2.a can only be used to connect sequential resonators in the series filter architecture [31, 35, 45]. Sophisticated mechanical coupling schemes providing coupling between non-adjacent resonators using extra coupling beams were shown to improve frequency spectrum characteristics with sharper roll-offs and improved stopband rejections [44]. However, the capacity to deliver mechanical coupling between non-adjacent resonators using coupling beams is limited even with an innovative filter layout. Thus, a coupling scheme delivering mechanical coupling for any resonator pair irrespective of resonator number for any beam-based filter configuration would be a significant improvement. Currently no solution

exists in the literature at the nanoscale level for both mechanical coupling and arraying of individual resonators while keeping the oscillator real estate shrinking.

This thesis describes design, fabrication, electrical characterization and numerical modeling of an innovative composite resonator architecture at the nanoscale. Chapter 2 discusses the two important aspects of the developed device namely vertical arraying and mechanical coupling. A nanomechanical resonator array is formed by stacking resonators perpendicular to the surface of a substrate. Mechanical coupling between NWs in a vertical array is achieved through use of membrane-type coupling elements. Development and process characterization of the fabrication flow used to realize designed coupled vertical NW arrays is considered in Chapter 3. Frequency spectrum measurements presented in Chapter 4 are implemented not only for fabricated coupled vertical NW arrays but also for single clamped-clamped NWs to understand the effects of mechanical coupling and multiple resonators in an array on frequency spectrum characteristics. Comparison of measured spectrum responses of various single and coupled array samples coupled with numerical simulations is performed in Chapter 5 to extract the conclusions presented in Chapter 6.

Chapter 2: Vertical Coupled NW Arrays

2.1. Mechanical Coupling by Coupling Membrane at the Nanoscale

Instead of the traditional coupling beam of Fig. 2.1.a, the use of membrane-type coupling elements of Fig. 2.1.b is proposed as a new and versatile coupling scheme. Suggested coupling membrane (CM) corresponds to a significant expansion to the rather limited mechanical coupling toolkit at the nanoscale.

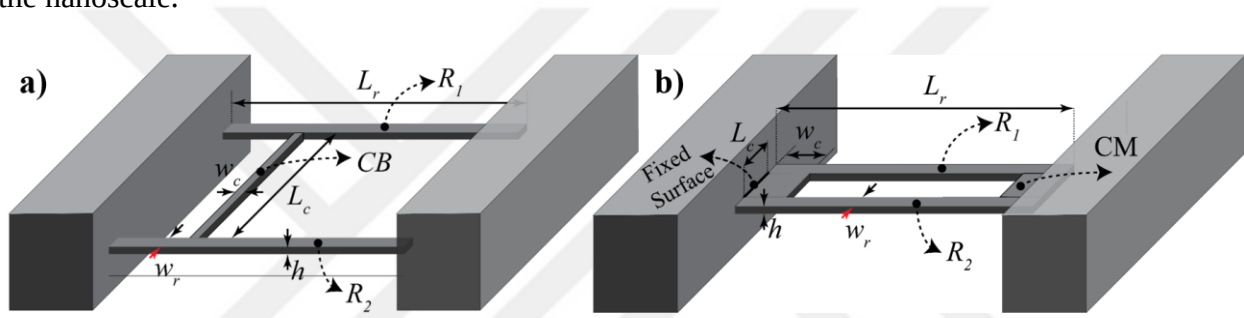


Figure 2. 1: (a) Schematic of a second-order electromechanical filter together with resonator and coupling beam design parameters, (b) Proposed filter structure employing CMs to deliver the desired level of mechanical coupling at the nanoscale.

Contrary to the coupling beam of Fig. 2.1.a, one of the side surfaces of each CM is fixed as shown in Fig. 2.1.b. Thus, this boundary condition modification effectively sets the attachment location of a CM fixed at the end of resonators. Number of resonators in any composite resonator architecture can be increased at will. However, CMs with lengths of only a fraction of adjoined resonator length enable very large resonator density. The compactness of the resonator configuration of Fig 2.1.b thanks to short CMs becomes even more advantageous considering the downscaling from the micro to the nanoscale. Switching from horizontal to vertical arrays of resonators as shown in Fig. 2.2 seems instrumental to reach even higher resonator densities.

In this thesis, an innovative and flexible mechanical coupling scheme is proposed at the nanoscale as shown in Fig. 2.2. A nanomechanical resonator array is formed by stacking resonators perpendicular to the surface of the substrate that holds the array. Mechanical coupling is achieved through the use of CMs between one-dimensional nanomechanical resonators in a vertical array as depicted in Fig. 2.2 for the case of double-clamped nanomechanical resonators. In this way, all adjacent or non-adjacent beams are connected by common CMs at their ends. Then, the resulting nanomechanical resonator array is placed between a pair of electrodes, one for actuation and one for readout to ensure electronic compatibility.

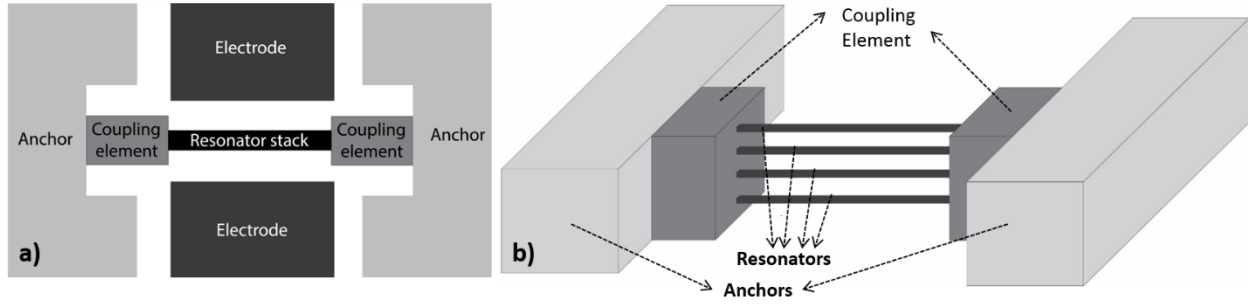


Figure 2. 2: Top (a) and perspective (b) view of the proposed composite resonator configuration consisting of vertical NW array coupled with CM at their ends

Employment of mechanical coupling to eliminate the decoupling of the vibration modes of a NW array due to fabrication-based limitations is demonstrated as follows. The effect of resonator-to-resonator variation on the frequency spectrum response of a vertical stack of NWs are shown in Fig. 2.3. Vertical NW array consists of beams having a common length of $10\text{ }\mu\text{m}$ and diameters ranging from 85 nm to 100 nm . Absence of any coupling between NWs by elimination of CMs altogether leads to a frequency spectrum featuring individual modes of these non-identical resonators *i.e.* decoupling of the vibration modes. Moreover, limited number of resonators in motion at any mode frequency results in lower readout signals measured from a gate electrode. On the other hand, some mechanical coupling between these non-identical nanoresonators is introduced through a CM of the width, height and length of $0.13\text{ }\mu\text{m}$, $1.6\text{ }\mu\text{m}$ and $5.0\text{ }\mu\text{m}$ at both ends of the resonators. A three-fold signal amplitude increase is realized for the resonator array at a lower frequency mode where all resonators vibrate in-phase.

Vertical stacking of nanoresonators together with common actuation and readout electrodes occupy a much less real estate than horizontally-stacked arrays along the plane of a substrate irrespective of number of resonators in an array for the proposed resonator array design. Small footprint of this composite resonator architecture enables laying multiple arrays with their specific frequencies in an ultra-small area on a chip. Moreover, collection of such arrays with their own operation frequency covering a wide frequency range can be connected to a common frequency manipulation circuitry on the same chip.

The maximum number of nanomechanical resonators in a vertical NW array is primarily determined by the diameter of and distance between nanomechanical resonators and thickness of the layer in which nanomechanical resonators are fabricated. In resonator designs that require employment of identical resonators in a vertical stack, uniformity challenges between resonators is also a deciding factor for the maximum number of resonators.

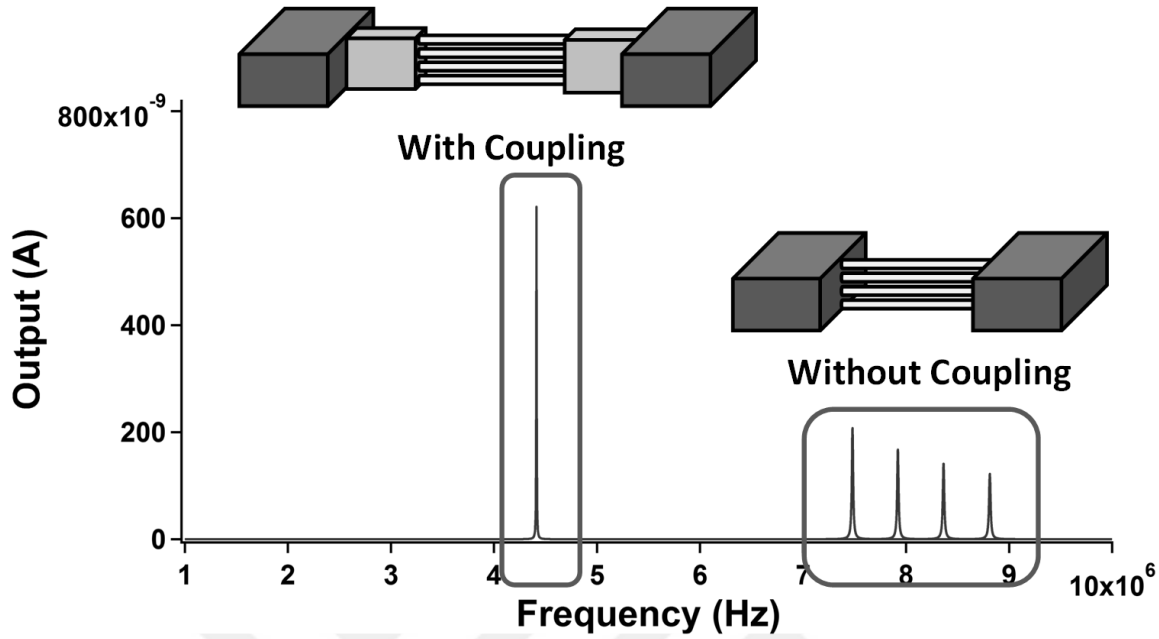


Figure 2. 3: Introduction of some mechanical coupling through the use of CMs provides a common mechanical mode and resulting increase in output signal amplitude.

2.2. Coupled Vertical NW Array Design

Electromechanical filter design is a complex process that has analytical, experimental and simulation fronts. Moreover, selections of actuation and readout schemes dictate certain constraints over the layout and operation of a filter requiring further revisions and optimizations for successful filter operation.

Let us consider any series electromechanical filter consisting of an arbitrary number of identical resonators. While the filter bandwidth (BW) is centered around the common resonance frequency of resonators (f_0), BW is determined by coupling beam stiffness (k_c) according to Eq. 2.1.

$$BW = f_0 \frac{k_c}{k_{rc}k_{12}} \quad (2.1)$$

where k_{rc} and k_{12} are resonator stiffness at a coupling location and normalized coupling coefficient for a given filter type, respectively [49]. Thus, it seems that coupling element stiffness can be set to get a desired BW for a given filter architecture and coupling beam attachment location. Moreover, modifying the resonance frequency of constituent identical resonators in a stack is enough to regulate the filter f_0 while keeping a coupling beam fixed.

Fig. 2.4.a shows the mode shapes of a simple system consisting of pure masses and connecting springs. Each mode corresponds to a specific signal peak in the frequency spectrum of the system. Moreover, the effect of the coupling springs on the frequency spectrum of the system is outlined in Fig. 2.4.b. In accordance with Eq. 2.1, as the compliance of the springs increases, frequency

spectrum peaks begin to diverge from each other. It is also possible to fine-tune frequency spectrum characteristics of any filter system by modifying mass and spring properties of the system components in general.

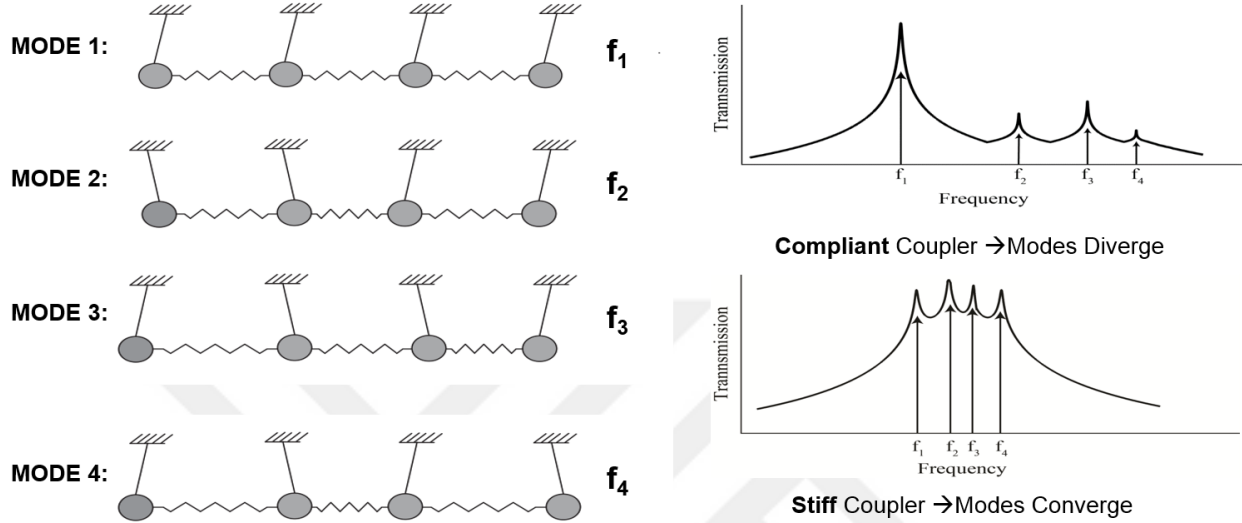


Figure 2.4: (a) Connection of pure masses with pure springs results in mechanical modes proportional to the number of masses. (b) Compliance of the coupling elements affects the resulting mode frequency distribution

Development of mechanically-coupled vertical NW stacks necessitates switching from the conventional coupling beam of Fig. 2.1.a to CMs of this work. Moreover, this transition also implies that analytical $\lambda/4$ approach for coupling beam modeling in MEMS filters can no longer be used. There is no analytical model in the literature to model the coupling element configuration of this work in order to predict the frequency response of a fabricated structure. Moreover, challenges associated with coupling modeling of this unorthodox structure involve changing filter mode shapes and filter f_0 with respect to CM dimensions. Alternatively, a numerical modeling methodology given in Appendix A is developed to have the array f_0 and BW as a function of coupling dimensions directly from modal analysis in finite element modeling (FEM).

Thus, coupled vertical NW array designs are performed based on FEM simulations. A commercial finite element software with three-dimensional (3D) free-tetrahedral mesh elements is employed to implement modal analysis simulations. Single crystalline anisotropic silicon following the $\langle 110 \rangle$ direction is used as the structural material.

Thus, the two fundamental design approaches are mainly pursued in NEMS array designs. Keeping a CM fixed and just changing the resonator aspect ratio *i.e.* resonator length over resonator width summarizes the first design strategy as shown in Fig. 2.5. This design scheme leads to a group of NW arrays whose center frequencies vary in a wide range but a certain common mechanical coupling is shared for each filter.

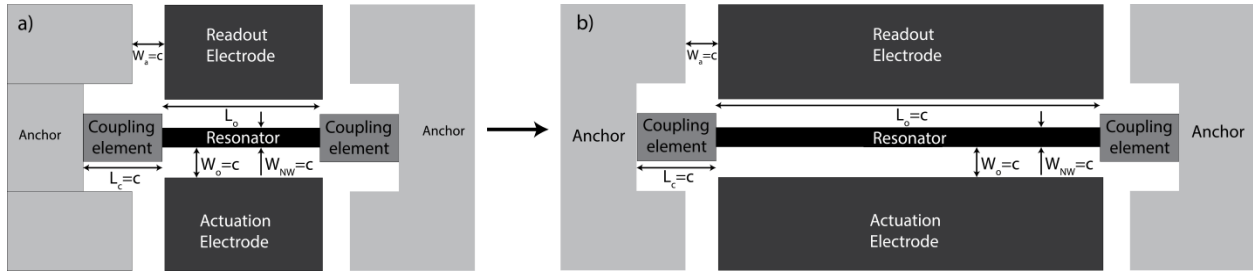


Figure 2.5: Changing the common length of NWs in an array for a given CM results in various filter center frequencies.

On the contrary, the second design set addresses the effect of mechanical coupling on frequency spectrum properties of NEMS vertical arrays by just changing the CM length while keeping resonators in a vertical stack unchanged as in Fig. 2.6. This design approach can be expected to produce another group of arrays in which the divergence of resulting array modes is proportional to the CM length.

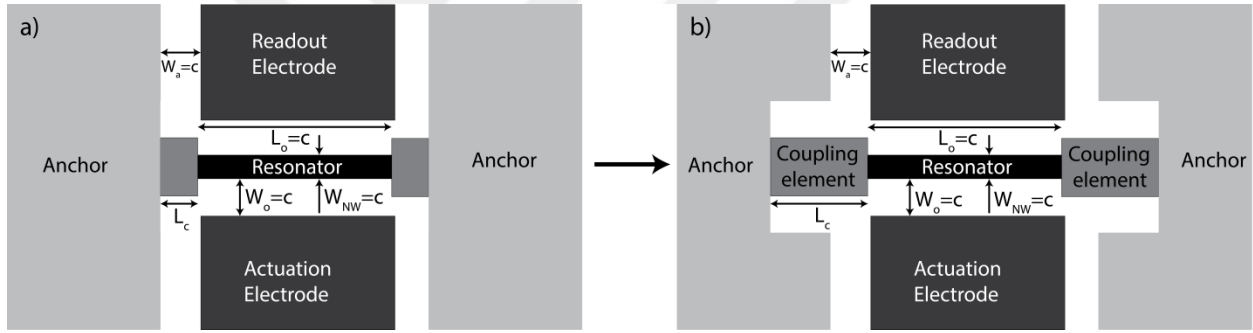


Figure 2.6: Gradual changing of the length of CMs in an array for a given NW length results in varying mechanical coupling between NWs.

Fabrication studies end up with vertical NW arrays consisting of 8 NWs as explained later. NWs in fabricated arrays are optimized successfully in terms of structural integrity, NW-gate electrical isolation and uniformity of a NW along its length and of various NWs within a vertical stack. All resulting samples have NWs with the common width of approximately 60 nm. As a result of the developed design approaches, resonators having the nominal aspect ratio *i.e.* nominal NW length over nominal NW mask linewidth of 100 nm, range of 20 - 50 were coupled with a CM whose length was fixed to 5% of the associated resonator length. On the other hand, the fabricated CMs feature lengths from 5% up to 50% normalized to the associated fixed resonator length of 2 μm .

As stated previously, CM stiffness is adjusted simply by changing its length to get a desired level of mechanical coupling between resonators in a vertical stack. Fig. 2.7 depicts the dependence of mechanical coupling in a vertical nanoresonator array on CM length for the in-phase mode.

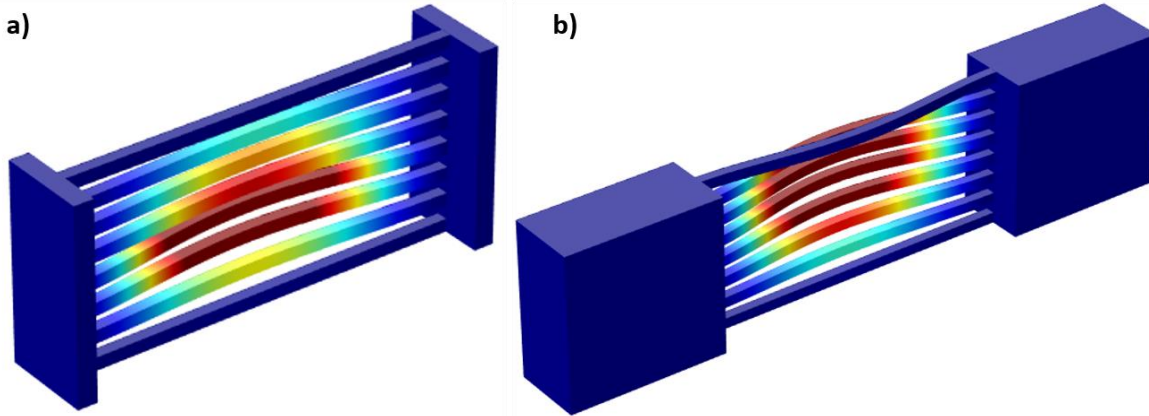


Figure 2.7: Increase of the CM length from 100 nm in (a) to 1000 nm in (b) corresponds to more interactions between resonators in an array. NW: 60x65x2000 nm (wxhxL), CM: 500x1000x1000 nm (wxhxL)

If the bottom surface of each employed CM is released from an underlying substrate, effective increase for the compliance of employed coupling elements corresponds to even further mechanical coupling between resonators as shown in Fig. 2.8.

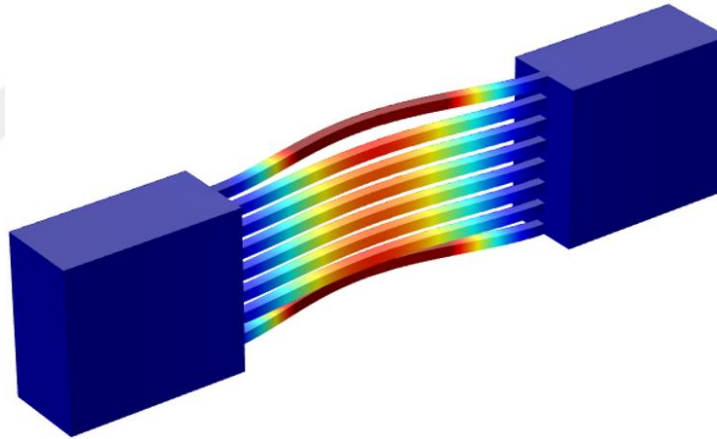


Figure 2.8: Releasing CMs from an underlying substrate leads to more mechanical coupling in general.

Actuation of a vertical NW array with a common side-gate electrode corresponds to a parallel resonator architecture which can be used to implement motional output signal increase if enough mechanical coupling between resonators in the array is provided. Moreover, at least two mechanical modes of a NW array in close proximity can form a bandpass filter behavior.

Piezoresistive frequency downmixing schemes are used to sense high frequency miniscule mechanical motion of resonators of measured NW samples. Room temperature piezoresistive coefficients in the (100) plane of n-type Si is shown in Fig. 2.9.a. Fig. 2.9.a implies that longitudinal piezoresistive coefficient is approximately three times higher along the $\langle 100 \rangle$ direction than $\langle 110 \rangle$ direction. Proportional relation of a transduced measurement signal amplitudes with longitudinal piezoresistive coefficient given in Fig. 2.9.a suggests employment of the highest gauge factor possible to have best signal-to-noise ratio outputs. On the other hand,

faster decrease in temperature coefficient of piezoresistive coefficient than piezoresistive coefficient itself shown in Fig. 2.9.b-c as a function of doping concentration encourages the selection of higher doping levels for piezoresistors at the expense of smaller gauge factors. Use of higher doping levels to have smaller temperature sensitivities for piezoresistive sensors is well-established in the literature [51]. Hence, the very high doping level of more than $1 \times 10^{20} \text{ cm}^{-3}$ is employed for the fabrication of single NW and NW array samples to limit thermal induced noises. This kind of doping results in very low Si NW resistivity on the order of $10^{-5} \Omega\text{cm}$ and a few $\text{k}\Omega$ resistances R_u for fabricated nano structures. In turn, such small undeflected NW resistances are instrumental to boost the resistance change sensitivity $\Delta R/R_u$.

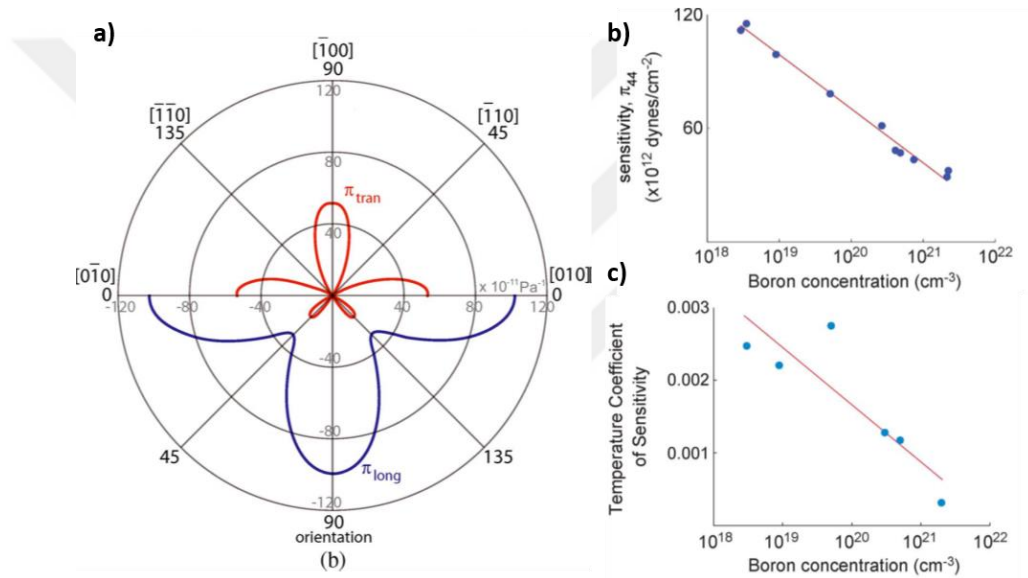


Figure 2.9: (a) Longitudinal and transverse piezoresistive coefficients as a function of crystallographic directions for n-type Si, (b-c) dependence of longitudinal piezoresistive coefficient and its temperature coefficient on doping levels.

Chapter 3: NEMS Vertical Stack Fabrication

3.1. Fabrication of Vertical Coupled NW Arrays

The fabrication aspect of the development of a coupled vertical NEMS arrays were performed in Center of MicroNanoTechnology (CMI) cleanroom facility in EPFL (École Polytechnique Fédérale de Lausanne) in Lausanne, Switzerland with the grant by the scientific and technological research council of Turkey (Tübitak) 2214 scholarship program.

The very first step of a fabrication process in any cleanroom is to develop a fabrication flow. The developed fabrication flow is then presented to the cleanroom technical committee to check its compatibility to available equipment, process constraints minimizing potential risk of cross contamination, material and human resources available. The fabrication flow proposed to realize vertical NW resonator arrays with proper actuation and readout schemes is presented schematically in Fig. 3.1 and as a runcard in Appendix C. Only after the approval of the suggested fabrication flow, training requests to each necessary device stated in the fabrication flow were authorized.

The fabrication of a coupled NEMS array starts with a silicon-on-insulator (SOI) wafer. The employed SOI wafer was selected and purchased from the CMI wafer inventory. The SOI wafer with the device, buried oxide (BOX) and handle layer thicknesses of approximately 1 μm , 1 μm and 725 μm were chosen over another SOI wafer having those layer thicknesses of approximately 0.34 μm , 2 μm and 725 μm respectively to fabricate greater number of resonators in a vertical array at the cost of more severe doping and spatial uniformity challenge between NWs.

The fabrication flow in Fig. 3.1 starts with initial cleaning of the SOI wafer by full RCA (RCA1+RCA2) and HF treatments to remove organic/metallic contaminants and native oxide layer on the wafer surfaces respectively (#0). Shortly after, the entire 1 μm thick device layer of the SOI wafer is doped with POCl_3 to have very high n doping (n^{++}) through a solid-state diffusion process at 900 °C. Afterwards, the wafer is annealed at 900 °C for 30 minutes to enhance the doping uniformity across the device layer thickness. Selection of the doping level of approximately 10^{20} cm^{-3} at the SOI wafer top surface is based on the electromechanical design of the NEMS array. In the literature, doping levels higher than approximately 10^{19} cm^{-3} are reported to provide ohmic rather than Schottky contact between Si and metal surfaces [52].

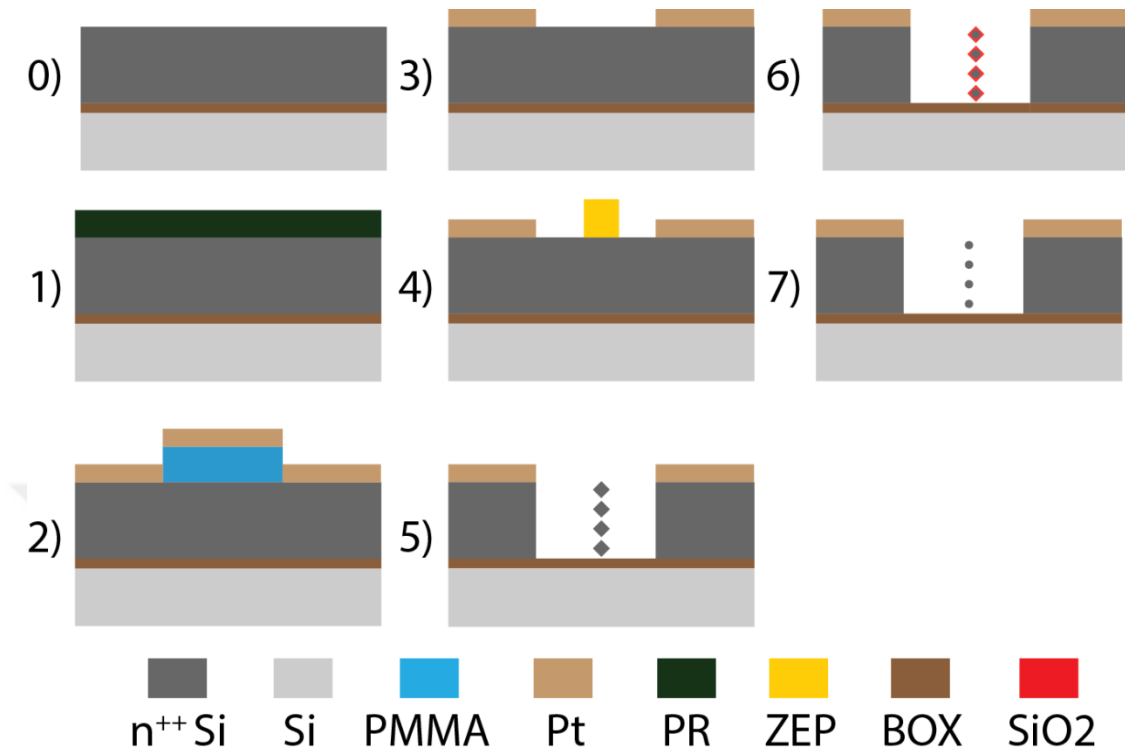


Figure 3.1: A three mask fabrication flow is developed to fabricate vertical coupled NEMS arrays consisting of NWs, CMs and actuation/readout electrodes.

Then either positive or negative alignment marks are patterned on the wafer surface by electron beam (e-beam) lithography to place different mask layers with an overlay accuracy of less than 20 nm. E-beam lithography processes are implemented with Vistec EBPG5000 e-beam lithography system. This first e-beam lithography process is carried out with a PMMA/PMMA (poly methyl methacrylate) bilayer positive e-beam resist to perform a lift-off process to deposit metal (5 nm Cr and 50 nm Pt) alignment marks on the wafer. Metal layers are deposited through e-beam evaporation at the room temperature by Leybold Optics LAB 600H e-beam evaporator having a high source-substrate distance chamber. The lift-off process is accomplished using an acetone bath along with a sonicator (2). Then, the wafer is cut into dice by Disco DAD321 automatic dicing saw after coating the wafer surface with a 2 μ m thick photoresist (PR) layer to protect the wafer surface from dicing related contamination. This process enables transforming of the 4" wafer to precise 1 cm x 1 cm chips. Processing of each chip separately under different fabrication parameters makes systematic characterization of fabrication processes easier. After dicing, the protective PR layer is removed by using acetone and isopropyl alcohol (IPA) baths for each chip.

Then the second e-beam lithography is implemented with the same PMMA/PMMA bilayer positive e-beam resist to perform another lift-off process again but this time to deposit metal (5 nm Cr and 50 nm Pt) touchpads, lines and electrodes on chip samples (2). Again this lift-off process is completed like the first one using an acetone bath together with a sonicator (3).

Then, NW pattern placed inside a trench is defined with a ZEP positive e-beam resist layer together with its anchors and CMs by another e-beam lithography process (4). Application of fluorine-based deep reactive ion etching (DRIE) plasma by Alcatel AMS200 SE with an optimized recipe results in not only a final NEMS array structure but also electrical isolation of doped NW array and adjacent electrode parts of fabricated samples between each other and from the rest of the chip (4). DRIE process parameters such as etch step time and layout parameters such as mask linewidth and resonator-to-electrode gap are optimized for best dimensional uniformity along the NW length and between various NWs within a stack. A vertical coupled NEMS array design is realized when the ZEP mask layer is removed with oxygen plasma (5). However, the uniformity of a NW along its length and of various NWs within a stack may be improved through an additional wet/dry oxidation step (6). NWs can then be released by removing oxide envelope with HF VPE-100 hydrofluoric acid vapor phase etcher (7).

Metrology measurements performed primarily with the help of Zeiss LEO 1550 and Zeiss Merlin Scanning Electron Microscopes (SEM), Bruker Dektak XT surface profiler, Veeco Wyko NT1100 optical profiler and Nanospec AFT-6100 spectroscopic reflectometer equipment were employed to characterize the processes in the fabrication flow and then fabricated structures.

3.2. Process Development

Pursuant to fabricate vertical coupled NW arrays, most of resources was channeled to develop most appropriate recipes for e-beam lithography, DRIE and lift-off processes from all the processes described in the Section 3.1 and summarized in the runcard in Appendix C. Each of these processes will be addressed in the following sections separately in detail.

3.2.1. E-beam Lithography Process Characterization

For all the equipment in the fabrication flow devoted to lithography, etching, deposition, metrology and packaging processes, most of the time was consumed with the complicated Vistec EBPG5000 e-beam lithography device to learn how to work with different e-beam resists (HSQ, MMA, PMMA, and ZEP), to create recipes for each employed resist and to get the best overlay accuracy for multiple mask processes.

First experiments in the cleanroom were the process characterization of each of e-beam resists (HSQ, PMMA, MMA and ZEP) presented to cleanroom users in the e-beam department of the cleanroom. Resist characterization was performed with a dose test experiment for each e-beam resist to get the highest throughput in terms of mask writing time, dimensional accuracy and structural integrity of a patterned mask by selecting proper process parameters such as dose, e-beam spot size, mask fracture size and development time.

Of the aforementioned supplied e-beam resists available in the cleanroom, HSQ (Hydrogen silsesquioxane) is a negative resist and has the highest resolution with a resolution of less than 10 nm. Very good dry etch selectivity of HSQ comes at the expense of low resist sensitivity *i.e.* very high doses. Thus, employment of this resist is effectively limited to small working areas if the mask printing time is a priority. A representative dose test experiment implemented for HSQ resist reveals optimum e-beam lithography and development parameters in Fig. 3.2.

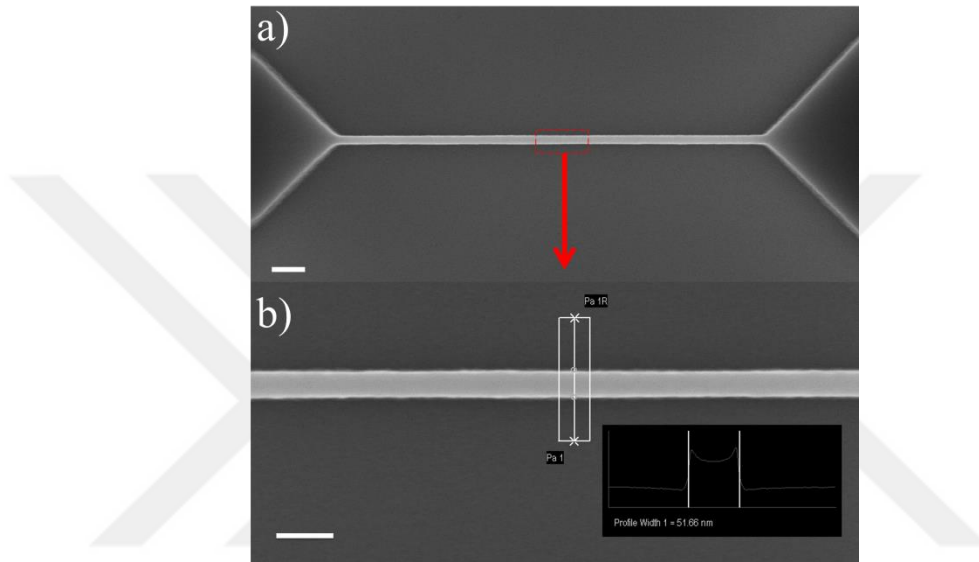


Figure 3.2: a) HSQ NW pattern fabricated with the dose of 4000 $\mu\text{C}/\text{cm}^2$ and e-beam spot size of 9.032 nm. Scale Bar: 200 nm b) Linewidth of the printed pattern is approximately 51.66 nm which deviates slightly from the nominal linewidth of 50 nm Scale Bar: 100 nm.

Among the positive resists, ZEP has higher resolution, sensitivity and dry etch selectivity than PMMA, MMA resists. On the other hand, PMMA and MMA resists consisting of long polymer chains of carbon atoms and having various molecular weights are mainly combined into PMMA/PMMA and MMA/PMMA bilayers to deposit a metallization layer by a lift-off process thanks to larger undercut profile of a bilayer. A large undercut profile is necessary for a resist to eliminate coating of an evaporated metal layer on the sidewalls of the resist. However, one consequential limitation of employment of a bilayer resist structure for a lift-off process is confronted while considering requirement of a lower resist thickness being more than double of a deposited metal thickness.

E-beam resist patterns having a resolution of less than 10 nm, resist thickness of up to 600 nm and overlay accuracy of less than 20 nm were fabricated successfully with the available e-beam resists thanks to the performed dose tests in order to make subsequent etching and deposition processes possible. Positive e-beam resists of ZEP and PMMA/PMMA bilayer are selected to generate e-beam masks for fabricating vertical coupled NW arrays and depositing metallization layers through DRIE and lift-off processes respectively.

3.2.2. NW Uniformity Optimization in a Vertical Stack

A vertical array of nanomechanical resonators can be fabricated by various techniques such as time multiplexed alternating process namely Bosch process. Bosch process originally developed to enable high aspect ratio vertical walls may result in a vertical stack of NWs through patterning two windows or openings in a layer by means of the scalloping effect. A dividing mask line between the two openings is employed as a protective layer for subsequent etching cycles.

Bosch process is essentially a fluorine-based DRIE plasma process alternating repeatedly between isotropic plasma etching (Sulfurhexafluoride (SF_6) gas) and passivation (Octafluorocyclobutane (C_4F_8) gas) steps. Main parameters of the process are chamber base pressure, plasma power, gas flow rates and step times, window/opening width *i.e.* distance of a mask line from a sidewall, and dividing mask linewidth. Bosch process may result in a vertical stack of NWs or fin formation with respect to dividing mask linewidth whether etch scallops from both sides meet or not along the centerline of the dividing column respectively [53-55]. The number of process cycle sets the number of NWs in a stack. NW diameter and distance between two NWs in a vertical stack are set primarily by chemical etch step parameters such as gas flow rate and duration. A subsequent oxidation process may be exploited to form vertically-stacked NWs from a fin structure and/or to modify NW geometrical characteristics such as nonidealities, diameter and cross section properties when a following oxide etching process releases NWs from oxide envelope [54, 56-60]. If required, a sacrificial or protective layer can be carved out from NWs with another oxidation process at any time. Thus, vertical resonator density can be adjusted easily by the number of Bosch process cycles. Field effect transistors (FET) fabricated from a vertical NW array and featuring multiple gate-all-around electrodes were also reported in the literature [61, 62].

The etch rate of a Bosch process and resulting NW profile are governed by loading, microloading and ion induced defluorination of the passivation film phenomena. The loading effect corresponding to the exposed portion of a substrate surface has an inverse relationship with the DRIE process etch rate [63]. However, replenishment difficulty of etchant species inside a trench denominated as the microloading effect manifests itself as local etch rate degradation when the etching window/opening width keeps reducing [63, 64]. Thus, NW horizontal density adjusted by NW pitch and etching gas flow rate are among the DRIE parameters to control the local DRIE etch rate by the microloading effect.

The step time and flow rate of SF_6 can be used to slow down Si etch rate. A fraction of the time of the SF_6 step is spent to remove the passivation layer at the bottom of a trench deposited at the previous passivation step. This fraction becomes considerable for etching at the nanoscale. Thus, thicker passivation layers translate itself as low Si etch rates in addition to micrograin formation [65]. On the other hand, ion bombardment of very thin passivation layers leads to desorption of

fluoride from a passivation film *i.e.* defluorination, to build up etchant species in it to etch the underlying Si away [66, 67]. Thus, some optimization for the passivation layer thickness is required.

As a result, the aforementioned governing physical phenomena for Bosch process lead to various optimum etching recipes for NWs having different linewidths, aspect ratios and trench openings. In other words, it is absolutely necessary to find correct DRIE process parameters to have a proper vertical NW stack. Otherwise it is quite likely to end up with problematic NW structures such as stiction of NWs in a vertical stack to each other or completely vanishing due to excessive etching. Even greater challenge for the fabrication of a vertical NW stack arises in case of resonators. Since uniformity between NWs in a vertical stack is utmost importance due to resonance frequency dependence of each NW on its profile. Fabricated NWs must be uniform along their length and within a vertical stack for better one-to-one correspondence to performed FEM simulations optimized for highest readout signal levels.

Thus, seeking the best NW uniformity in a vertical stack is the key to the realization of a properly designed NEMS resonator array. The developed NEMS array is composed of double clamped NWs. Mechanical coupling is provided with coupling elements attached to both extremes of a vertical resonator stack. Actuation and readout electrodes are fabricated at either side of the vertical stack with any desired electrode-NW gap as in Fig. 3.3.

As explained, Bosch process is used to carve out vertical NEMS resonator stacks from bulk silicon. In addition to the DRIE process parameters of etching and passivation step times, layout parameters of NW linewidth (W_{NW}), opening width (W_o) *i.e.* electrode-to-resonator gap, and opening length (L_o) and anchor-to-electrode gap (W_a) illustrated in Fig. 3.3 are examined to extract the best uniformity of a NW along its length and of various NWs in a vertical stack on a 1 cm x 1 cm Si chip surface.

However, the mask layout template in Fig. 3.3 is not enough to extract frequency spectrum properties of vertical NW resonator stacks. Metal pads and lines, and labels should also be incorporated into a specimen layout to provide/get voltage signals to/from NWs and electrodes as shown in Fig. 3.4. Fig. 3.4 features a specific vertical NW array design having a unique combination of layout parameters of resonator and coupling element lengths, anchor-to-electrode and resonator-to-electrode lengths, and opening lengths in addition to common metal pads and lines, and label structure.

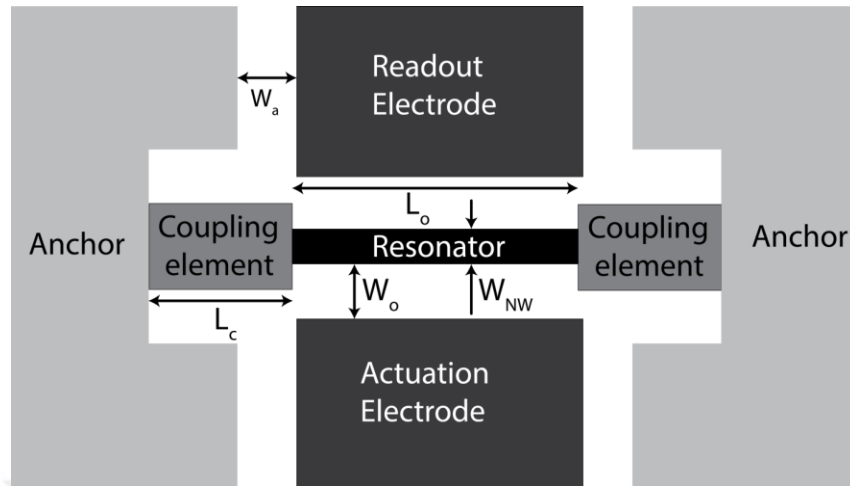


Figure 3.3: Mask layout of a NW and its immediate surroundings is demonstrated together with the examined layout parameters

When the employed expensive SOI wafer was cut into 1 cm x 1 cm chips, the building block of Fig. 3.4 is printed several times on a chip surface to investigate the effect of the layout parameters of Fig. 3.3 on NW uniformity in a vertical stack efficiently. Thus, each chip consisting of 24 building blocks of Fig. 3.4 enables 24 unique combinations of the layout parameters as in Fig. 3.5.

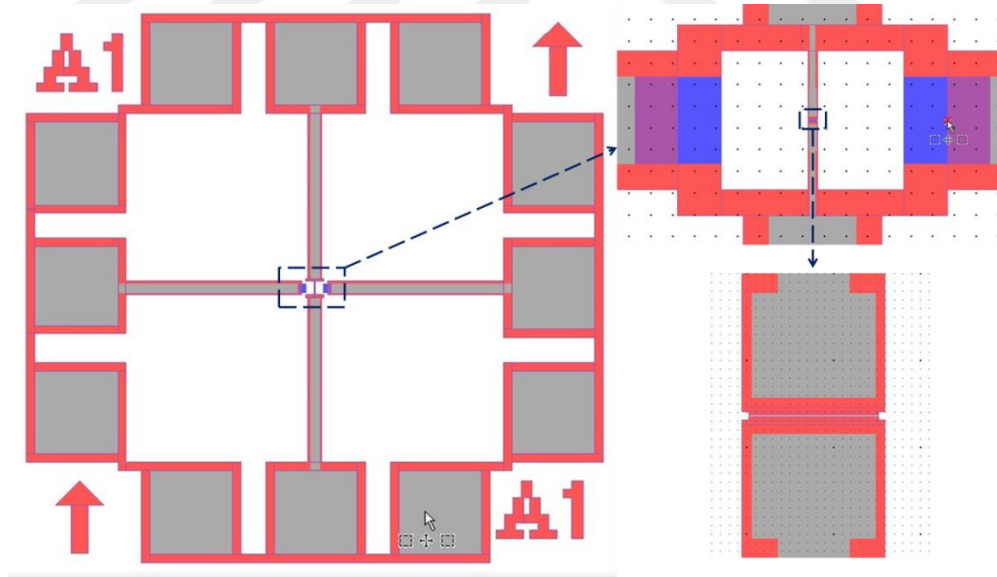


Figure 3.4: The layout used a building block to fabricate robust coupled NW array structures

The layout parameters of opening width (W_o) and length (L_o), and anchor-to-electrode gap (W_a) of Fig. 3.3 determine local DRIE etch rate and NW profile through microloading. Hence, each unique combination of these layout parameters results in a different DRIE etch rate at least at some region across the specimen. Thus, fabrication of vertical NW array specimens together on a common 1 cm x 1 cm chip makes the uniformity matter worse. As a result, it is impossible to optimize NW uniformity for all specimens with a common set of process parameters. However,

since NW uniformity in a vertical array does not depend on each layout parameter equally, proper selection of etch parameters may converge to best NW uniformities for some similar array designs.

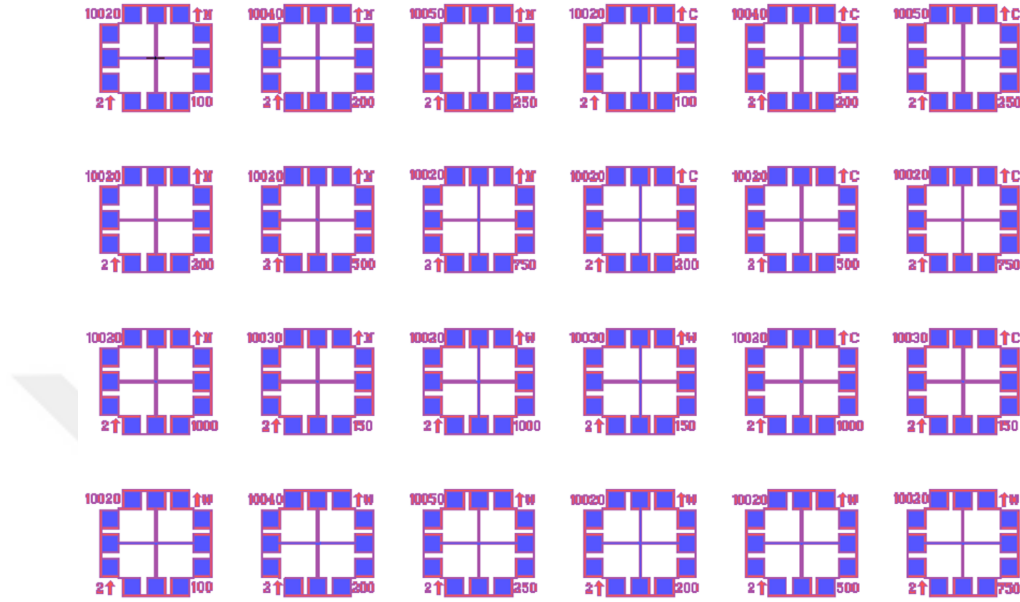


Figure 3.5: Each processed 1 cm x 1 cm chip consists of 24 combinations of the layout parameters of Fig. 3.3 to make systematic DRIE process characterization convenient.

Fabrication experience of vertical nanoresonator arrays clearly underlines the importance of the opening width (W_o) and length (L_o), and anchor-to-electrode gap parameters (W_a) on uniformity of NWs in a stack. Effect of these parameters on NW uniformity is investigated separately in detail. Fig. 3.6 illustrates etch rate difference between the center and end portions of the NWs in a vertical stack for two identical specimens fabricated simultaneously on a same SOI chip except the resonator length corresponding to a different opening length (L_o) for each specimen.

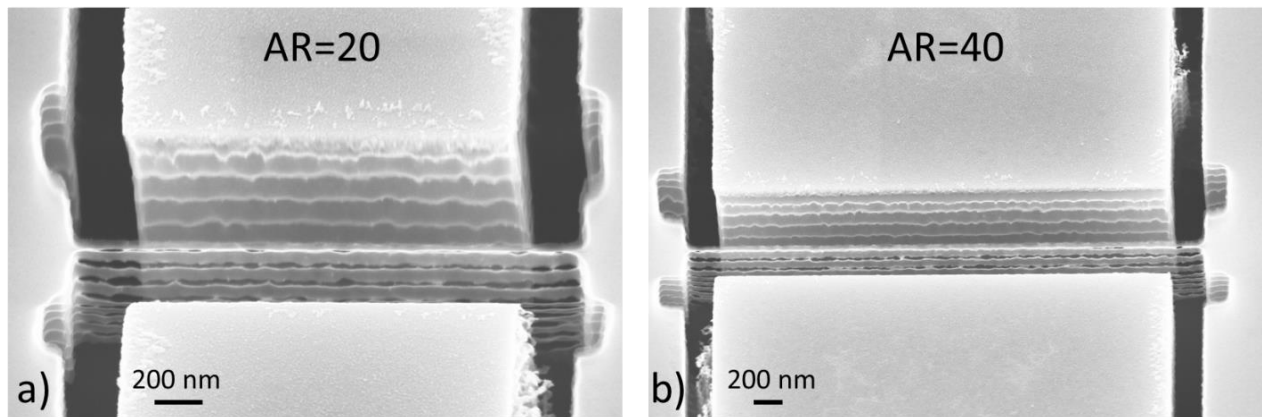


Figure 3.6: Increasing nominal aspect ratio of the NWs from 20 in (a) to 40 in (b) results in partial release at the center section of the fabricated array.

Fig. 3.7 demonstrates the effect of the anchor-to-electrode gap on local etch rates in the neighborhood of NW-CM junction. Keeping the gap relatively large ends up with faster local etch

rates at NW-CM junction regions than the center portion of a vertical stack. Thus, this difference of local etch rates at the ends and middle of a NW array shows that non-uniformity in the cross section of a NW exists not only along the NW length but also between NWs in a stack at NW-CM junction region as in Fig. 3.7.b.

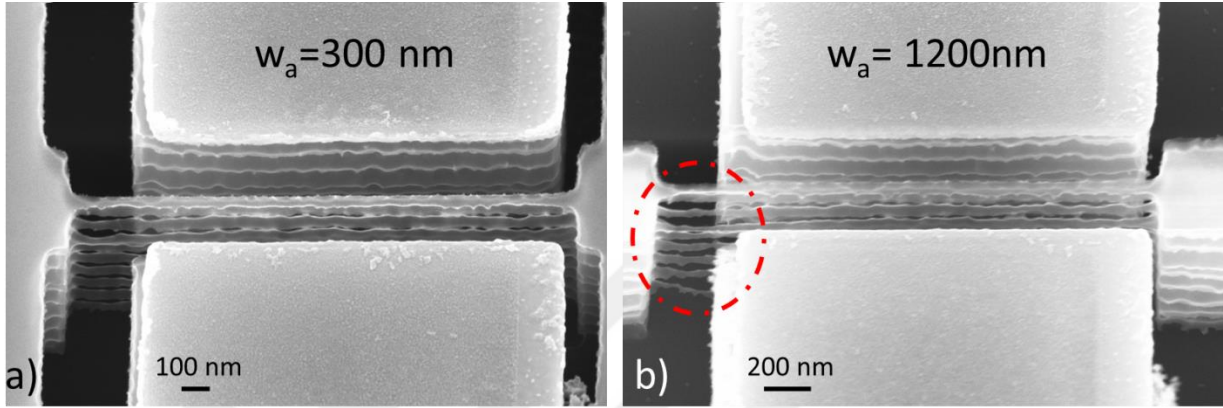


Figure 3. 7: Increase of the anchor-to-electrode gap from 300 nm in (a) to 1200 nm in (b) severely disrupts NW cross-section uniformity between NWs in the array at a NW - coupling beam junction region

Opening width *i.e.* resonator-to-electrode gap (W_o) and NW linewidth (W_{NW}) also play a crucial but subtle role in uniformity optimization experiments. The opening width (W_o) together with the opening length (L_o) is the most fundamental layout parameter to determine DRIE process etch rate by microloading effect. An increase in the resonator-to-electrode gap as shown schematically in Fig. 3.8 leads to an increase in scallop size resulting in higher roughness and etch rate. In turn, higher roughness and etch rate of a Bosch process yield greater NW non-uniformities along a NW length and between various NWs in a stack and it may even compromise the structural integrity of a NW as shown in Fig. 3.9.

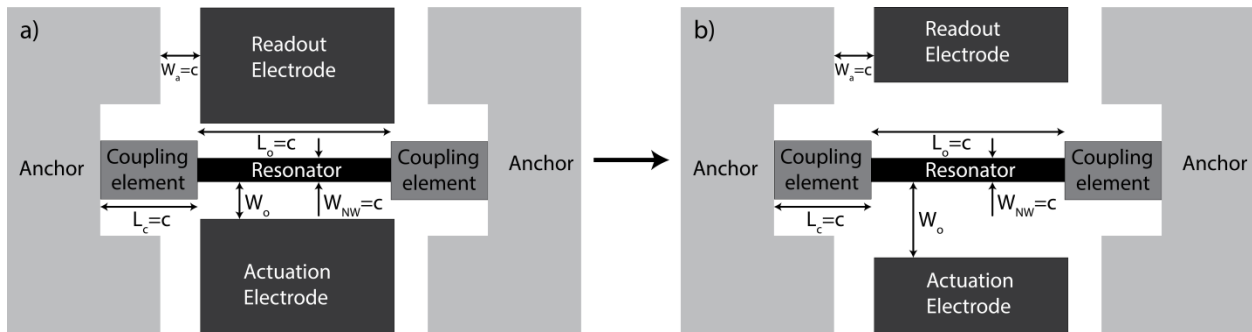


Figure 3.8: The resonator-to-electrode gap is the most critical layout parameter to determine DRIE etch rate and the uniformity of a NW along its length through adjusting the scallop size.

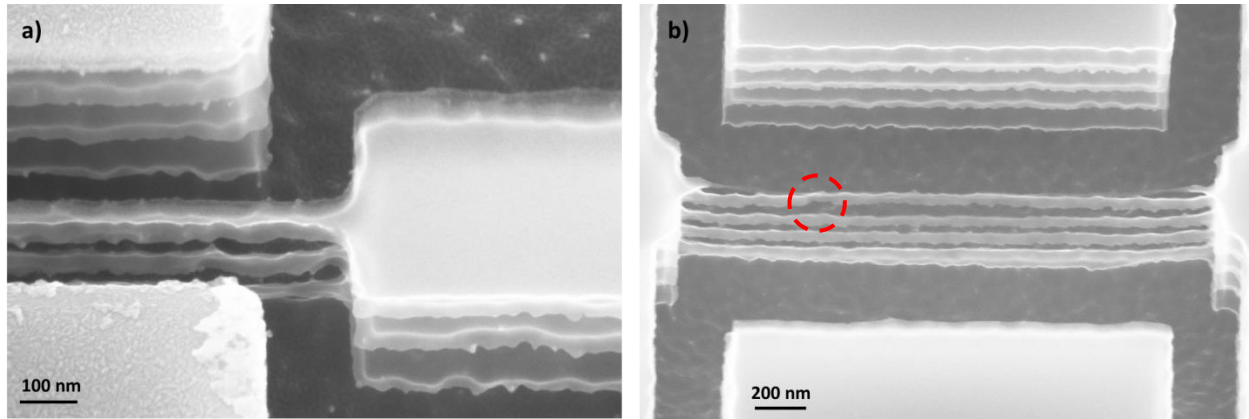


Figure 3.9: Increase of the nominal resonator-to-electrode gap from 200 nm in (a) to 500 nm in (b) leads to higher frequency of NW non-idealities such as weak spots that compromise the structural integrity of NWs

On the other hand, the effect of the NW linewidth (W_{NW}) on NW spatial uniformity is also significant. When the NW linewidth is getting smaller as shown schematically in Fig. 3.10, minimum scallop size resulting in released vertical NW arrays by meeting from the both sides along the centerline of a dividing column also shrinks.

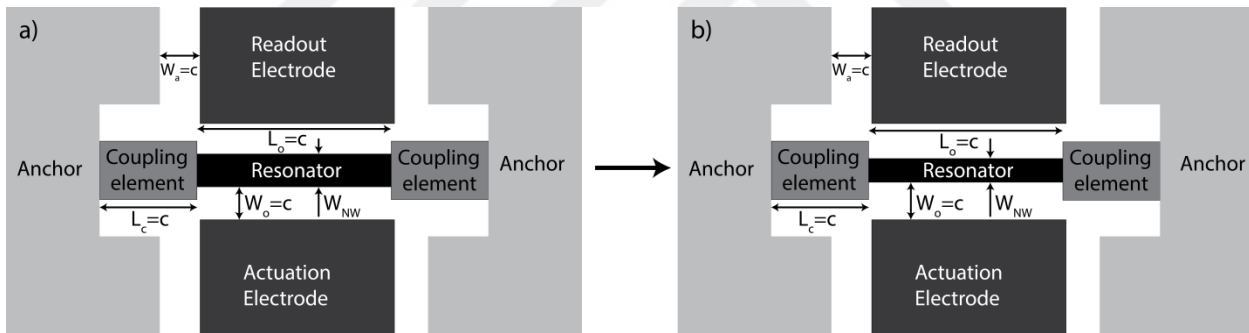


Figure 3.10: As the mask linewidth gets smaller from (a) to (b), lower minimum scallop size to release NWs of a vertical stack corresponds to lower DRIE etch rate resulting in lower roughness and better NW uniformity.

Similar to the opening width, smaller minimum scallop size corresponds to lower etch rate leading to a more controllable etch process with lower roughness and higher NW uniformity. However, when the etch rate is too low or too high with respect to a NW linewidth, one gets either a fin structure or structural deformities such as partially released NWs, stiction of released NWs to each other, broken NWs or complete etch of NWs. Sensitivity of the fabrication of vertical Si NW arrays on employed Bosch process recipes is illustrated in Fig. 3.11.

One other source of NW non-uniformity in a vertical array stems from the misalignment of different layers patterned with the e-beam lithography. As described in section 3.1, while PMMA/PMMA bilayer positive e-beam resist is patterned to deposit a metallization layer, a DRIE mask layer is formed using ZEP positive e-beam resist. As shown in Fig. 3.12.a, any misalignment between these two layers compromises designed symmetrical structures of the opening width (W_o)

and anchor-to-electrode gap (W_a) at each side of a vertical stack and an electrode respectively. Resulting different gaps at each side manifest itself as different etch rates due to microloading effect corresponding to non-uniformities for a NW along its length and scallop size at each side of a vertical stack.

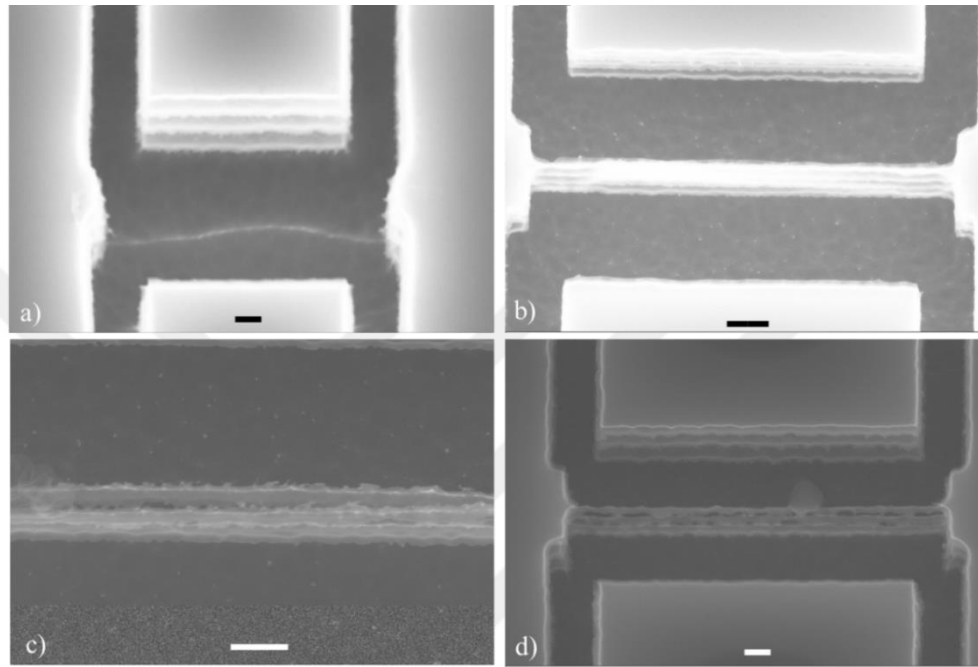


Figure 3.11: Improper etching parameters lead to complete etching of a NW array in (a), fin formation in (b) and partially released arrays in (c) and (d).

Parallel to gradual mastery over the complicated e-beam lithography process and machine, alignment errors between deposited metal and etched Si layers shrank by proper e-beam software manipulations and employment of multiple e-beams within a single writing job. Utilization of multiple e-beams subsequently enables writing the most critical regions delicately with a smaller beam while patterning the rest of a specimen with a fast beam. As a result, the overlay accuracy of the employed fabrication flow approaches to the specified machine overlay accuracy of less than 20 nm as shown in Fig. 3.12.

From the fabrication perspective, there are some fundamental differences between processing of Si test and SOI wafers that may pose extra challenges related to DRIE etch rate and uniformity of NWs within a vertical stack. The most conspicuous difference is the presence of an oxide layer that limits the etch depth of a DRIE process to the device layer of a SOI wafer for SOI wafers. More importantly, the oxide layer also forms an electric field functioned effectively as a shield which complicates the etching process. Moreover, it may result in a very thin Si membrane on top of the BOX layer adjacent to a fabricated vertical stack as shown in Fig. 3.13.

Complete elimination of this thin Si membrane requires some extra etching cycles. However, these extra etching cycles may deteriorate already optimized uniformity and structural integrity of the NWs in a vertical stack. Thus, the elimination requirement of this membrane by some extra etching cycles results in some difference in the developed etch recipes for SOI and Si chips. As a result, DRIE process and mask layout parameters optimized for the best uniformity of various NWs within a stack with Si test chips should be taken merely as a guide before the actual characterization of these factors with SOI chips. Thus, optimum DRIE and sample layout parameters extracted from DRIE experiments using Si test chips must be fine-tuned for SOI test chips in terms of structural integrity and NW uniformity.

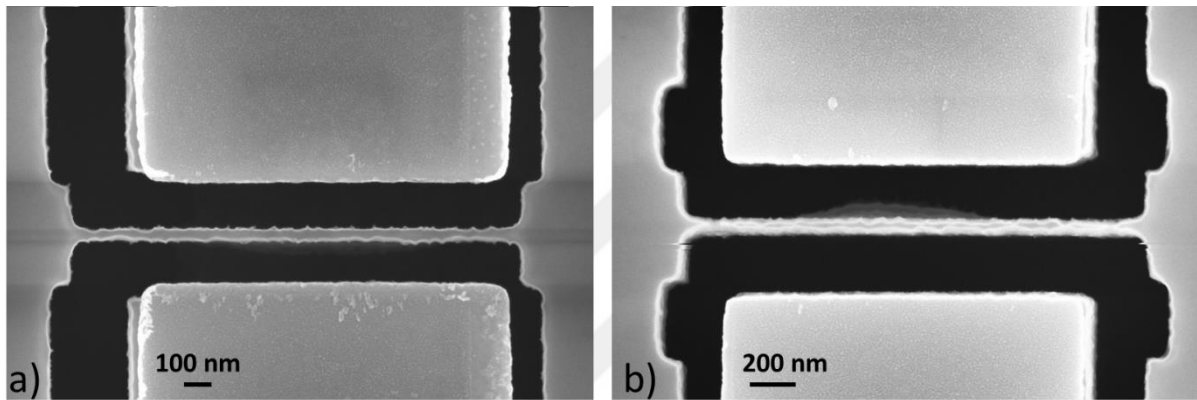


Figure 3.12: Obvious alignment errors in (a) are compensated by e-beam mask modifications and employment of multiple beams in (b)

It is crucial to note that complete elimination of a Si membrane existed between a vertical NW array and its electrodes is very critical. Since any remaining Si membrane may ruin the electrical isolation between a fabricated NW stack and gate electrodes. Complete elimination of a Si membrane can be checked quickly under SEM. Moreover, the existence of an electrical short or open circuit between a NW leg and a side-gate electrode through probe station measurements reveals the true nature of a sample conclusively.

Alternative to some extra etching cycles, oxidation of a Si membrane layer and subsequent brief etching of the resulting oxide by a hydrofluoric acid vapor phase etcher can be employed to get rid of problematic thin Si membrane layers without compromising optimized uniformity of the NWs in a stack.

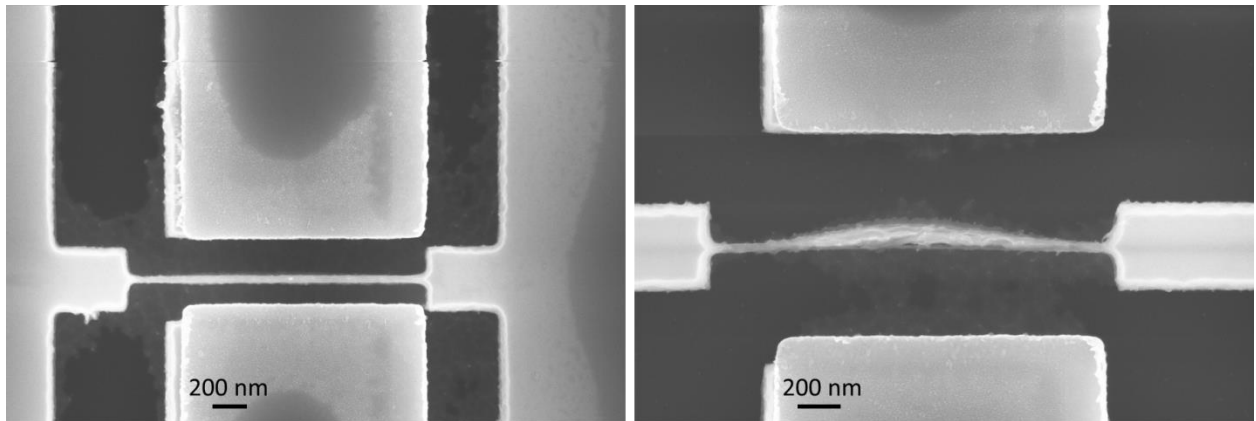


Figure 3.13: Si thin membranes left at narrow corners adjacent to a vertical NW stack after an etching process must be eliminated to ensure electrical isolation between electrodes and NWs.

Thus, DRIE process optimization by examining process parameters of the etch step time and the four layout parameters of mask linewidth, opening width and length, and anchor-to-electrode gap of Fig. 3.3 is performed to obtain not only the best uniformity of the NWs in a vertical stack but also complete elimination of thin Si membranes on a BOX layer as shown in Fig. 3.14.

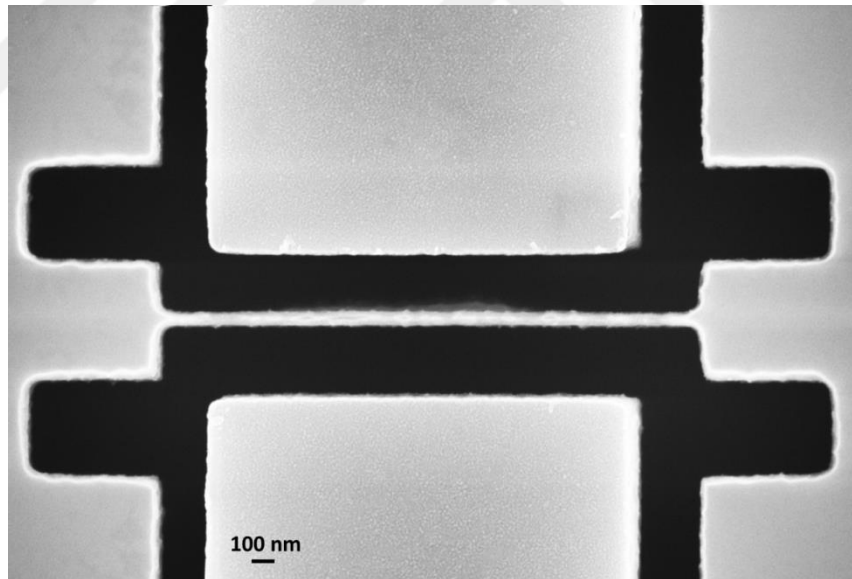


Figure 3.14: In addition to the examination of a SOI chip under SEM, electrical measurements are performed to ensure complete elimination of thin membrane remnants

An additional rather unexpected DRIE process parameter arises due to absence of a chip holder for the employed DRIE machine. There is only one 4" wafer holder present for the machine. Thus, it is impossible to work with chips directly. This obstacle is overcome by attaching a chip sample on a 4" blank carrier wafer. However, selection of an attachment technique such as employment of thermoplastic glue (Quick Stick) or using tapes (Kapton) seems to modify resulting DRIE characteristics differently by affecting heat transfer mechanism from a heated chip sample exposed to the plasma, to a base wafer underneath. Performed characterization experiments favored

employment of thermoplastic glue (Quick Stick) over Kapton tape with respect to structural integrity and NW uniformity within a vertical stack.

3.2.3. Metal Deposition Process Development

Development of an efficient lift-off process is crucial to deposit alignment marks and metal lines, touchpads and electrodes while maintaining good adhesion to an underlying layer. Undercut resist profile is necessary to protect sidewalls of a resist pattern from deposition of a metal layer at a subsequent deposition step. Although an undercut resist profile can be achieved using a monolayer resist, bilayer resist structures such as MMA/PMMA or PMMA/PMMA pairs provide larger undercuts. Individual layer thicknesses, applied dose, e-beam spot size, development time, deposited metal thickness and adhesion strength of a deposited metal to a layer underneath are among numerous parameters that determine the success of a lift-off process significantly.

Although MMA/PMMA bilayer has a higher inherent resist resolution, processing practicability of PMMA/PMMA bilayer resist is found more significant. Very low molecular weight of MMA resists leads to structural integrity related reliability concerns. High MMA resist sensitivity to resist development and subsequent metal deposition conditions causes high susceptibility to failure due to collapse of the resist.

Platinum (Pt) selected as the metallization element is deposited by e-beam evaporation to form electrodes, metal lines and touch pads. However, the adhesion of Pt to silicon surfaces is found weak after some unsuccessful lift-off attempts. In order to enhance the adhesion of Pt layer on silicon surfaces, a very thin Cr or Ti layer (~5 nm) is deposited on a Si surface prior to Pt layer by e-beam evaporation. One subtle fabrication facility related issue is that materials that deteriorate easily upon exposure to oxygen such as Cr are not allowed to be processed in some machines such as oxidation furnaces to avert cross contamination concerns. Thus, employment of Ti as an adhesion promoter is preferred whenever possible.

Sensitivity of a lift-off process on process parameters can be appreciated with the help of Fig. 3.15 where a bilayer resist thickness is much greater than a deposited metal thickness. Metal particles previously deposited on sidewalls of the bilayer resist structure landed on the deposited metal layer and underlying substrate itself after the lift-off process and led to severe contamination as shown in Fig. 3.15.

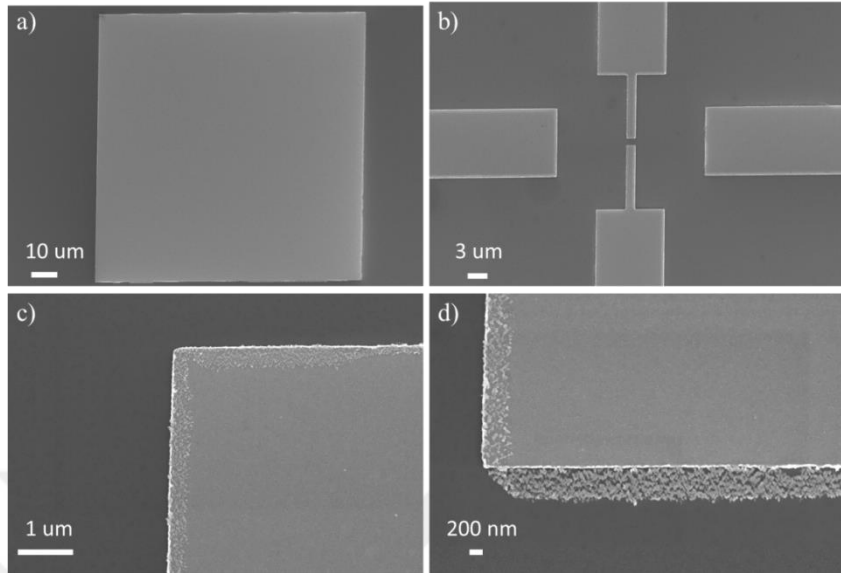


Figure 3.15: Depositing a thin layer as a metal pad in (a) and metal lines and electrodes in (b) using a lift-off process results in scattered particles on the surfaces of a substrate and layer itself as shown in (c), (d)

Importance of these scattered metal particles is fully acknowledged when a vertical NW array are fabricated adjacent to these scattered metal particles as shown in Fig. 3.16. Some scattered metal particles adjacent to the vertical NW stack prevented proper dry etching of Si such that some part of the vertical stack was not even released at all. Thus, particles stemming from a lift-off process must be suppressed by selecting of a proper set of resist deposition parameters resulting comparable resist and metal thicknesses.

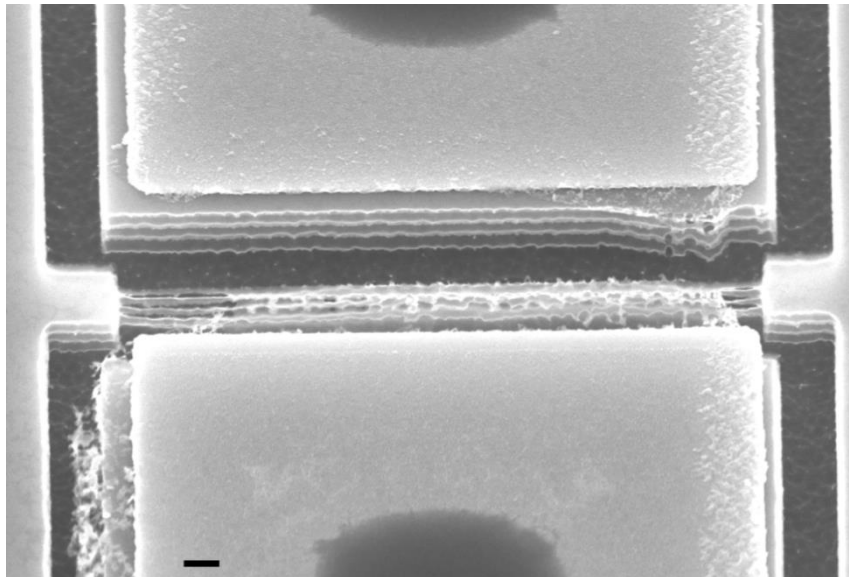


Figure 3.16: Bosch process is affected by scatter particles from a previously deposited metal layer such that some part of resulting NW array does not release properly. Scale bar: 200 nm

Improper e-beam lithography process parameters such as beam dose, beam diameter and development recipe etc. lead not only to problematic results for a deposited metal layer but also affect structural integrity and uniformity of NWs in a vertical stack as shown in Fig. 3.17.

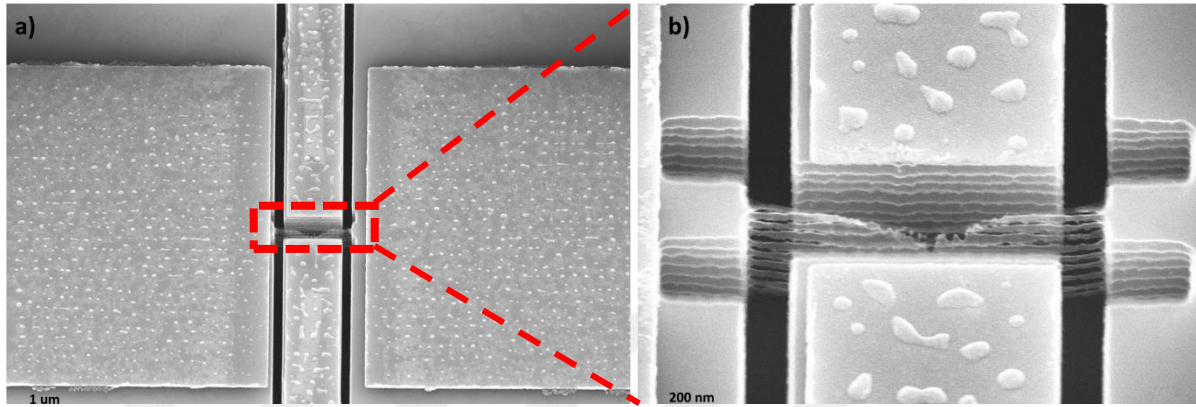


Figure 3.17: Coating and processing of a lift-off resist has profound effect on not only a subsequently deposited metal layer (a) but also later DRIE process characteristics (b).

Another metal deposition related issue arises if the device layer thickness of the employed SOI wafer is considered. The device layer thickness of approximately 1 μm corresponds to the height of the vertical NW stack as shown in Fig. 18.a. Best electrostatic transduction to a vertical NW array is provided by a side-gate fabricated from a metal layer and having the same thickness with the vertical array. On the other hand, the lower layer thickness of a bilayer resist is suggested to be more than two times thicker than the thickness of a deposited metal as a rule of thumb. Thus, the maximum allowable metal thickness with a lift-off process using a PMMA/PMMA bilayer resist falls far short from the required 1 μm SOI device layer thickness. Alternatively, thicker photolithography resists can be employed coupled with some other metal deposition techniques such as sputtering to have thicker metal layers. However, switching from e-beam lithography to photolithography process comes at an expense of much greater alignment errors that cannot be tolerated if tight overlay accuracy demands shown in Figs. 3.12-14 are considered. A compromise solution of depositing a thin metal layer on the highly doped (n^{++}) SOI device layer as shown schematically in Fig. 3.18.b is adopted in the fabrication of coupled vertical NW arrays at the cost of weaker transduction.

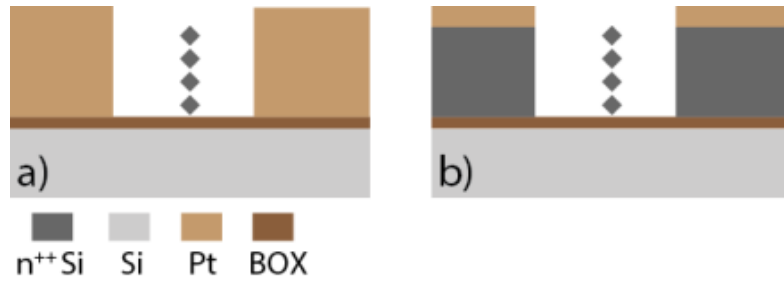


Figure 3.18: The maximum deposition thickness limitation imposed by the employed e-beam lift-off process requires switching from full metal electrodes in (a) to highly-doped Si electrodes with a top metal film in (b).

3.3. Fabrication Results

Initial DRIE process characterization experiments are performed using Si test chips prior to SOI chips for cost-effective research purposes. At first, Si samples such as those shown in Fig. 3.19 do not have any metallization layer. Instead, coupled vertical NWs arrays are fabricated between pure Si electrodes. The first set of DRIE experiments is oriented to select a common, proper NW linewidth value to limit the scope of future systematic experiments effectively considering the demonstrative aspect of the research. Three mask linewidths of 50 nm, 100 nm and 150 nm are selected to carve out NW vertical stacks consisting of up to 4 NWs.

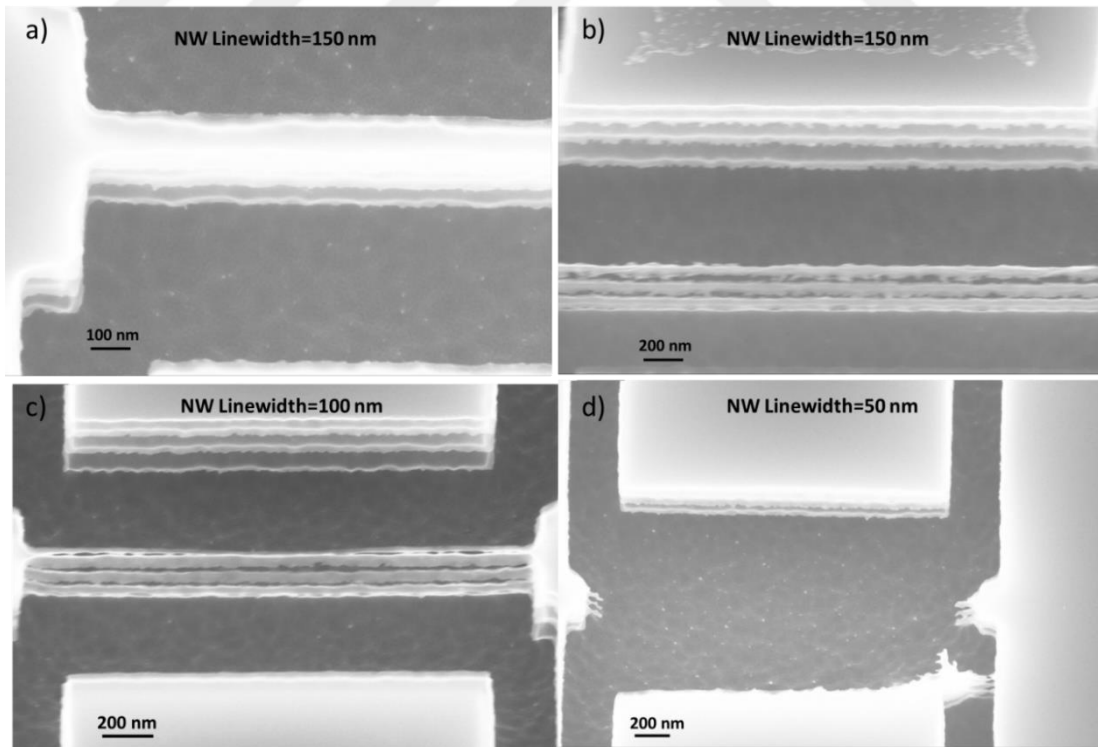


Figure 3.19: DRIE recipes were investigated to produce vertical NW arrays from the mask linewidths of 50, 100 and 150 nm. The 100 nm linewidth shown in (c) is selected as a compromise.

As a result, Bosch process recipes are developed to fabricate vertical NW stacks successfully from the mask linewidths of 150 and 100 nm as shown in Fig. 3.19.b-c. On the other hand, initial experiments cannot slow down DRIE Si etch rate enough to ensure the structural integrity of vertical stacks fabricated from the 50 nm mask linewidth as shown in Fig. 3.19.d. Thus, the mask linewidth of 100 nm is selected to realize vertical NW stack based composite resonators.

Number of NWs within a vertical stack can be adjusted easily by just setting number of cycles of a DRIE process as shown in Fig. 3.20. However, maximum number of NWs is determined by the device layer thickness and mask linewidth parameters for SOI samples. In accordance with the literature [59], (N) number of DRIE cycles results in (N-1) NWs in a vertical stack.

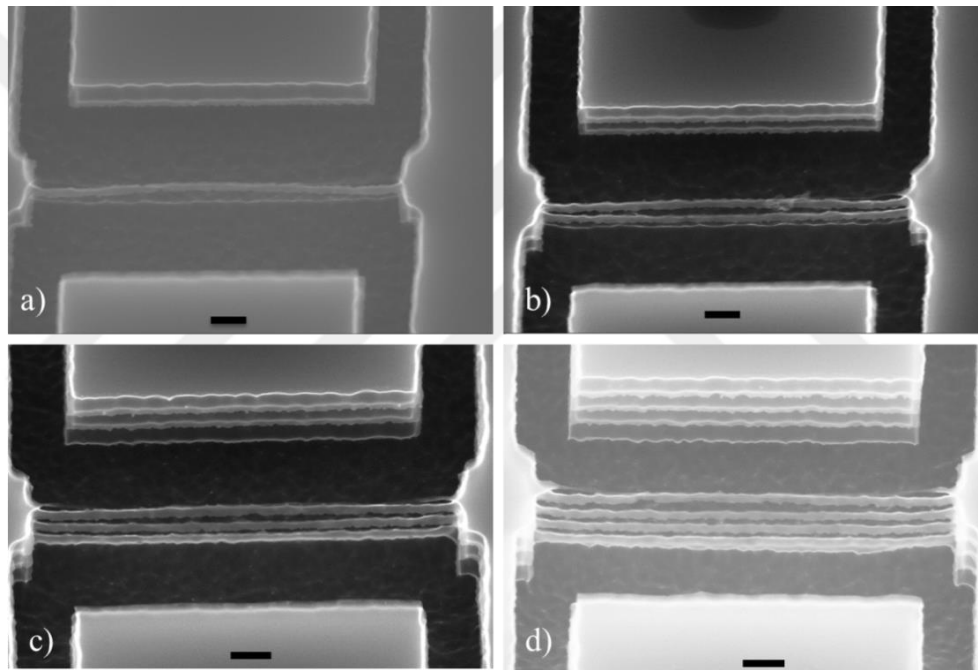


Figure 3.20: Vertical stacks consisting of one (a), two (b), three (c) or four (d) NWs are demonstrated. Scale bar: 200 nm

In order to realize vertical NW arrays spanned between metallized electrodes, integration of a NW vertical stack with metallized electrodes was studied with Si test chips following to prior lift-off characterization experiment results. Metal deposition issues of scattered metal particles and weak adhesion of Pt on Si surfaces are solved by employing a thinner PMMA/PMMA bilayer structure together with optimized e-beam lithography process and a thin layer (~5nm) of Ti or Cr as an adhesion promoter. Representative vertical NW stacks carved out from Si chips alongside metallized electrodes are illustrated in Fig. 3.21 with the nominal resonator-to-electrode gaps of 200 and 500 nm.

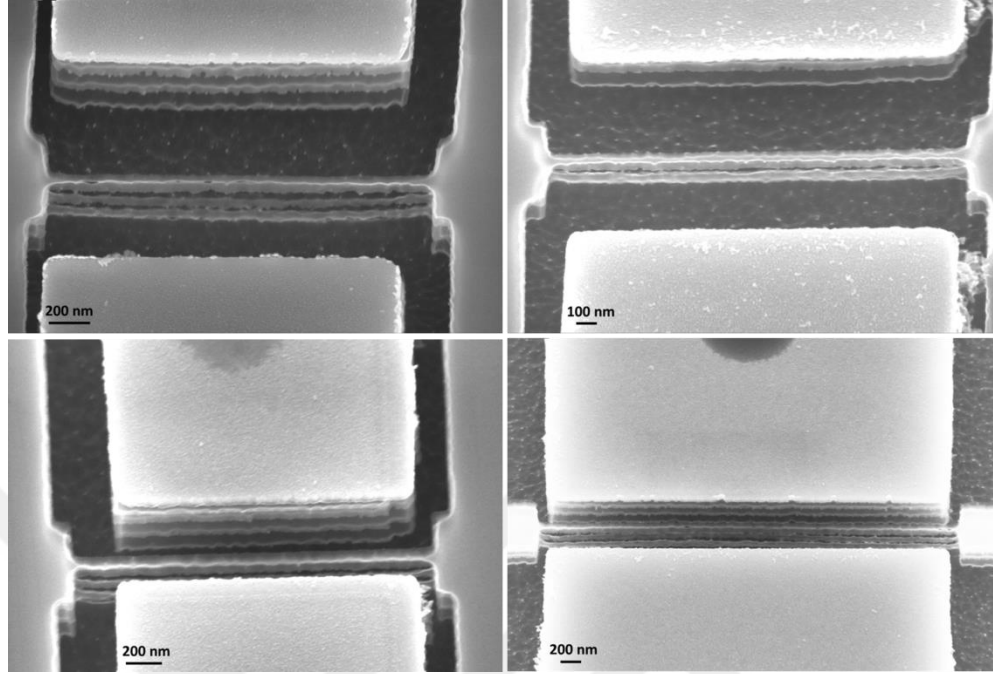


Figure 3.21: Successful integration of a vertical NW stack with metallized electrodes nearby is demonstrated with the nominal resonator-to-electrode gaps of 200 nm and 500 nm

Combination of a vertical NW array and a pair of CMs forms the basis for the proposed coupled NEMS array architecture. Effect of each component of this composite resonator configuration on frequency spectrum characteristics is studied separately by parameterizing the CM and NW lengths. In accordance with the proposed NW array design approaches, the CM length (L_c) is varied from 5% to 50% of the associated resonator length to have different coupling stiffness *i.e.* mechanical coupling, while keeping the length of the resonator fixed to 2 μm as shown in Fig. 3.22. On the other hand, resonators having the length of from 2 μm to 5 μm are coupled with a CM whose length is fixed to 5% of the associated resonator length as shown in Fig. 3.23.

Unlike previous preliminary NW vertical stack fabrications with Si test chips, proper implementation of a NEMS array demands an additional requirement of electrical isolation of coupled NWs from adjacent gate electrodes and an underlying substrate for SOI chips. This necessity should be ensured by complete removal of a SOI device layer until the underlying BOX layer is exposed by DRIE etching. Thus, utilization of a SOI wafer with a device layer thickness of 1 μm requires more etching cycles than silicon test chips studied so far, producing more resonators in fabricated vertical stacks as a byproduct. Therefore, a new set of Bosch process and layout parameters is required to protect NW uniformity while almost doubling number of DRIE process cycles and time. From the layout parameters shown in Fig. 3.3, the nominal resonator-to-electrode gap is eventually reduced from 500 to 200 nm to make the DRIE process more controllable.

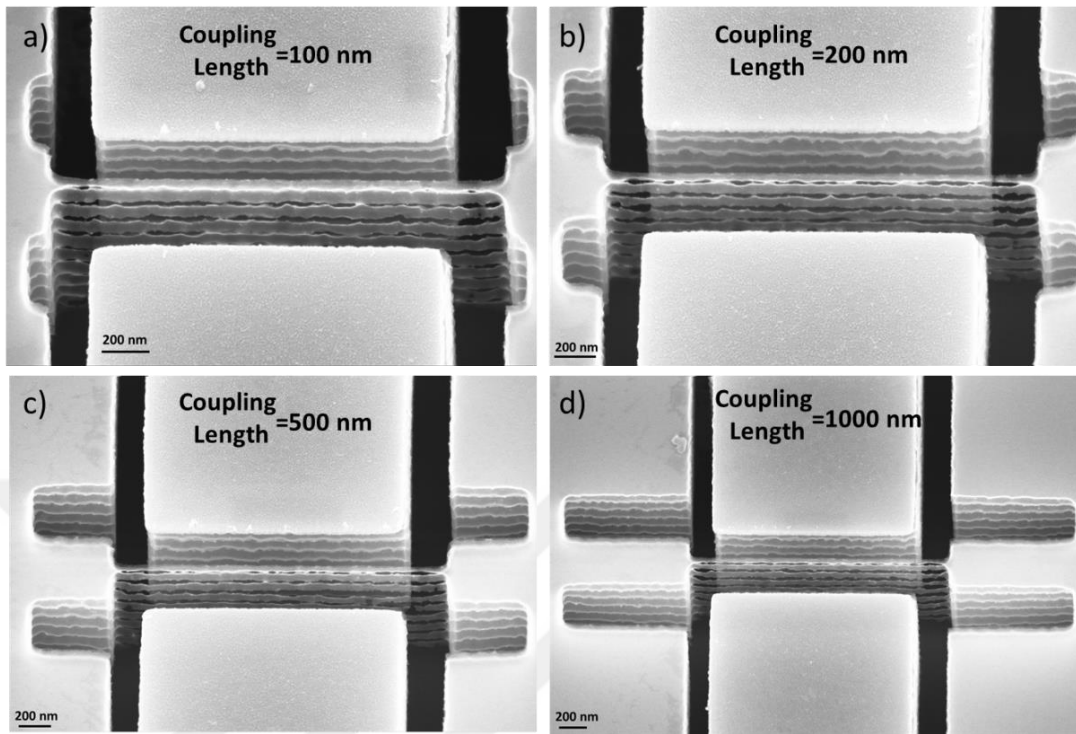


Figure 3.22: Setting the CM length of 100 nm (a), 200 nm (b), 500 nm (c), 750 nm (not shown), 1000 nm (d) corresponds to normalized lengths from 5% to 50% considering a fixed resonator length of 2000 nm

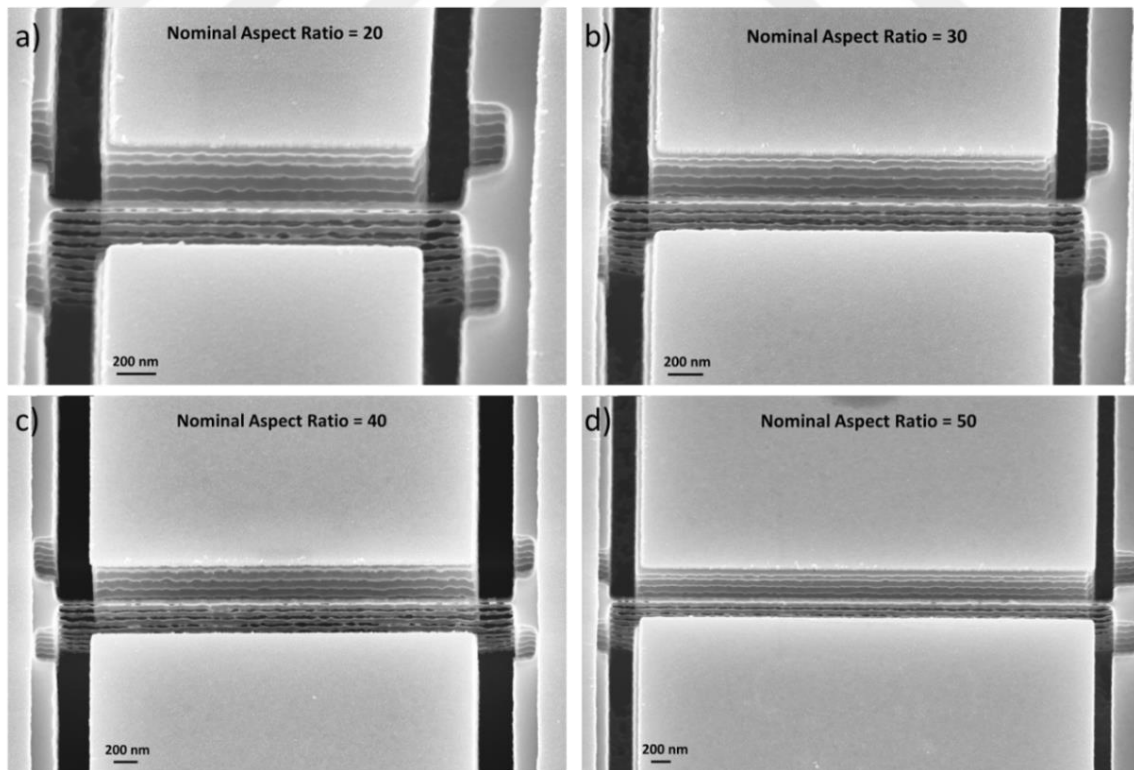


Figure 3.23: Coupled vertical arrays consisting of NWs having lengths from 2 μm (a), 3 μm (b), 4 μm (c) and 5 μm (d) for a fixed CM length of 5% of the associated resonator length.

Apart from apparent DRIE process and layout parameters shown in Fig. 3.3 and discussed so far, one subtle and substantial DRIE parameter partly determining NW profile and uniformity of NWs within a vertical stack emerges while considering how to apply or organize etch cycles during a DRIE process. The employed DRIE equipment of Alcatel AMS200 SE limits users to set the process time for a recipe only to an integer second. This simple but fundamental deficiency of the equipment encourages a user to use of a continuous etch process that is one cycle after another without adjustable purge step in between. Thus, it is impossible run a single etch/passivation cycle and a specific purge step directly one after another for most of the cases. Alternatively, splitting a DRIE process into some etch/passivation cycle groups can be performed such that total etching/passivation time of each group takes an integer second to elapse and inserting a purge step between cycle groups can be employed. Real impact of this seemingly minor difference between DRIE processes with or without a purge step between some process cycles can be appreciated by comparing Figs. 3.24 and 3.25.

A DRIE process consisting only of subsequent etch/passivation cycles without any purge step in between *i.e.* continuous process leads to a smaller scallop size corresponding to a smaller diameter NW and NW interval at higher etch depths as shown in Fig. 3.24. Increasing difficulty of removing etch reaction by-product gases with increasing etch depths slows down DRIE etch rate leading to NWs with smaller diameters.

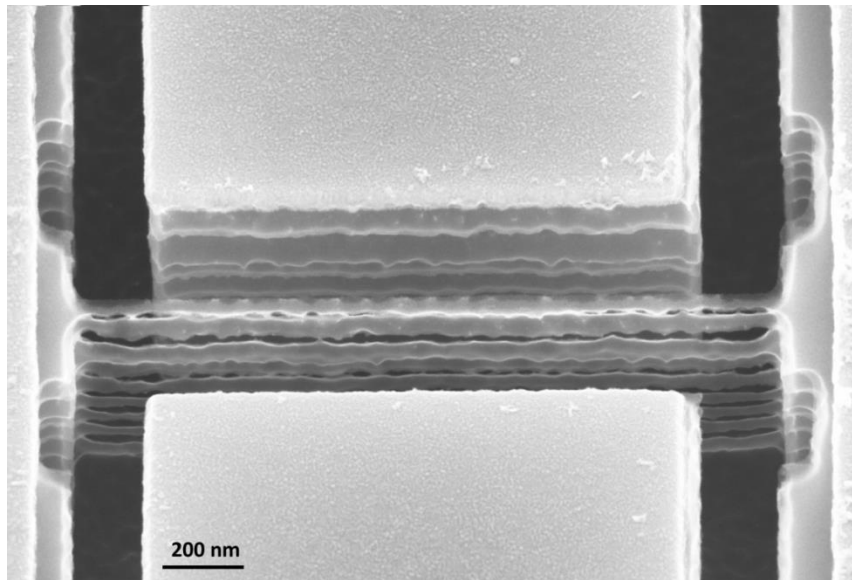


Figure 3.24: A DRIE process consisting only of non-stop etch and passivation cycles leads to smaller diameter NWs as the process continues.

On the other hand, utilization of a purge step between some cycle groups helps to alleviate this effect and resulting non-uniformity as shown in Fig. 3.25. However, dividing a DRIE process into some etching/passivation cycle groups which have overall integer elapsed time for each group is

not an option such as a single etching/passivation cycle time of 3.1 s. In other cases, an optimization about how to organize etch/passivation cycles is required to extract the best uniformity of NWs within a vertical NW stack.

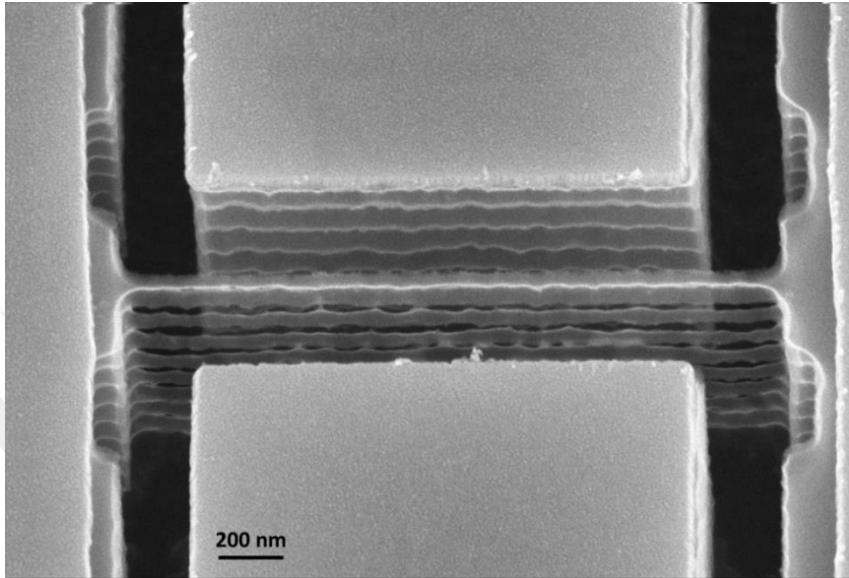


Figure 3.25: Addition of a purge step between DRIE process cycle groups enhances uniformity of NWs within a vertical stack.

Some other representative examples of coupled vertical NW arrays fabricated with or without purge steps in between some DRIE cycles are provided in Figs. 3.26-3.28 together with the applied DRIE recipe strategies and some layout parameters.

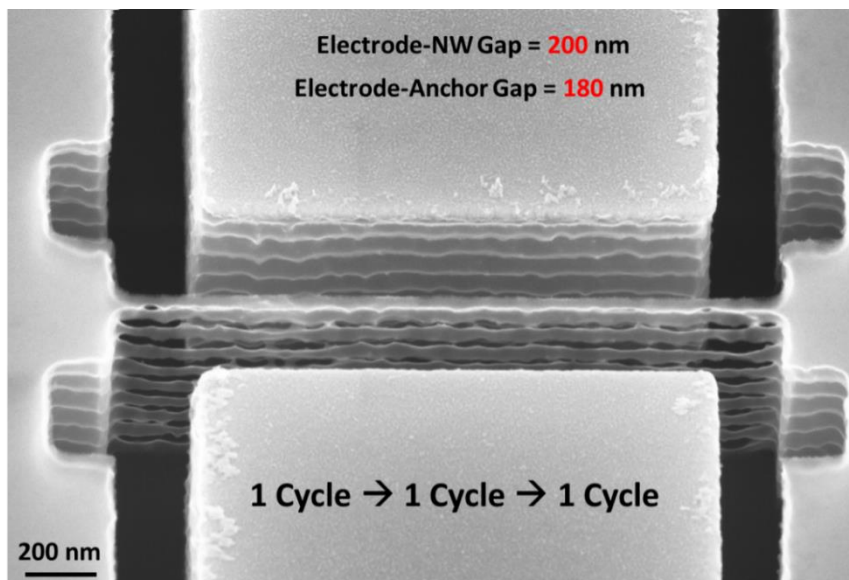


Figure 3.26: Another example of a vertical NW array fabricated with a continuous process displays the non-uniformity of NWs in the neighborhood of the NW-CM junctions.

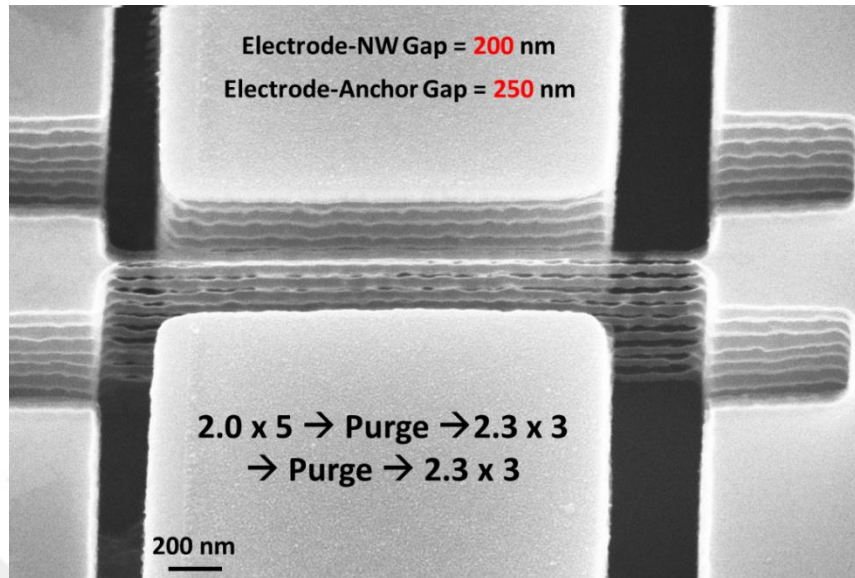


Figure 3.27: Application of different etch step times for each etch/passivation cycle groups can be exploited to have better NW uniformity in a vertical stack.

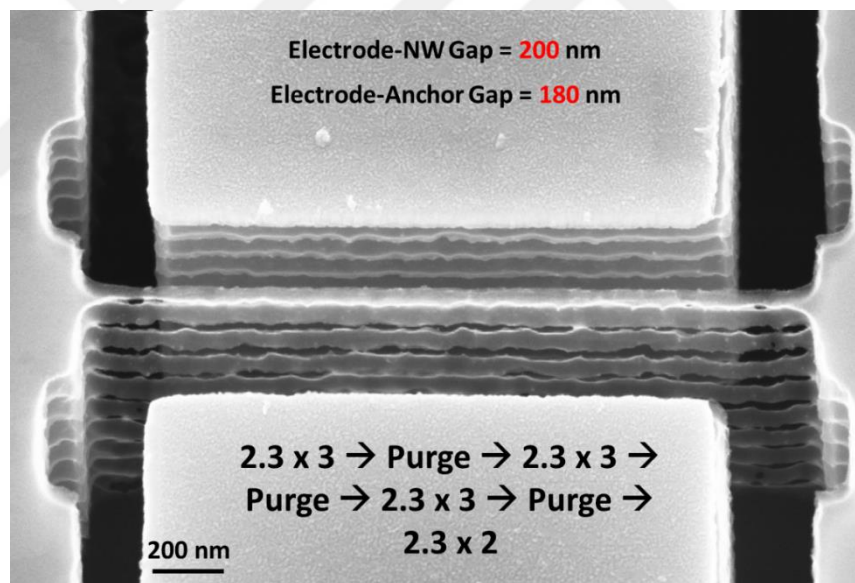


Figure 3.28: Employment of multiple purge steps between short cycle groups results in very good uniformity for the NWs in this vertical stack.

A clever solution to bypass the integer overall DRIE process time limitation of the equipment can be the introduction of a third process gas into a recipe to permit a purge step after each etch/passivation cycle. Moreover, the effect of the new process gas can be made negligible by setting the flow rate of this gas equal to zero. Although this approach seems promising in terms of NW uniformity in a vertical stack and reducing complexity of a DRIE process, initial DRIE experiments having this etch-passivation-purge pattern lead to some variations from previous DRIE etch characteristics such as DRIE etch rate as shown in Fig. 3.29. This process scheme

clearly deserves further examination with more experiments to develop a fine-tuned DRIE recipe to have the best NW uniformity in a vertical stack.

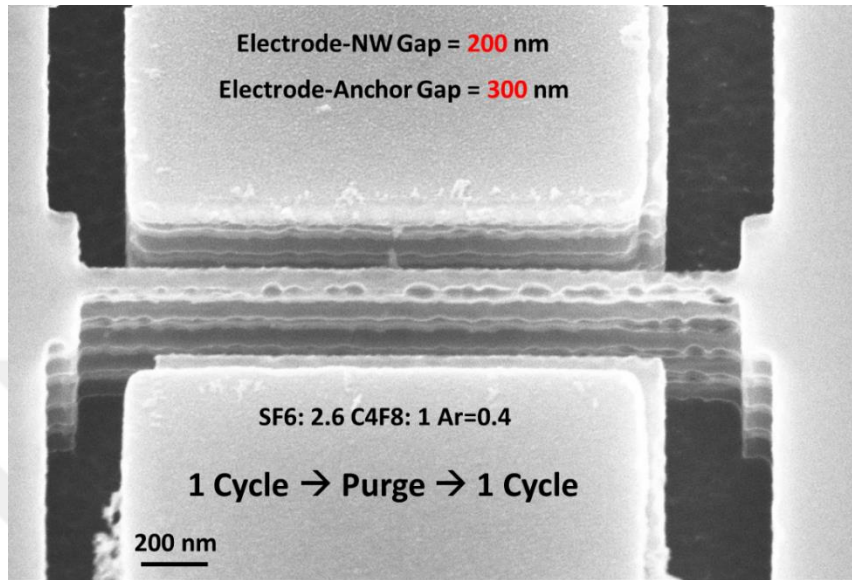


Figure 3.29: Introduction of a third gas such as Ar in a DRIE recipe enables a purge step right after each etch/passivation cycle without any change on resulting etch characteristics if the flow rate of this gas is set to zero.

Moreover, DC probe station measurements between touchpads connected to fabricated NW arrays result in the representative current-voltage relationship shown in Fig. 3.30 being reminiscent of the response from a diode. Further investigations trace this behavior to the existence of a Schottky contact rather than an ohmic contact at metal-doped Si interfaces. A residual dielectric layer on the wafer surface after the employed doping process is suspected as the origin of this contact problem. Scratching of some part of a metallization layer on a touchpad by a probe and then establishing direct contact to the underlying doped Si layer through wirebonding result in ohmic contacts with a NW resistance of approximately 2 k Ω .

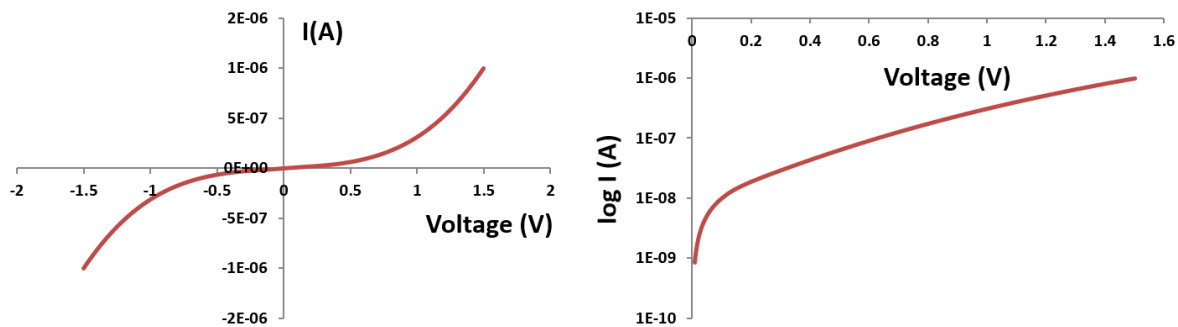


Figure 3. 30: Existence of a dielectric layer at metal-Si interfaces is suspected as the cause of the shown I-V relation similar to the typical behavior from a diode.

3.4. Fabrication Conclusions

As a result of the fabrication characterizations, coupled vertical arrays of Si NWs consisting of 8 NWs are optimized successfully in terms of uniformity of a NW along its length and of various NWs within a stack, structural integrity and electrical isolation with the help of the layout parameters of Fig. 3.3 for SOI 1 cm x 1 cm chips. Resulted DRIE recipes having a scallop size of approximately 20 nm lead to formation of vertical NW stacks with the actual NW width of approximately 65 nm as shown in Fig. 3.31 from the nominal mask linewidth of 100 nm. NWs with aspect ratios of up to 50 (up to 77 if the actual width of NWs of approximately 65 nm after a usual DRIE process is employed) coupled with CMs with percent lengths of up to 50 % of the associated resonator length of 2000 nm are carved out in a vertical array configuration. Insertion of a purge step between small groups of etch/passivation cycles gives the best results in terms of NW uniformity in a vertical stack. The fabrication flow of coupled vertical NEMS resonators presented in Fig. 3.1 is found quite reliable and repeatable with the developed recipes.

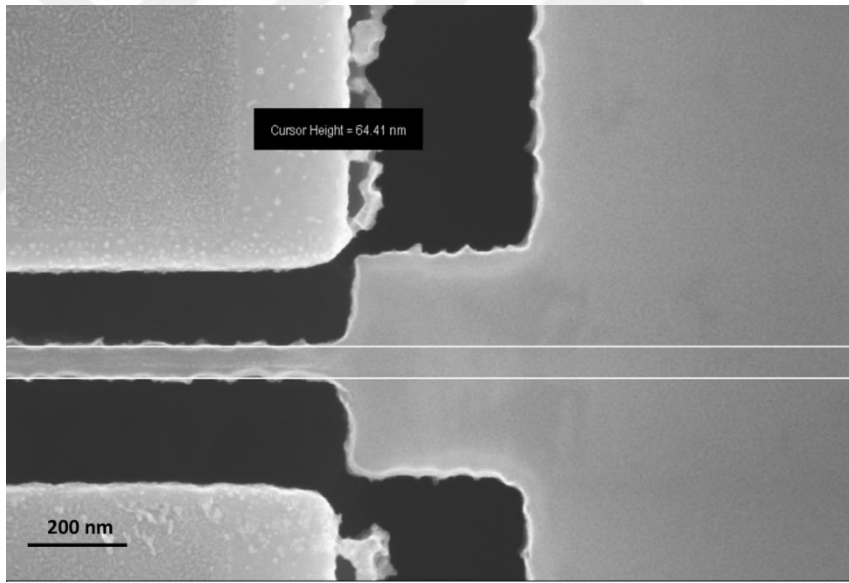


Figure 3.31: Actual width of NWs in a vertical stack is determined primarily by the parameters of initial mask linewidth and recipe-dependent scallop size.

Table 3.1 summarizes the optimized DRIE process and layout parameters for SOI and Si test samples. The employed DRIE processes are optimized at 25 °C using Quick Stick to attach a 1 cm x 1 cm sample to an underlying blank carrier wafer. Etching of the device layer thickness of the utilized SOI wafer of 1 μm together with the complete removal of any formed Si membranes takes 11 DRIE cycles or corresponding DRIE process time of approximately 37 s with the given etch and passivation step times in Table 1.

Table 3.1: Mask layout and DRIE process parameters optimized for the best uniformity and structural integrity of NWs in a Si vertical stack are different for Si test and SOI samples.

Mask Layout & DRIE Parameters	Si Test Samples	SOI Samples
Etching (SF ₆) Step Time (s)	2.6	2.3
Passivation (C ₄ F ₈) Step Time (s)	1	1
Nominal Electrode-NW Gap (nm)	500	180
Nominal Electrode-Anchor Gap (nm)	300-1200	180-250
Number of NWs within a Vertical Stack	4	8
Number of Cycles	5	11
Process time (s)	19	37

Chapter 4: Frequency Spectrum Measurements

4.1. NW Frequency Spectrum Measurements

Among various transduction techniques, higher integration capability to on-chip electronics and compatibility with batch fabrication make electromechanical transduction the preferential scheme whenever possible. While integration of resonators to on-chip electronics enables utilization of various functions such as signal conditioning, multiplexing and amplification, compatibility with batch fabrication leads to favorable manufacturing costs for micro and nano systems having reliable and low noise operation.

Although the capacitive readout is the traditionally dominating transduction technique for MEMS, technical issues such as ever-decreasing motional capacitance embedded in significant parasitic capacitance and increasing impedance mismatch with measurement equipment requiring extremely small gaps or very high operation voltages hinder employment of the capacitive detection for nano structures. Fortunately, efficient conversion of high frequency miniscule resonator motion of few nanometers into resolvable electrical signals can be achieved with piezoresistive transduction.

Thus, electromechanical characterization of the fabricated resonators is performed using electrostatic actuation and piezoresistive readout in order to ensure the best integration possibility with on-chip electronics in the future. While electrostatic actuation is implemented to initiate resonance vibration using only one of two adjacent gate electrodes at each side of resonators, the other gate is grounded. Frequency downmixing enables indirect measurement of a high frequency signal by demodulating it to low frequency components. Low frequency detection signals arise from mixing of high frequency signals with the vibration of resonators. In this way, challenges such as impedance mismatch and large parasitic capacitances inherent to the capacitive readout of high frequency minute motion detection of nanoresonators are handled.

Two piezoresistive frequency downmixing techniques namely two-source/ 1ω and two-source/ 2ω detection scheme are employed. The experimental setup for each piezoresistive frequency downmixing scheme are shown in Fig. 4.1 schematically. Next, equations for these time-varying low frequency detection signals are derived for the utilized downmixing schemes.

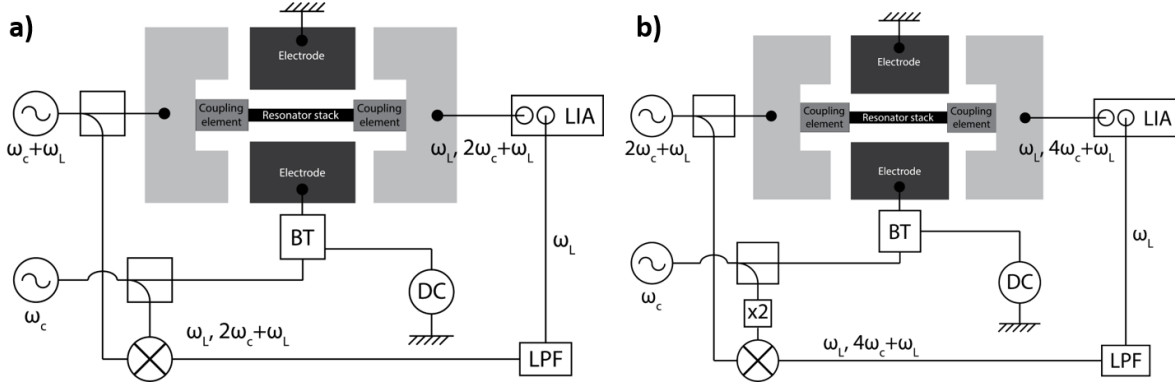


Figure 4.1: The experimental setups of two-source/ 1ω (a) and two-source/ 2ω (b) detection schemes are shown schematically. Frequency mixing leads to low-frequency motional components detected by a lock-in amplifier. LIA: Lock-in Amplifier, LPF: Low Pass Filter, BT: Bias Tee

Let us begin with the consideration of a beam profile at any moment. A beam profile can be modeled as if the combination of the two deflection components. First, static forces stemming from an adopted fabrication flow yield asymmetric beam profile at rest. Second, electrostatic driving forces in case of electrostatic actuation result in a vibration mode shape. Superposition of these displacements can be used to define a resonator beam profile at any time as in Eq. 4.1 [68].

$$w(x, t) = d_0 \phi_0(x) + a_n(\omega) \phi_n(x) \cos(\omega t) \quad (4.1)$$

where x is the coordinate along the beam's length, and $a_n(\omega)$ is the maximum vibration amplitude at a driving frequency ω and d_0 is the maximum static deflection at rest in the vibrational plane of a given mode. Moreover, $\phi_0(x)$ and $\phi_n(x)$ are the asymmetric beam profile at rest normalized to d_0 and the n th-order vibration mode profile normalized to $a_n(\omega)$ respectively. The piezoresistance can be simplified as the change in electrical resistance of a material as a function of applied mechanical strain. Periodic elongation of a vibrating beam is a case where the same relation between the time-varying resistance change $\Delta R(t)$ and the total net strain $\epsilon(t)$ can be established as in Eq. 4.2.

$$\Delta R(t)/R_u = G\epsilon(t) \quad (4.2)$$

where G corresponds to the proportionality constant also called gauge factor and R_u is the undeflected beam resistance. The total net strain can be calculated using the beam deflection model in Eq. 4.1 as in Eq. 4.3 [69].

$$\epsilon_d = \frac{1}{2L} \int_0^L w'^2(x, t) dx \quad (4.3)$$

where prime denotes derivative with respect to the spatial coordinate x , and L is the undeflected beam length. Current through the beam can be determined using Ohm's law from the time-

dependent parameters of voltage applied to the beam $V_{NW}(t)$ and total resistance $R_{NW}(t)$ as in Eq. 4.4.

$$I_{NW} = \frac{V_{NW}(t)}{R_{NW}(t)} = \frac{V_{NW}(t)}{R_u \left(1 + \frac{\Delta R(t)}{R_u}\right)} \cong \frac{V_{NW}(t)}{R_u} \left(1 - \frac{\Delta R(t)}{R_u}\right) \quad (4.4)$$

$V_{NW}(t)$ is a harmonic signal at frequencies $\omega + \omega_L$ and $2\omega + \omega_L$ for the two-source/ 1ω and two-source/ 2ω detection schemes respectively where ω_L is the low frequency of the modulated voltage signal.

$$V_{NW,2s1w}(t) = V_0 \cos[(\omega + \omega_L)t] \quad (4.5)$$

$$V_{NW,2s2w}(t) = V_0 \cos[(2\omega + \omega_L)t] \quad (4.6)$$

Electrostatic actuation is accomplished by combining DC bias and AC input voltages applied to a gate electrode and the resonator input respectively. Sweeping the driving frequency across the frequency spectrum enables resonator vibration when it coincides with the natural frequencies of the resonator.

Eq. 4.4 indicates that in general, multiplication of the time-varying beam input voltage and resistance terms results in signal mixing and eventually low frequency current signals at frequency ω_L during resonance. Thus, the transduction scheme dependence of the voltage waveform given in Eqs. 4.5 and 4.6 yields distinct low-frequency motional current components by mixing with different time-varying resistance components. Substitution of the associated voltage and resistance change parameters in Eq. 4.4 leads to the following low-frequency current signal equations for each downmixing scheme.

$$I_{2s1w} \cong -G \frac{1}{2L} \frac{V_0}{R_u} a_n(\omega) d_0 \int_0^L \phi'_0(x) \phi'_n(x) dx \quad (4.7)$$

$$I_{2s2w} \cong -G \frac{1}{8L} \frac{V_0}{R_u} a_n^2(\omega) \int_0^L \phi_n'^2(x) dx \quad (4.8)$$

Thus, Eqs. 4.7-4.8 indicate that the time-dependent current variation has two components irrespective of a beam profile at rest and vibration mode shape in case of any asymmetric beam deflection profile at rest. First, the two-source/ 1ω transduction leads to a current signal at the driving frequency (ω) which is proportional to the vibration amplitude and deflection at rest. The second current signal is at the frequency of 2ω and proportional to the square of the vibration amplitude. As a result, while linear relation of the current signal with the vibration amplitude makes the two-source/ 1ω detection a linear transduction technique, the two-source/ 2ω detection corresponds to quadratic transduction.

If the fundamental flexural mode shape is assumed to be the case for a beam profile at rest, Eqs. 4.7-4.8 can be reduced to Eqs. 4.9-4.10 for the fundamental resonance mode ($n=1$) for each transduction technique.

$$I_{2s1\omega} \cong -2.44 \frac{V_0 G}{R_u L^2} d_0 a_1(\omega) \quad (4.9)$$

$$I_{2s1\omega} \cong -0.61 \frac{V_0 G}{R_u L^2} a_1^2(\omega) \quad (4.10)$$

The ratio between both low frequency current signals reduces to Eq. 4.11.

$$\frac{I_{2s1\omega}}{I_{2s2\omega}} = \frac{4d_0}{a_1} \quad (4.11)$$

Eq. 4.11 shows that when the asymmetric beam deflection at rest is greater than the quarter of the vibration amplitude, there is an amplification effect on the piezoresistive transduction. This amplification certainly helps to detect high frequency minute nanoresonator motion.

SEM is a commonplace tool to characterize an asymmetric beam profile at rest. In this way, device-dependent maximum static deflection amplitude d_0 can be classified and quantified accurately. Tensile stress stemming from the undercut parts of anchoring structures was shown to lead to higher static deflections for top-down resonators than bottom-up structures in the literature [68]. The SEM micrograph of Fig. 4.2 exemplifies the representative top view of a fabricated vertical NW array sample having a clear asymmetric beam profile at rest.

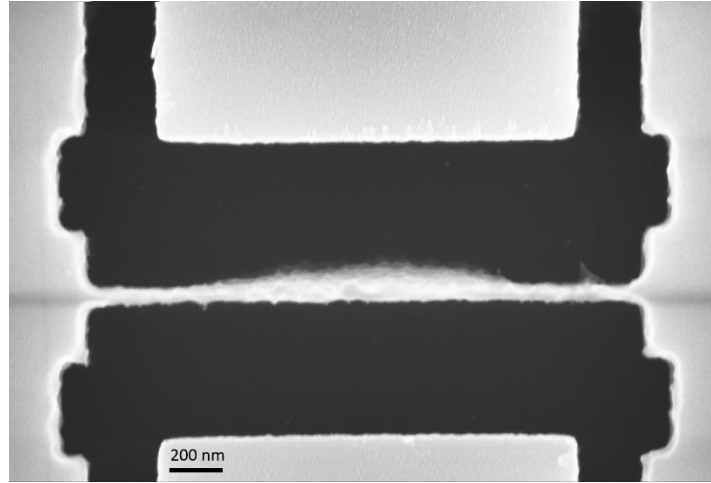


Figure 4.2: Asymmetric NW profile of a fabricated vertical NW array yields linear and quadratic time-varying resistance components.

In this work, the piezoresistive frequency downmixing techniques of two-source/ 1ω and two-source/ 2ω are employed to determine frequency spectrum responses of single fixed-fixed NWs and coupled vertical NW stacks. One to one correspondence of the two-source/ 1ω and two-

source/ 2ω transduction schemes to linear and quadratic current variation components respectively enables to quantify the relative magnitude of these components. As a result, the position of in-plane and out-of-plane resonance peaks of fabricated resonators are determined in the frequency spectrum through electromechanical characterization.

Electrical detection of fabricated single NWs and coupled vertical NW arrays is performed using electrostatic actuation and piezoresistive downmixing transduction in Bilkent University in collaboration with Prof. Hanay. The common specimen layout of fabricated NW arrays of Fig. 3.4 and Fig. 4.3.a depicts a vertical NW array in the middle, Pt touchpads at the perimeter and Pt metal lines connecting these two features. A simple printed circuit board (PCB) featuring SMA connector ports, central sample seating space and $50\ \Omega$ Cu metal lines is used to mechanically support and electrically connect of fabricated samples to measurement equipment. A typical employed PCB shown in Fig. 4.3.b also provides electrical grounding to the handle layer of fabricated SOI chips. Interconnection between fabricated devices and measurement equipment is achieved by first seating samples on a PCB and then performing wirebonding between a $100\ \mu\text{m} \times 100\ \mu\text{m}$ Pt touchpad on a sample and a metal line lying between the central seating space and a SMA connector port on a PCB. Four such wirebonding connections using gold wires are implemented for each sample to realize the experimental setups shown schematically in Fig. 4.1.

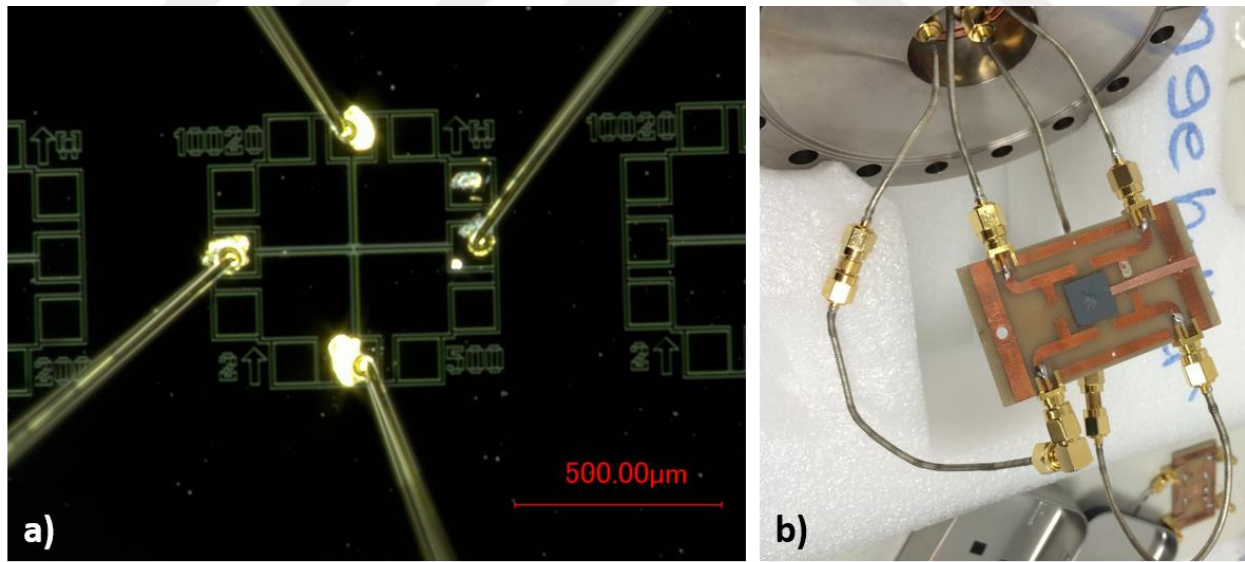


Figure 4.3: Wirebonds in (a) connect fabricated samples to measurement equipment through a PCB and a flange adaptor in (b)

Then, the PCB is connected to a flange adaptor shown in Fig. 4.3.b and placed in a vacuum chamber. The flange adaptor having several embedded SMA feedthroughs is used to support the PCB in the vacuum chamber and ensure electrical connections between the inside and outside of the vacuum chamber.

Frequency spectrum measurements of single NW and vertical NW array samples are performed at atmospheric and vacuum conditions. Vacuum pressures as low as 1×10^{-9} torr are achieved. Moreover, a vacuum chamber equipped with liquid nitrogen cooling enables electrical measurements at cryogenic temperatures as low as 76 K.

Two probe DC probe station measurements indicate very low power handling capacity for fabricated NW structures such that the DC voltage of 0.5 V is enough to damage single NW samples. Hence, very low peak-to-peak AC voltage around 0.3 V is applied to a NW input. On the other hand, DC and peak-to-peak AC voltages applied to a side-gate are swept up to 10 and 15 V respectively. The other gate electrode is grounded to decrease parasitic capacitances. The low frequency of the modulated voltage signal ω_L is also optimized at approximately 37k to get the cleanest electrical signals.

4.2. Determination of Mechanical Resonance Modes

Preliminary frequency spectrum sweeps are conducted in wide frequency windows as shown in Fig. 4.4 to demonstrate various signal peaks simultaneously. In general, any fabricated NW sample of this study may have various frequency spectrum peaks which can be associated with either in-plane and out-of-plane flexural mechanical modes. These spectrum peaks are classified as mechanical or electronic depending on their behavior with measurement parameters. For example, the signal peak at 101 MHz shown in Fig. 4.4 indicates a possible mechanical origin due to its resonance frequency dependence on varying gate AC voltages.

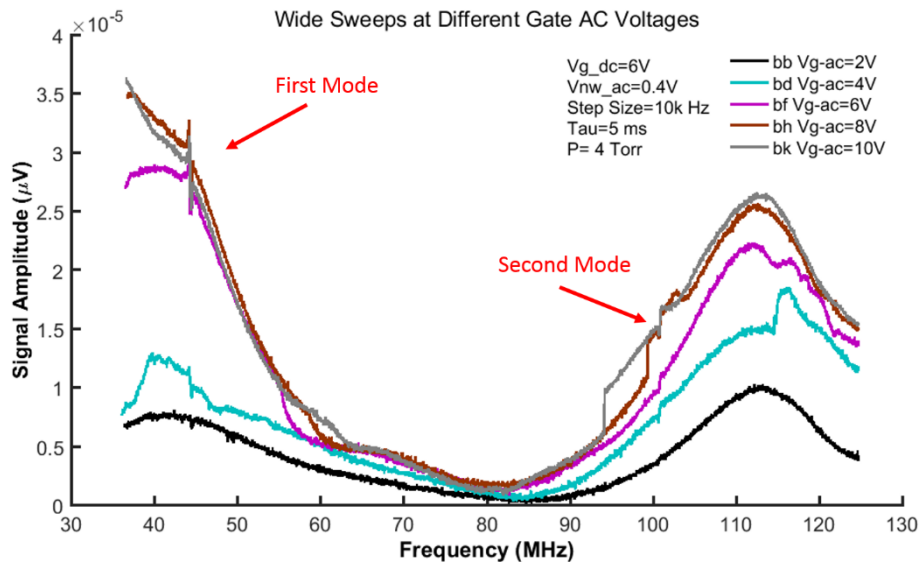


Figure 4.4: Wide range frequency spectrum sweeps at different gate AC voltages are employed to pinpoint possible mechanical resonance modes.

Each item in the following list provides some evidence to corroborate the mechanical nature of a certain frequency spectrum peak.

- Resonance frequency tuning with respect to gate electrode voltages
- Quality factor and resulting signal amplitude dependence on viscous damping coefficients
- Signal transition from linear to nonlinear drive with increasing gate voltages.
- Existence of hysteresis for nonlinear signals
- Comparison of measurements using two-source/ 1ω and two-source/ 2ω detection
- Comparison of signal responses from either gate

Each item helps to identify some mechanical aspect of a true mechanical signal peak. For example, electrostatic spring forces subtract from mechanical stiffness of a resonator leading to a lower resonance frequency of a NW yielding spring softening. As a result, the resonance frequency of a mechanical resonator shifts as a function of gate AC and DC voltages. Thus, collecting frequency spectrum data of a specific signal peak at different gate voltages provides a simple mean to distinguish mechanical modes from electronic counterparts. Figure 4.5 exhibits frequency spectrum measurements at different gate AC voltages for the signal peak at approximately 44 MHz. Spring softening with increasing gate AC voltages is obvious from the figure. Moreover, the frequency peak seems to diminish gradually at smaller gate voltages as expected from any mechanical mode.

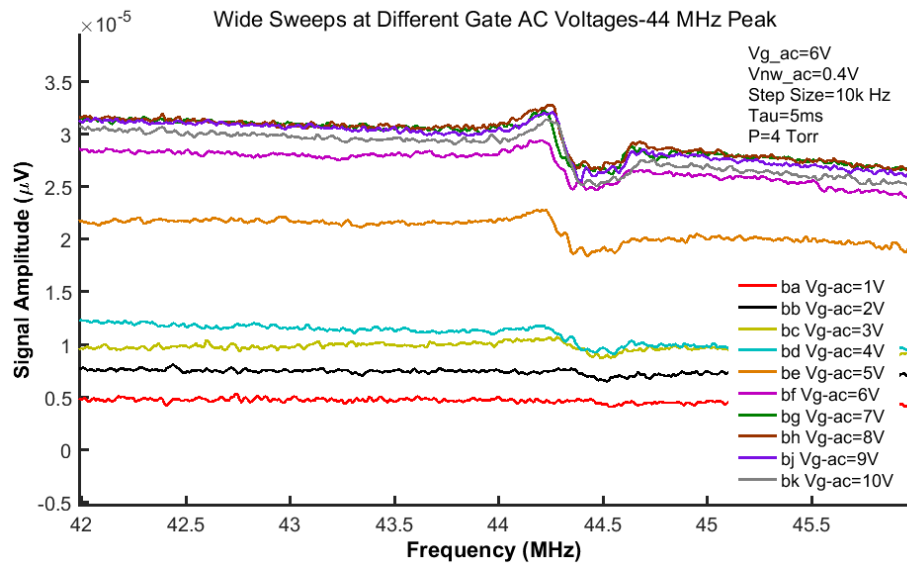


Figure 4.5: Frequency tuning of a detected spectrum peak with respect to gate AC voltages

Dependence of the Q of a damped oscillator on viscous damping coefficients obtained at various pressures can be used to validate mechanical nature of a detected signal. Such an analysis can be made simply by comparing device frequency spectrum responses at atmospheric and vacuum

pressures as shown in Fig. 4.6. Higher Q at a vacuum pressure implies the existence of a mechanical mode for this frequency spectrum peak.

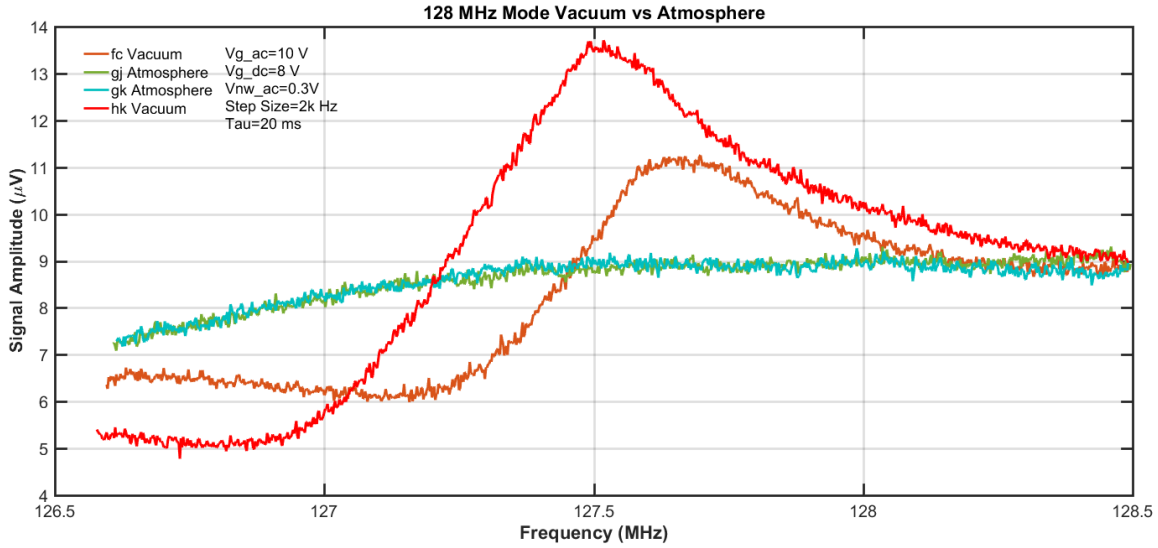


Figure 4.6: Comparison of the measurement signals at atmospheric and vacuum pressures

Resonance frequency of a mechanical mode changes linearly with small measurement voltages and a linear signal response ideally has the Lorentzian shape. Gradual increase in measurement voltages leads to nonlinear resonance frequency variation with applied voltages at some point. Moreover, a nonlinear signal response features discontinuity in the frequency spectrum. Thus, a linear signal response having the Lorentzian shape at smaller measurement voltages turns into a nonlinear response with discontinuity in the frequency spectrum by gradual increase in applied voltages. Transition of a signal response from linear to nonlinear regime is shown in Fig. 4.7.

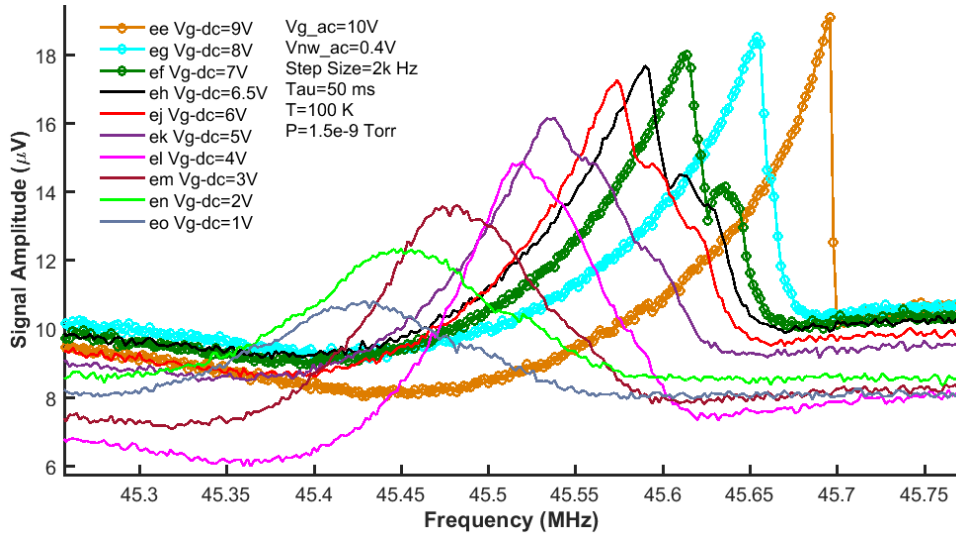


Figure 4.7: Transition of a spectrum peak from linear to nonlinear regime with increasing gate DC voltages

A nonlinear mechanical signal exhibits some hysteresis. Hysteresis characteristic of a mechanical mode can be revealed by taking frequency spectrum sweeps in the ascending and descending frequency directions. Thus, transition of a signal peak from the linear to nonlinear behavior coupled with hysteresis characteristic of a nonlinear signal response shown in Fig. 4.8 provide a strong claim on the existence of a mechanical mode.

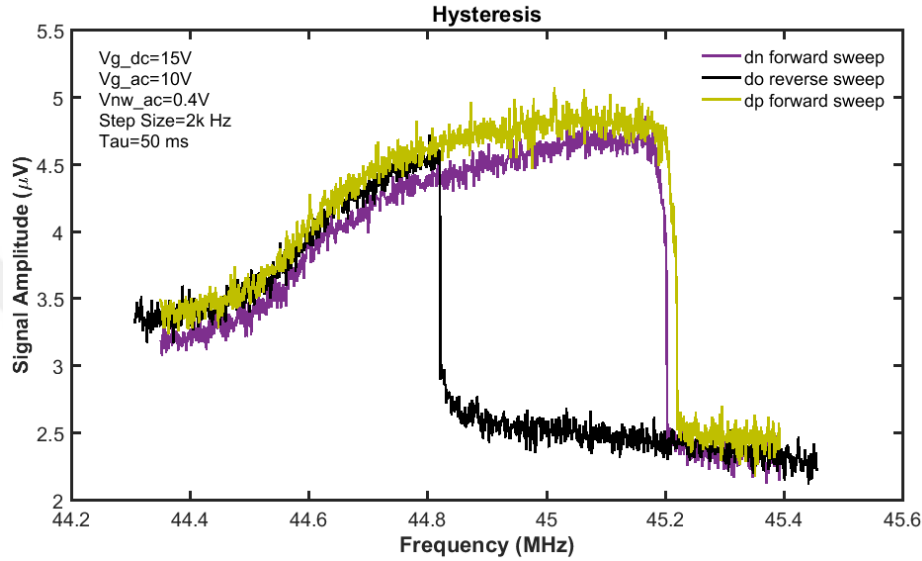


Figure 4.8: Frequency spectrum sweeps in the ascending (forward) and descending (reverse) directions are used to exhibit hysteresis characteristic of a signal peak

While the two-source/ 1ω detection scheme results in signal peaks at mechanical resonance frequencies, a mechanical spectrum peak is obtained at half of a resonance frequency using the two-source/ 2ω transduction. Therefore, simultaneous detection of frequency spectrum peaks at a resonance frequency and half of a resonance frequency using the 1ω and 2ω piezoresistive frequency downmixing schemes ensures the mechanical origin of a signal peak. However, smaller signal amplitudes resulting from the less efficient two-source/ 2ω detection scheme make it more difficult to detect NW mechanical modes in general. A representative comparison of signal outputs between the two-source/ 1ω and two-source/ 2ω detection schemes is shown in Fig. 4.9.

Electrostatic actuation and piezoresistive readout schemes necessitate employment of the only one of two gates electrodes. While AC and DC gate voltages are applied to a selected gate, the remaining gate is grounded. Since all sample layout parameters are symmetrical nominally along the NW longitudinal axis on employed fabrication masks, gate related layout parameters are identical nominally. However, finite overlay accuracy of an adopted fabrication flow results in some differences between any two gates on a sample such as a NW and gate electrode distance. Thus, switching of an employed gate can lead to some change in a signal response behavior and provide additional information about an examined signal peak. This is the case shown in Fig. 4.10 which compares the signal responses from either gate.

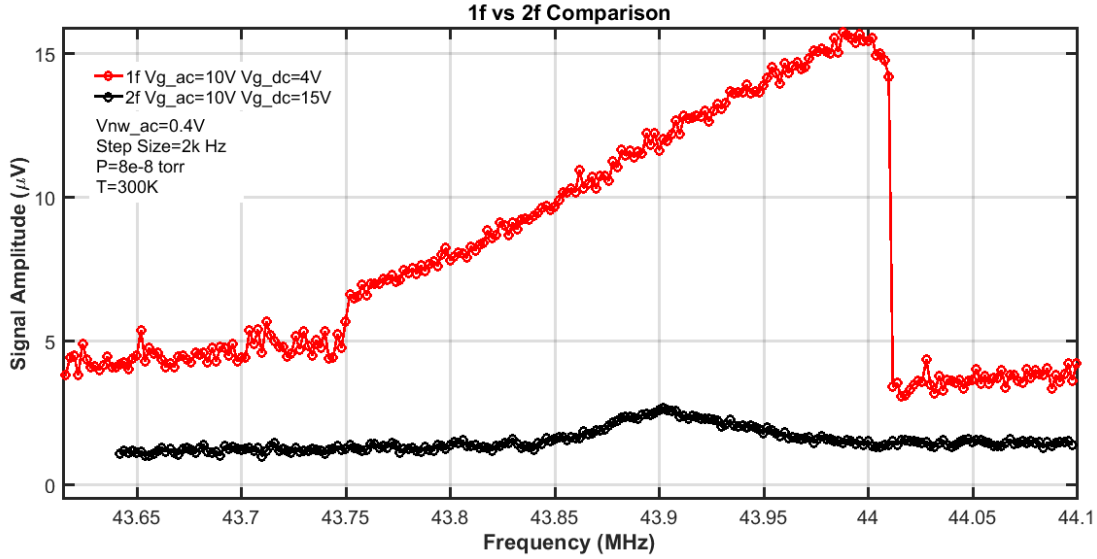


Figure 4.9: Demonstration of spectrum peaks using both of the transduction schemes to corroborate the mechanical character of a detected peak.

All of these points are taken under consideration to determine the origin of any signal peak on a frequency spectrum sweep whether it is mechanical or electronic conclusively. Thus, specification of a signal peak as a mechanical mode must meet the mentioned conditions simultaneously.

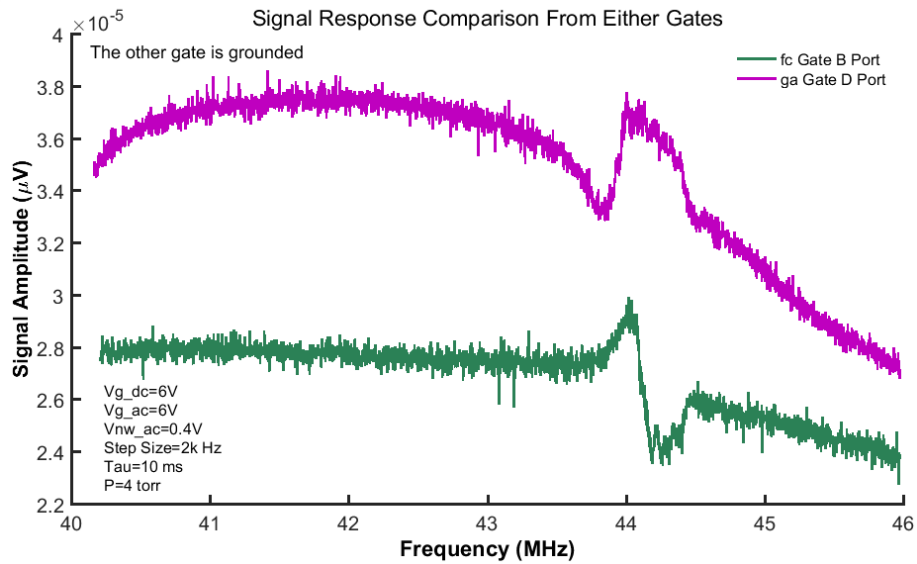


Figure 4.10: Comparison of detected signal responses from either gate may provide some information about a resonator structure on hand.

4.3. Single NW Frequency Spectrum Measurements

Electrical measurements are performed not only for fabricated coupled vertical NW arrays but also for single clamped-clamped NWs to examine effects of mechanical coupling and multiple resonators in an array on frequency spectrum characteristics. Hence, frequency spectrum

characteristics of single clamped-clamped Si NW samples fabricated by someone else [70] are investigated using electrostatic actuation and piezoresistive transduction as explained in Section 4.1 prior to coupled vertical NW array samples. Each suspended single Si NW spanned between two microscale electrodes was fabricated from a SOI substrate with a 10 μm thick device layer. The wafer was doped with phosphorous to a mean resistivity of $5 \times 10^{-4} \Omega\text{cm}$. A nominal gap of 400 nm between each Si NW and side-gate electrodes was achieved. Further fabrication details can be found elsewhere [71, 72].

Frequency spectrum measurements of single clamped-clamped NWs are performed using three samples having two different resonator geometries and crystal orientations. Some nominal device layout parameters consisting of NW width (w), height (h), length (L) and crystal orientation for each sample is summarized in Table 4.1.

Table 4.1: Dimensions and crystallographic orientation of the single NW samples employed in frequency spectrum measurements

Sample	Sample 1	Sample 2	Sample 3
w (nm)	80	80	80
h (nm)	200	200	200
L (μm)	5	5	8
Orientation	<100>	<110>	<100>

However, the adopted fabrication flow [70] resulted in a NW structure featuring Bosch process induced scallops and a thin oxide encapsulation layer. Moreover, a careful examination of the cross section of a fabricated NW sample using transmission electron microscope (TEM) revealed a trapezoidal cross section together with an excessive tail formed at the bottom [72]. Thus, actual NW geometry is far more complex than usual rectangular cross section with the nominal dimensions shown in Table 4.1 and should be considered accordingly.

In this section, frequency spectrum measurement results of the employed NWs are given sample by sample. Mechanical origin of detected spectrum peaks is investigated to explore frequency spectrum characteristics of the samples. In addition to points itemized in Section 4.2 to corroborate the mechanical origin of a frequency spectrum peak, frequency stability measurements are conducted by determining Allan deviation of certain mechanical peaks at ambient and cryogenic temperatures.

As specified in Table 4.1, Sample 1 has a clamped-clamped Si NW having the nominal dimensions of 80 nm x 200 nm x 5 μm (w , h and L) and the <100> crystal orientation. The wide range frequency spectrum sweep for the first sample is shown in Fig. 4.11. The frequency sweep designates two mechanical modes at approximately 46 MHz and 101 MHz.

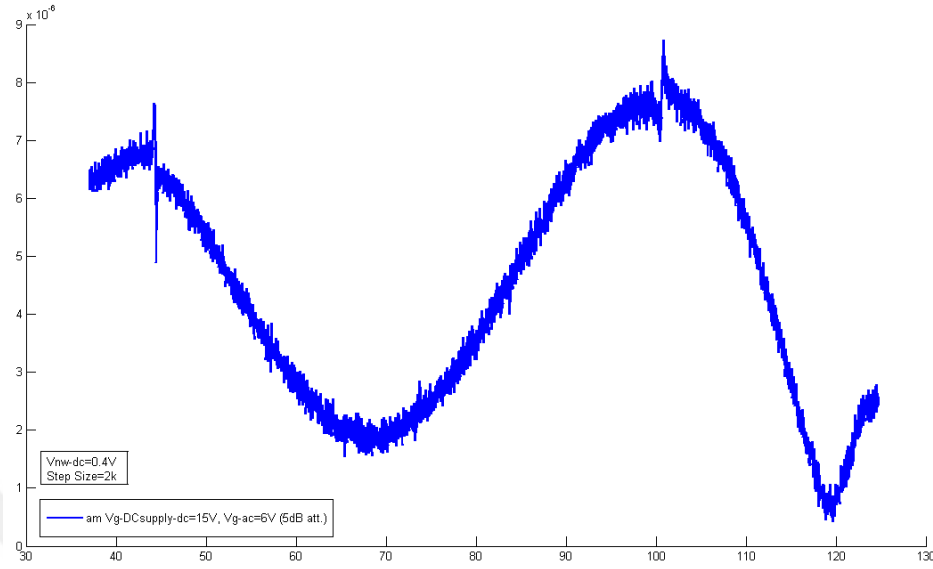


Figure 4.11: Sweeping a large part of the frequency spectrum results in two mechanical modes at approximately 46 MHz and 101 MHz

Resonance behavior of the first mode of the first sample with respect to gate voltages is examined at ambient and cryogenic temperatures. Fig. 4.12 summarizes frequency spectrum measurements at room temperature for various gate AC voltages. Increasing the amplitude of a gate AC voltage results in spring hardening and transition to the nonlinear oscillation mode.

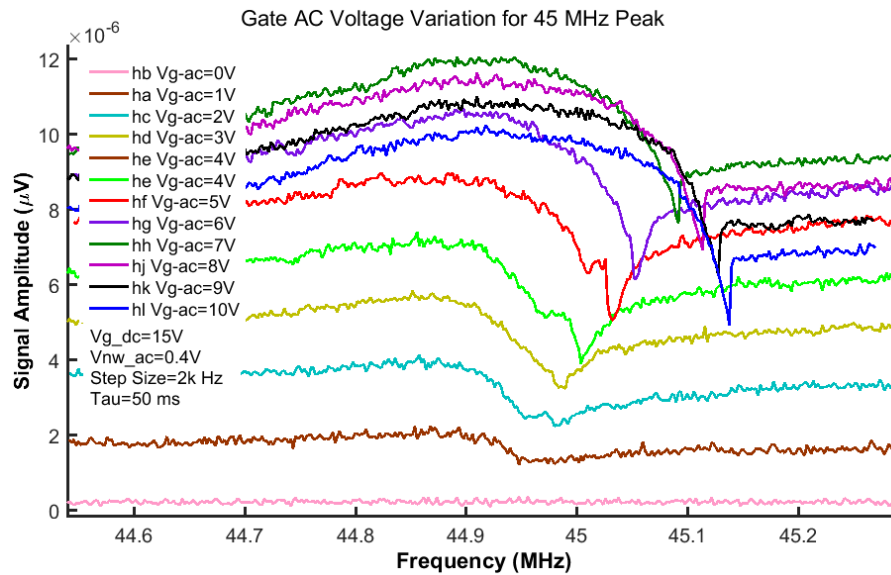


Figure 4.12: Resonance frequency tuning with respect to gate AC voltages demonstrates a linear character at small voltages for the 45 MHz peak

Resonance signal characteristics such as signal-to-noise ratio and Q are also investigated at cryogenic temperatures as low as 76 K and compared with room temperature results. Gate DC voltage effect on the resonance behavior of this mode performed at 125 K is given in Fig. 4.13.

Similar to the gate AC dependence of the 45 MHz peak shown in Fig. 4.12, transformation from the linear to nonlinear oscillation regime and spring hardening are observed. Thus, low temperature measurements yield similar results in terms of background signal level and spring hardening with increasing gate voltages.

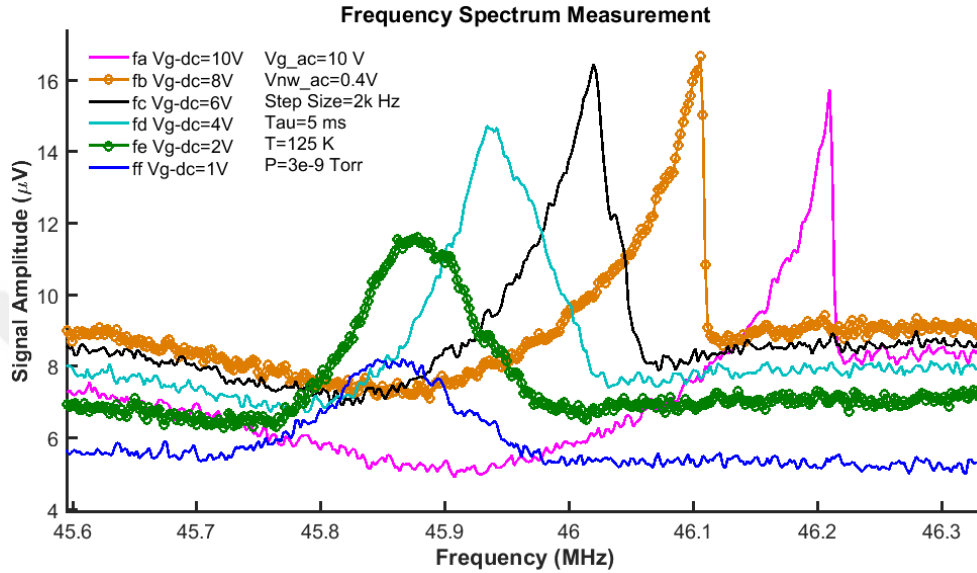


Figure 4.13: Dependence of the 45 MHz mode on gate voltages exhibits a spring hardening feature at 125 K

Measurements conducted at atmospheric and mild vacuum conditions verify the mechanical nature of the 45 MHz signal peak by confirming signal amplitude and Q dependence on the viscous damping coefficient as shown in Fig. 4.14. Moreover, the resonator has a still detectable measurement signal at the atmospheric pressure.

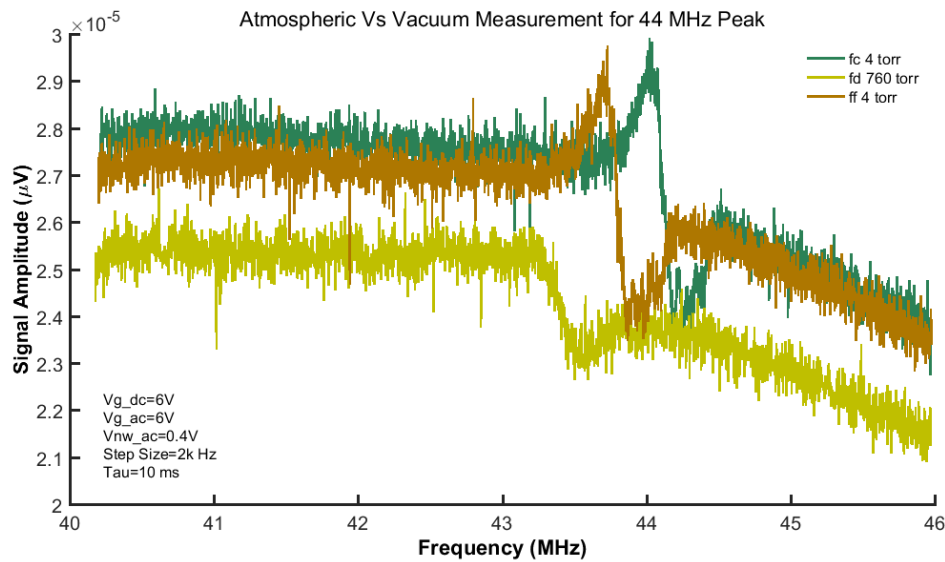


Figure 4.14: The Q and associated signal amplitude increase of the NW under vacuum conditions

The wide range sweep of Fig. 4.11 hints a second mechanical mode at approximately 101 MHz. Spectrum measurements carried out at several gate DC voltages for the second mechanical mode are shown in Fig. 4.15. Variation of the gate AC voltage also leads to similar spring softening behavior. In the literature, it is reported that when the resonance frequency of a clamped-clamped beam increases, increasing anchor losses result in lower Qs for mechanical modes [35]. This is certainly the case for the mechanical mode at 101 MHz.

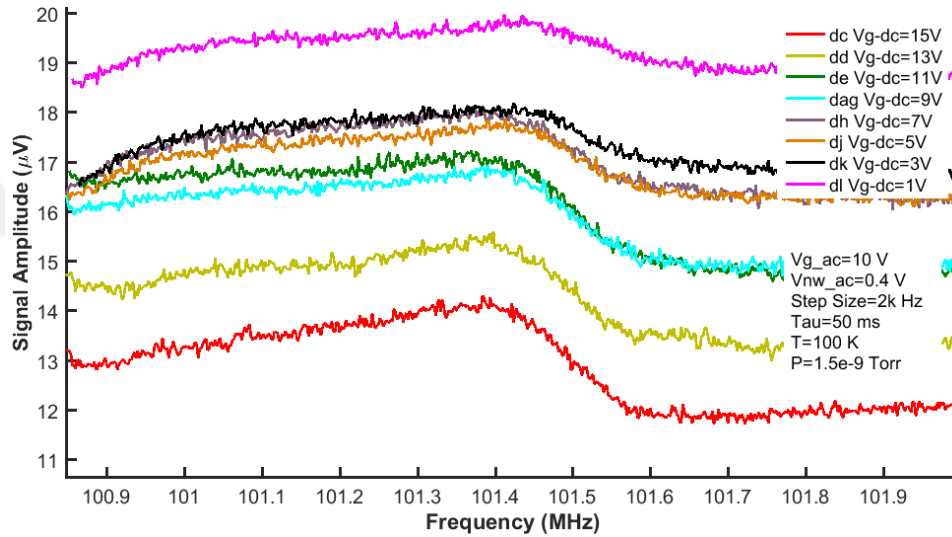


Figure 4.15: Spring softening for the second mechanical mode is realized with increasing gate voltages

Moreover, Fig. 4.15 indicates that application of 15 V DC and 10 V peak-to-peak AC voltages to a gate electrode is not enough to get a nonlinear response from the NW. However, the frequency spectrum measurements conducted at the atmospheric and mild vacuum pressures shown in Fig. 4.16 prove the mechanical nature of this 101 MHz peak conclusively.

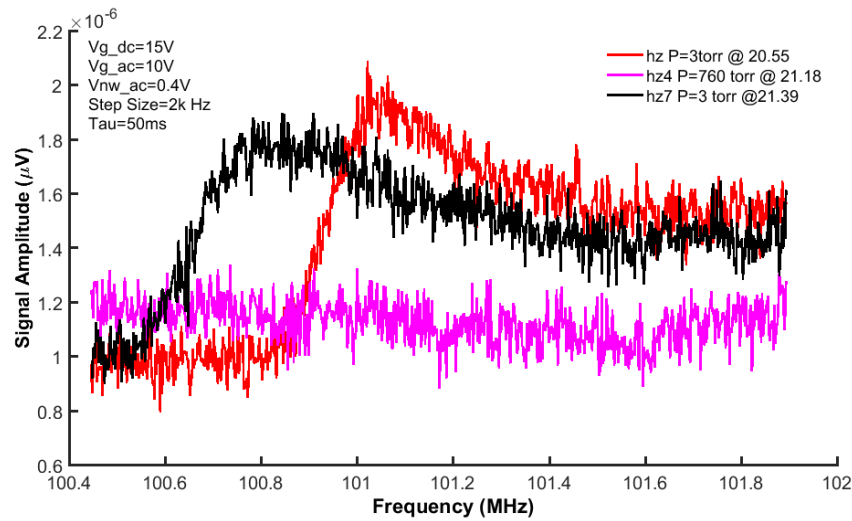


Figure 4.16: A significant increase in the Q of the NW is realized under even mild vacuum conditions

Moreover, the frequency spectrum measurements for the first and second mechanical mode at the atmospheric pressure contrast such that the second mode is not resolvable at the ambient pressure.

The Si NW on Sample 2 has the nominal geometry of the first sample except for the $\langle 110 \rangle$ crystal orientation. The wide range frequency sweep of Sample 2 shown in Fig. 4.17 indicates one clear mechanical mode at approximately 44 MHz. Spectrum characteristics of this peak are investigated to understand resonance features of this NW oriented along the $\langle 110 \rangle$ direction.

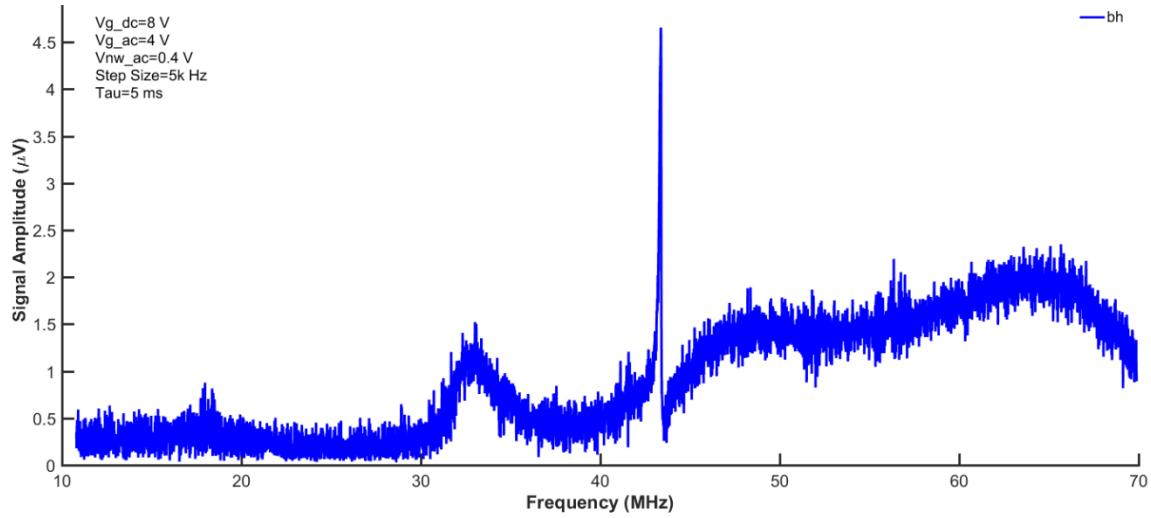


Figure 4.17: Spectrum measurements indicate one distinct mechanical peak at approximately 44 MHz.

Figure 4.18 shows the dependence of the 44 MHz mode with respect to DC voltages applied to one of the gate electrodes. Gradual resonance frequency increase with increasing gate voltages and transition to nonlinear regime are both observed. Gate AC voltage variation results in signal responses similar to the signal behavior shown in Fig. 4.18 for the gate DC voltage sweep.

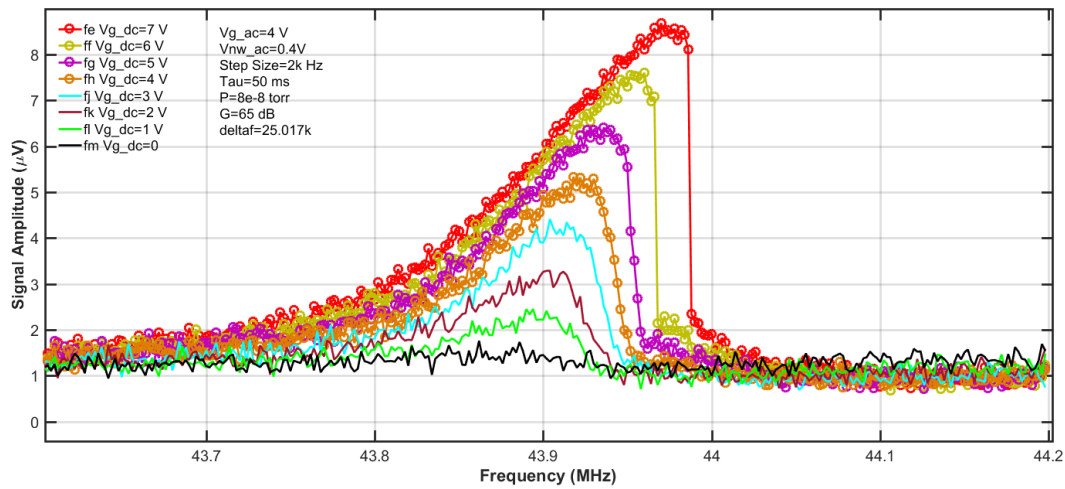


Figure 4.18: Capacitive coupling to a side-gate electrode results in spring hardening for the 44 MHz mode

Comparison of the detected signals measured through either of the frequency downmixing schemes at a common set of measurement parameters is given in Fig. 4.19. Fig. 4.19 demonstrates that both detection techniques result in resolvable signal peaks. However, the two source- 2ω transduction provides a signal with a significantly smaller amplitude. Thus, the two source- 1ω detection technique is a more efficient transduction scheme to convert nanomechanical motion into electrical signals for this sample. Existence of a signal peak at half of the resonance frequency eliminates any doubt in the mechanical nature of the 44 MHz peak.

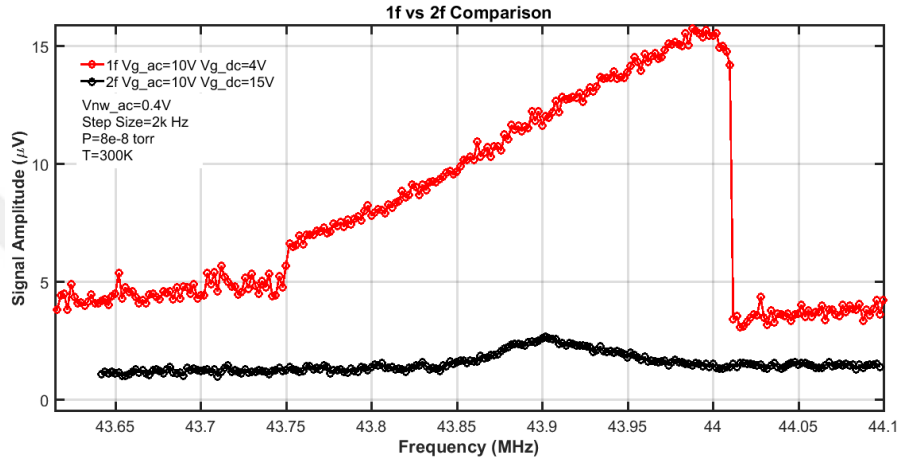


Figure 4.19: The two source- 2ω scheme results in a resolvable but low amplitude signal than 1ω scheme

Figure 4.20 shows the effect of gate AC voltages on the resonance behavior of the 44 MHz mode transduced with the two source- 2ω detection scheme. Moreover, application of the highest employed gate voltages cannot drive the NW in a nonlinear fashion with the two source- 2ω method. Besides, Fig. 4.20 depicts that slight spring softening is realized with increasing gate AC voltages using the two source- 2ω detection unlike the two source- 1ω transduced signal case.

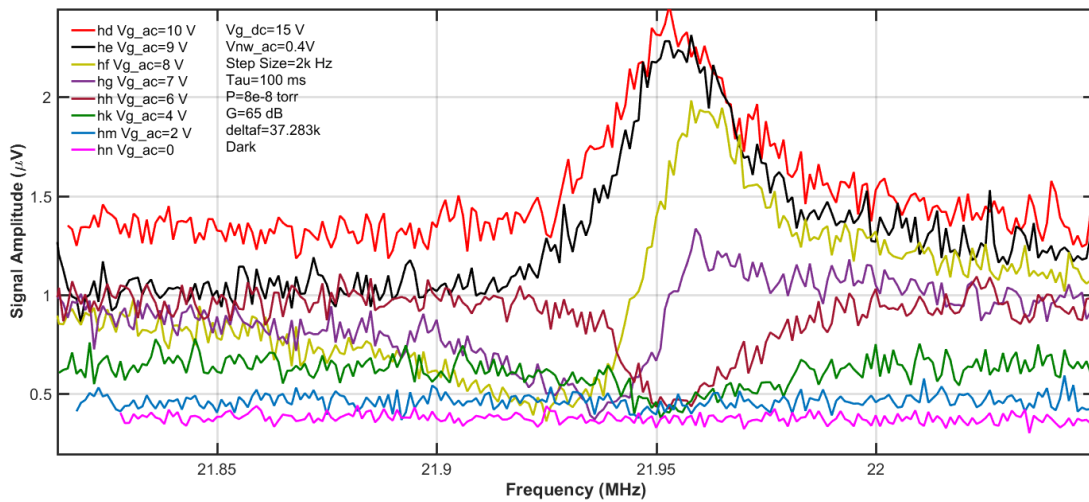


Figure 4.20: Resonance response of the 44 MHz peak displays slight spring softening with the 2ω detection.

Switching of the employed side-gate electrode results in a similar signal response for the 44 MHz mode as shown in Fig. 4.21. Fig. 4.21 implies that background signal level depends on a specific gate electrode used. Hence, selecting a correct gate electrode certainly helps to get cleaner measurements signals by minimizing background signals to obtain higher signal-to-noise ratios.

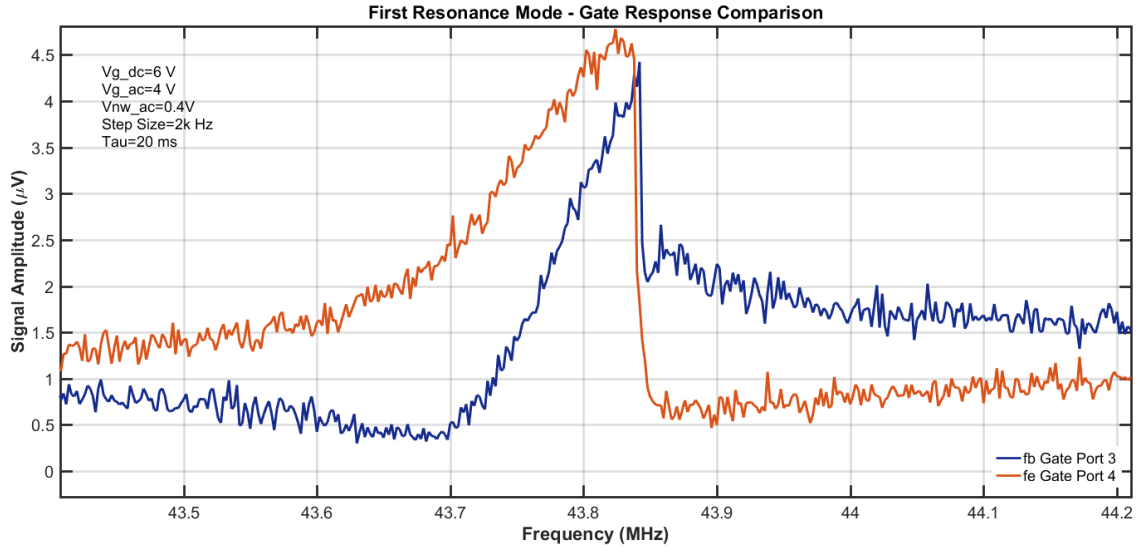


Figure 4.21: Background signal level may depend on a specific gate electrode employed

Sample 3 has a clamped-clamped Si NW having the identical nominal geometry of the first sample except for the NW length of 8 μm . The wide range frequency spectrum sweep of Fig. 4.22 presents two distinct mechanical peaks at approximately 18 MHz and 45 MHz.

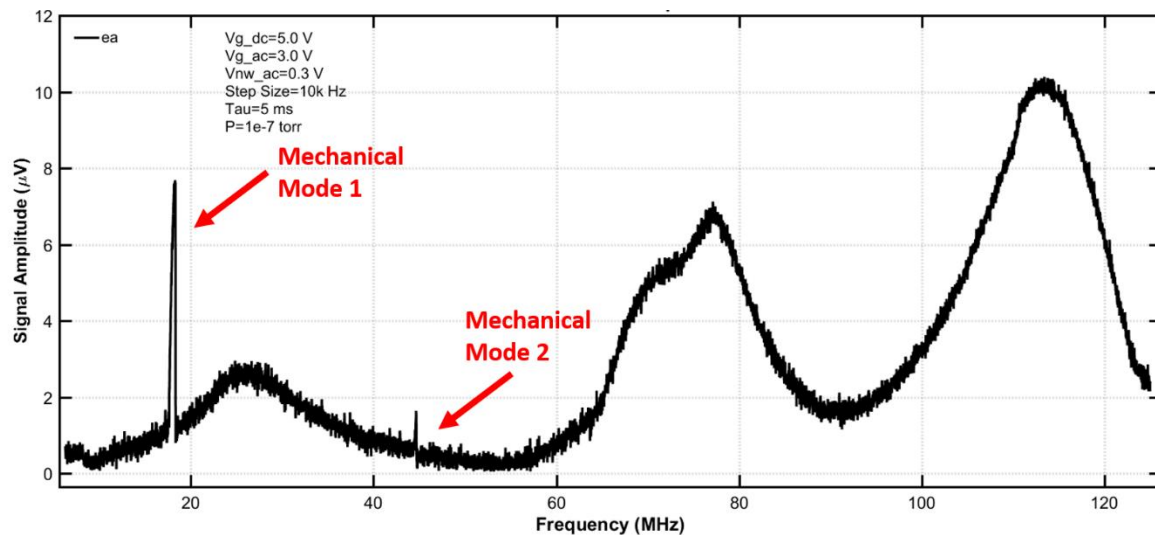


Figure 4.22: Changing the NW length from 5 μm to 8 μm results in lower frequency mechanical modes at approximately 18 MHz and 45 MHz.

A finer frequency sweep with a smaller frequency step size and a higher lock-in time constant as shown in Fig. 4.23 reflects frequency spectrum characteristics of the first mode more accurately. The resonator has a Q of approximately 1400.

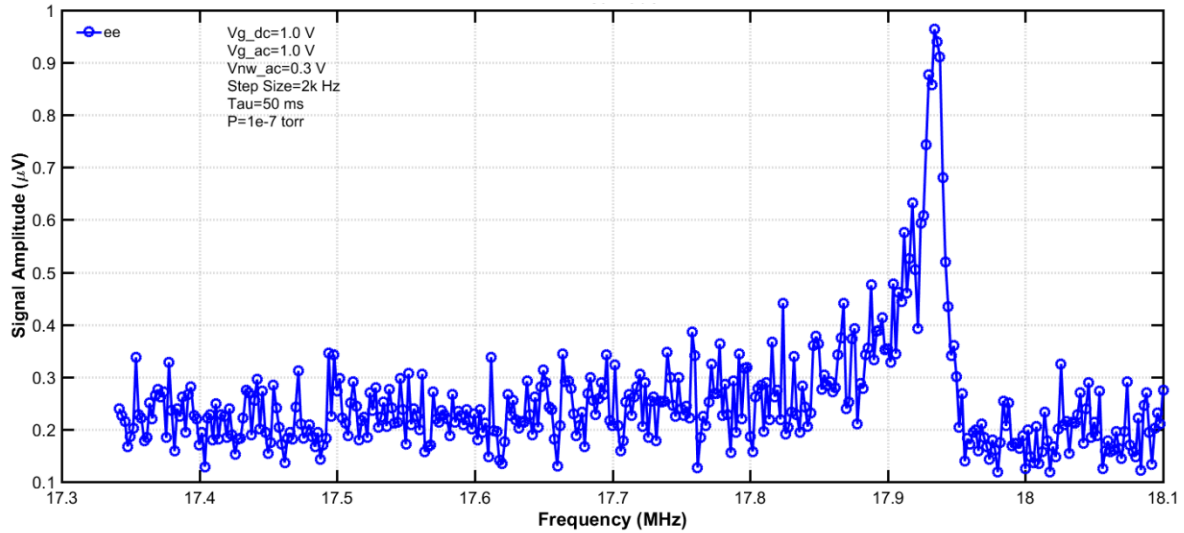


Figure 4.23: The first mechanical mode of the 8 μm long NW is found at approximately 18 MHz.

The resonance frequency of this mode with respect to AC voltages applied to a gate electrode is shown in Fig. 4.24. Spring hardening and transition from the linear to nonlinear response with increasing voltages are evident from the Fig. 4.24. Signal response dependence on gate DC voltages for this mode is similar to its dependence on gate AC voltages shown in Fig. 4.24.

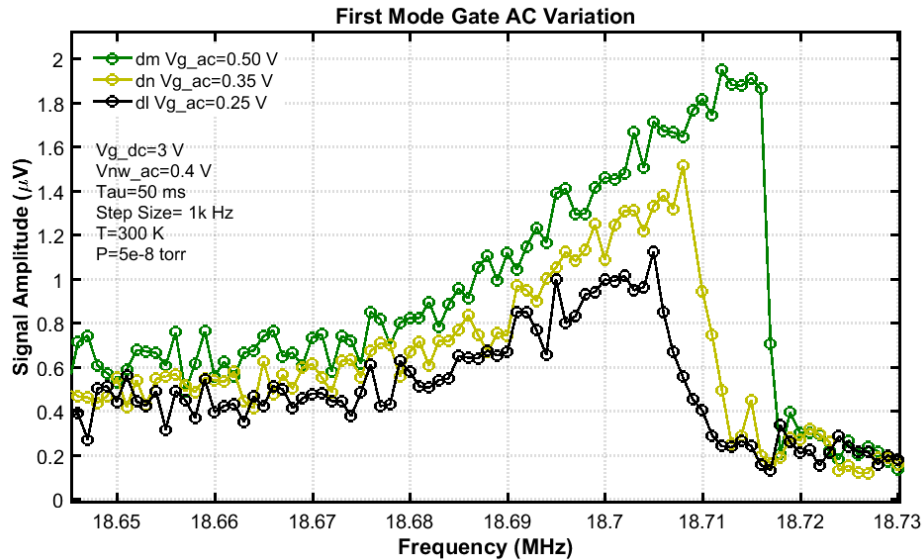


Figure 4.24: Limited dynamic range of compliant beams is underlined at the nanoscale.

The signal responses taken with the identical measurement parameters using either of the side-gates are compared in Fig. 4.25. Interestingly, a nonlinear NW response is obtained only from one

gate at the given voltages. Moreover, it can be attributed to finite overlay accuracy of the adopted fabrication flow resulting in different electrode-NW distances and asymmetric beam profile at rest.

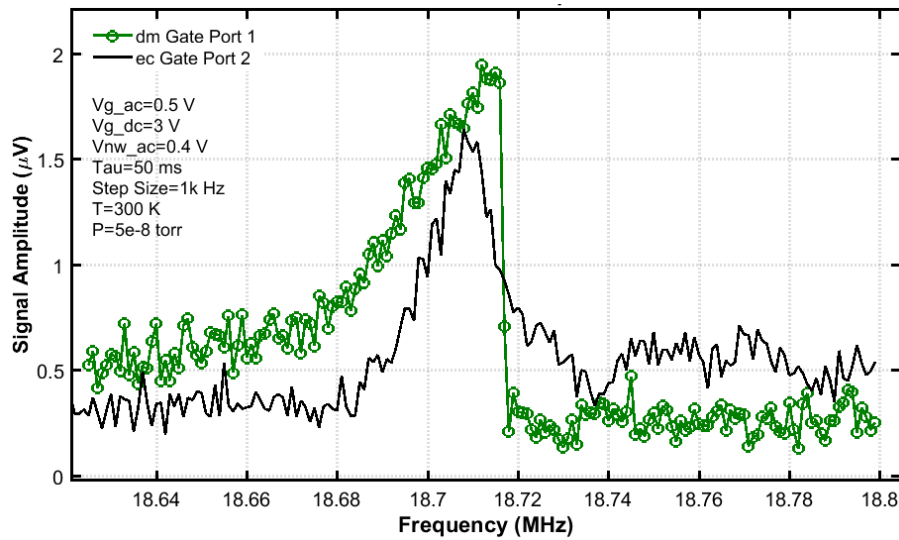


Figure 4.25: Layout and NW asymmetries may be related to different signal responses from either gate

Comparison of the signal responses detected using the 1ω and 2ω schemes yields a much smaller signal amplitude for the 2ω transduction case similar to previous results as shown in Fig. 4.26.

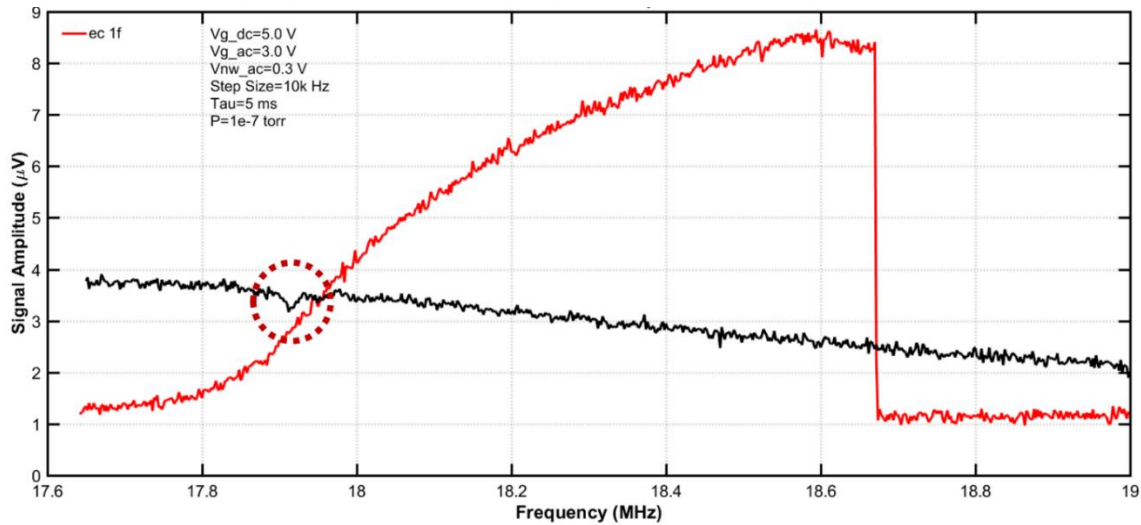


Figure 4.26: The 1ω scheme delivers a sharp signal peak having a higher amplitude and a lower background level than the 2ω transduction.

Frequency spectrum characteristics are also investigated for the second mechanical mode at 45 MHz for this sample shown in the frequency spectrum sweep of Fig. 4.22. The resonance frequency of the second mechanical mode with respect to AC voltages applied to a gate electrode is shown in Fig. 4.27. Transition to nonlinear response regime cannot be obtained even by applying the highest voltages to any gate electrode for this mode. However, there is slight spring hardening

with increasing AC voltages. Resonance signal relation with gate DC voltages is similar to that obtained for gate AC voltages shown in Fig. 4.27.

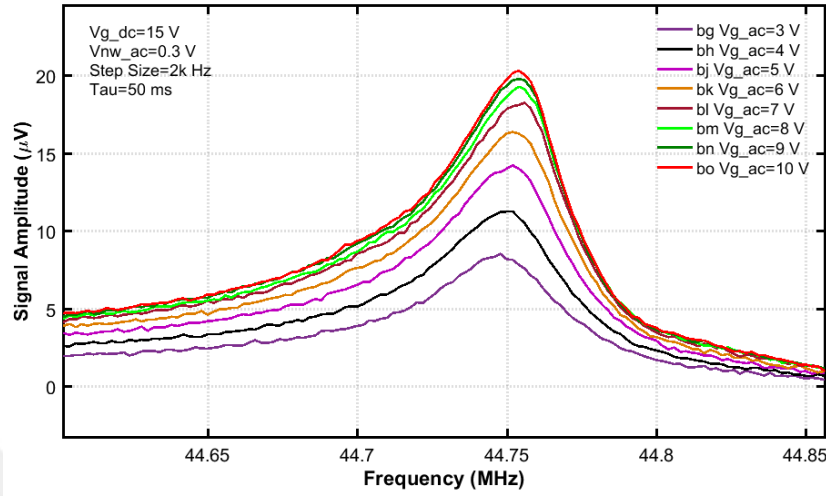


Figure 4.27: A slight frequency shift is realized as a result of increasing gate voltages for the 45 MHz mode

Sweeping the frequency spectrum in the ascending and descending frequency directions reveals clearly the hysteresis feature of a spectrum peak driven in a nonlinear fashion. Thus, hysteresis characteristic of a signal peak in addition to other spectrum characteristics such as signal amplitude and resonance frequency dependence on gate voltages, and transition to nonlinear response form a strong case to corroborate the mechanical origin of any detected signal peak. Existence of the hysteresis feature for the nonlinear drive of the 44 MHz signal peak of Sample 2 is shown in Fig. 4.28. All of the measured mechanical modes having a linear-to-nonlinear transition exhibit similar kind of hysteresis behavior.

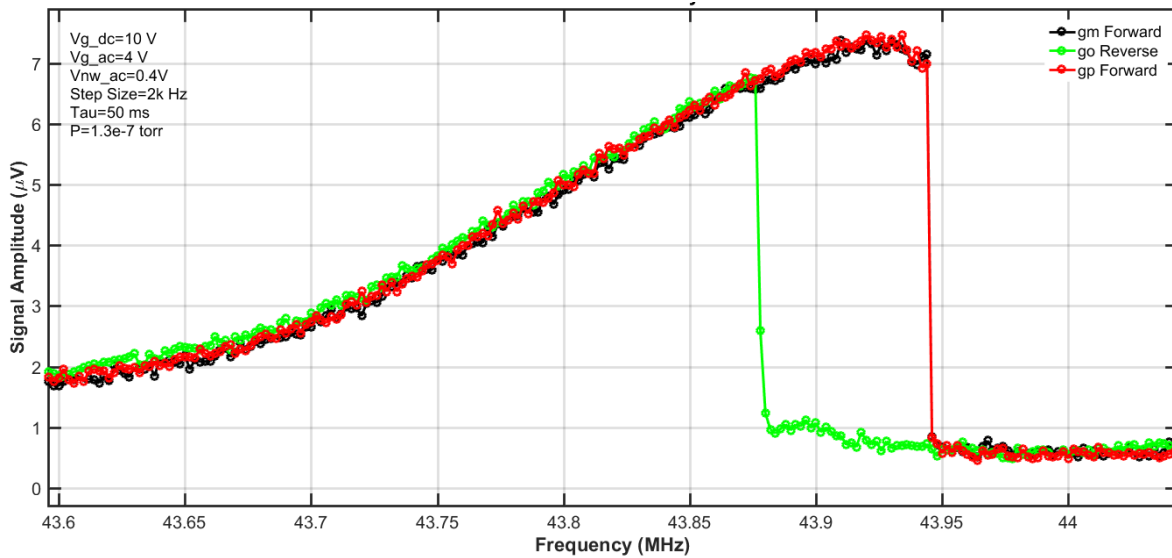


Figure 4.28: Driving of a mechanical mode in a nonlinear fashion results in a hysteresis behavior.

Allan deviation is measured to determine the resonance frequency stability of a mechanical mode for the single NW samples. Measurements are implemented at both ambient or cryogenic temperatures in vacuum. Frequency stability measurements result in Allan deviation of approximately 3-10 ppm which corresponds to a mass detection limit of approximately 1.0 ag.

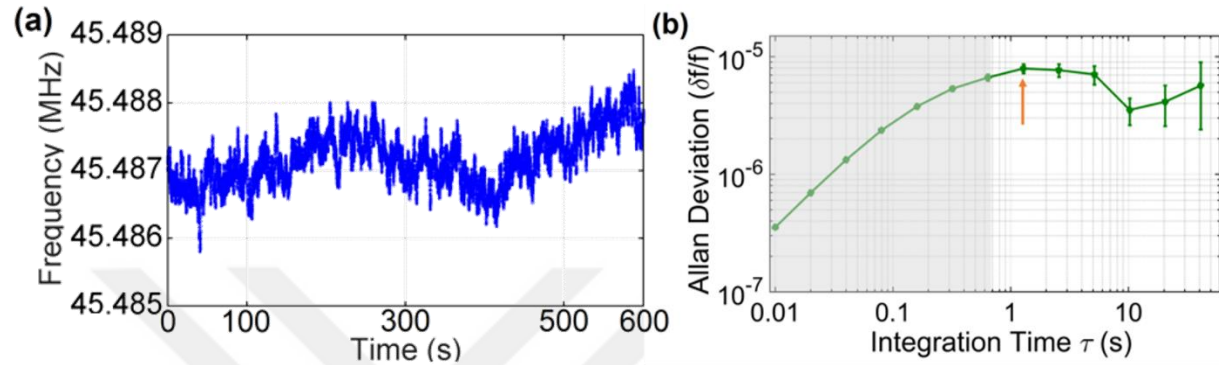


Figure 4.29: Phase lock loop (PLL) measurements are performed to track the resonance frequency of a mechanical mode in (a) and to determine the frequency stability by calculating Allan deviation in (b).

4.4. Frequency Spectrum Measurements of Coupled Vertical NW Arrays

In this section, the frequency spectrum measurement results of the fabricated four coupled vertical NW arrays are given sample by sample. The width (w), height (h) and length (L) of the fabricated NW and CM of each sample is summarized in Table 4.2. The width and thickness of the fabricated NWs and CMs are essentially same for all of the fabricated devices and the coupled NW arrays are fabricated along the [110] crystallographic orientation. While the NW length of the first sample is 3 μm , all of the remaining samples have the common NW length of 2 μm . Moreover, Sample 2,3 and 4 have an identical NW array structure except for the CM length of 1000 nm, 500 nm and 100 nm respectively.

Table 4. 2: Nominal dimensions of the fabricated NW and CM of each sample employed in frequency spectrum measurements

	Dimensions	Sample 1	Sample 2	Sample 3	Sample 4
NW	w (nm)	60	60	60	60
	h (nm)	65	65	65	65
	L (μm)	3	2	2	2
CM	w (nm)	500	500	500	500
	h (μm)	1	1	1	1
	L (nm)	150	1000	500	100

Thus, Sample 1 has a vertical NW array featuring NWs with the width, height and length of 60 nm x 65 nm x 3 μm and a pair of CMs with the width, height and length of 500 nm x 1 μm x 150 nm as shown in Table 4.2. The wide range frequency spectrum sweep of Fig. 4.30 presents two

mechanical modes approximately at 46 MHz and 58 MHz for the first vertical NW stack sample. The first mode clearly has an amplitude much higher than the second mechanical mode.

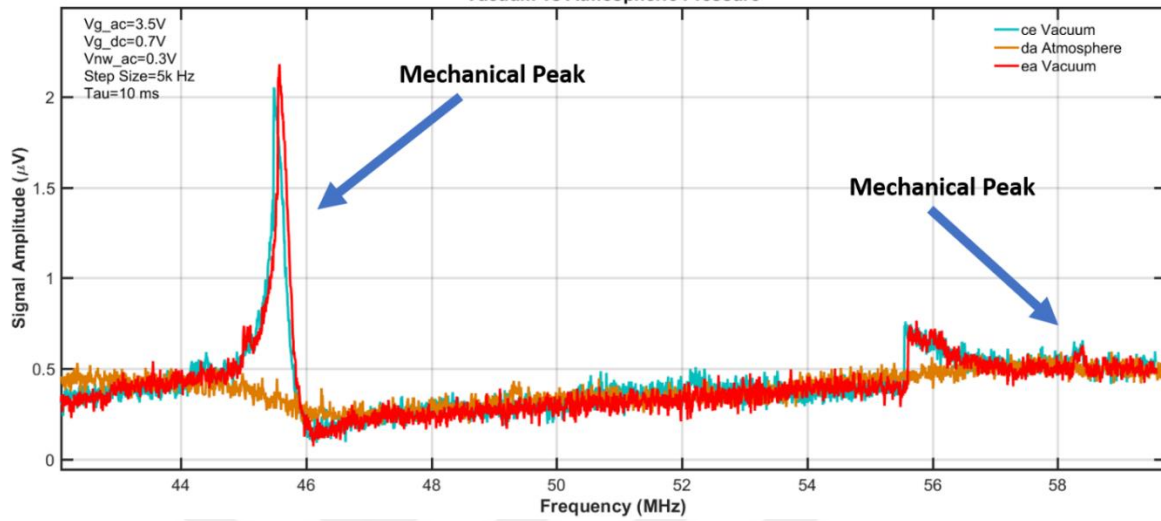


Figure 4.30: The wide range frequency spectrum sweep results in two mechanical modes approximately at 46 MHz and 58 MHz for the first coupled NW stack sample

In line with the previous single NW frequency spectrum measurements, examination of frequency spectrum characteristics of each mechanical mode is started by investigating resonance frequency and signal amplitude relation with gate voltages. Figure 4.31 and 4.32 show the effect of gate AC and DC voltages on the detected signal respectively. The Q is approximately 400 for this mode. It is interesting note that an increase in a gate AC voltage results in spring softening leading to a decrease for the resonance frequency of the NW array. On the other hand, resonance frequency dependence on a gate DC voltage is unusual and spring hardening is realized as a DC voltage applied to a gate electrode increases.

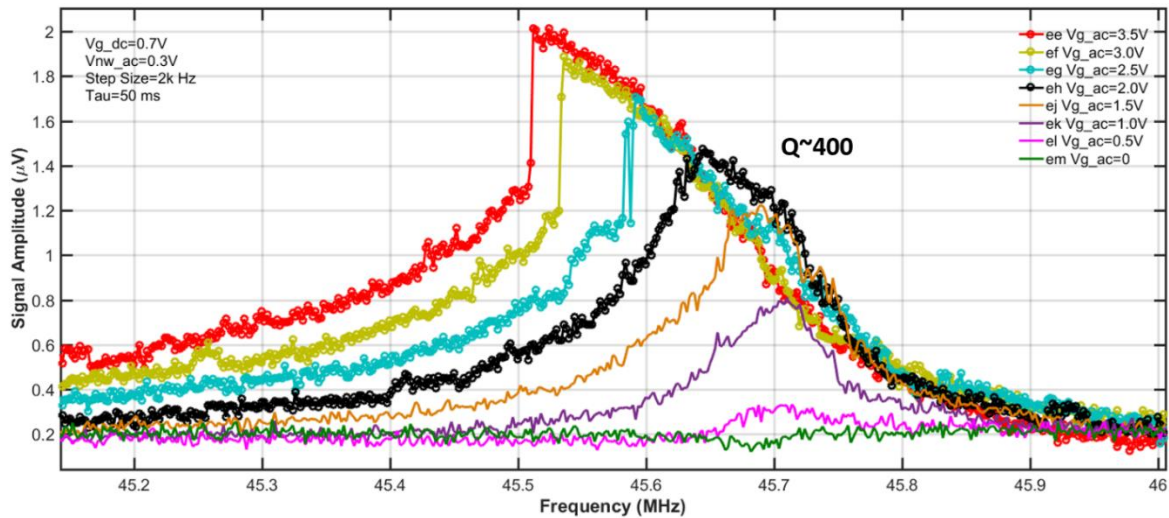


Figure 4.31: Resonance response of the first mode with respect to gate AC voltages

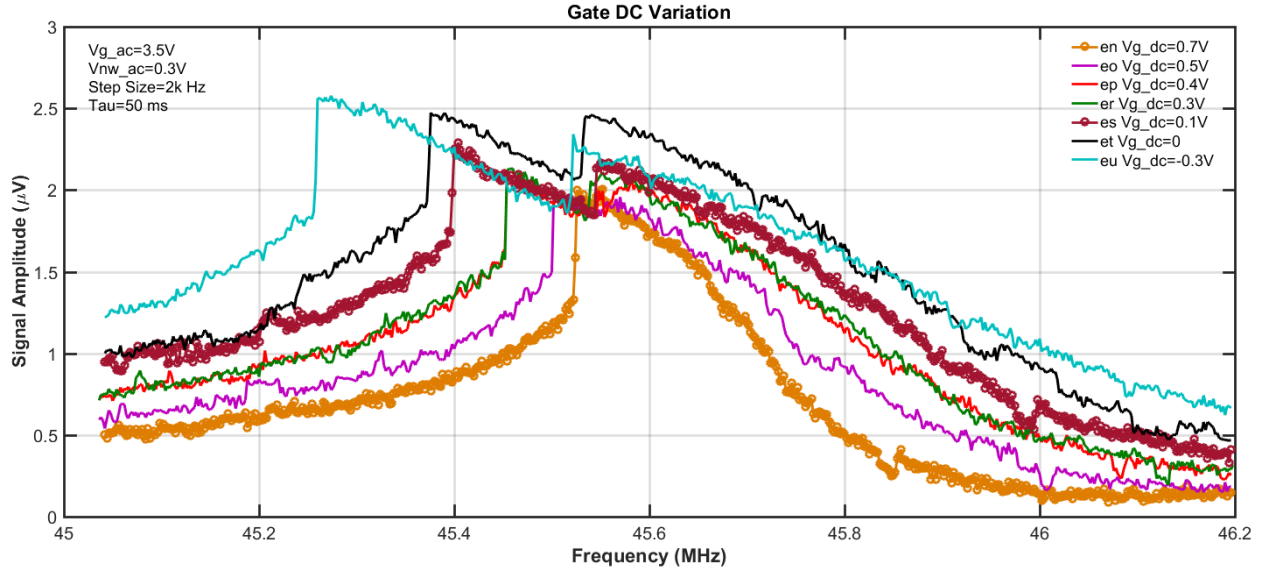


Figure 4.32: Effect of gate DC voltages on the rather unusual resonance signal of the 46 MHz mode has some spring hardening disposition.

On the other hand, frequency spectrum characteristics of the second mechanical mode with respect to gate AC and DC voltages are given in Fig. 4.33 and 4.34. In this case, a gradual increase in a gate AC voltage leads to spring hardening. Therefore, comparison of the resonance response relation of both mechanical modes with gate AC voltages demonstrated in Figs. 4.31 and 4.33 reveals that the effect of a gate AC voltage on each of the mechanical modes is clearly different.

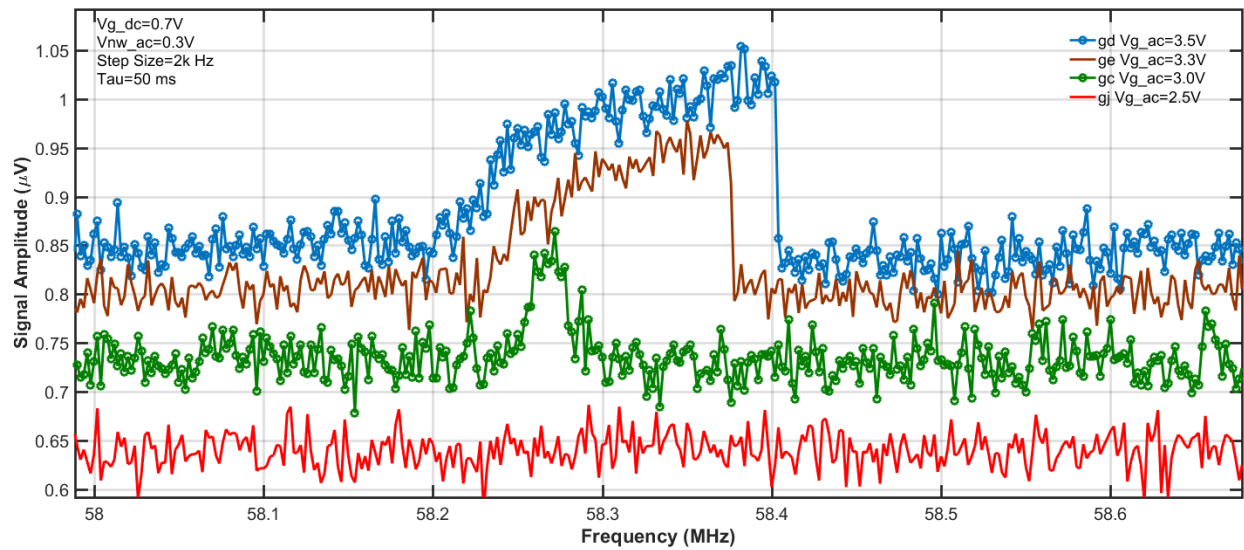


Figure 4.33: Frequency spectrum response of the second mechanical mode features both spring hardening and nonlinear transition characteristics

Interestingly, both the signal amplitude and the resonance frequency of the second mechanical mode seem independent from the considered gate DC voltages as shown in Fig. 4.34.

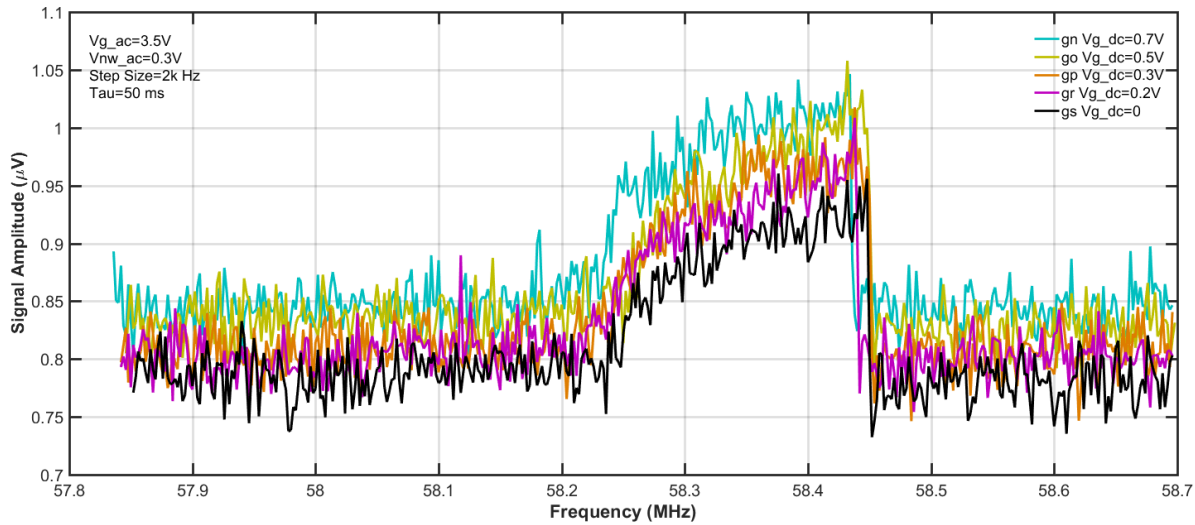


Figure 4.34: Detected signal at 58 MHz is found independent from the considered gate DC voltages

The frequency spectrum measurement using the two source/ 2ω setup of Fig. 4.1.b provides a spectrum peak at half of the resonance frequency of the first mode as shown in Fig. 4.35. Hence, it confirms the mechanical nature of the 45 MHz peak. Figure 4.35 indicates that the two source/ 2ω detection technique clearly results in a smaller signal-to-background ratio signal than the two source/ 1ω detection in accordance with previous measurements using single NW samples. No detectable signal is obtained for the second mechanical mode using the two source/ 2ω detection.

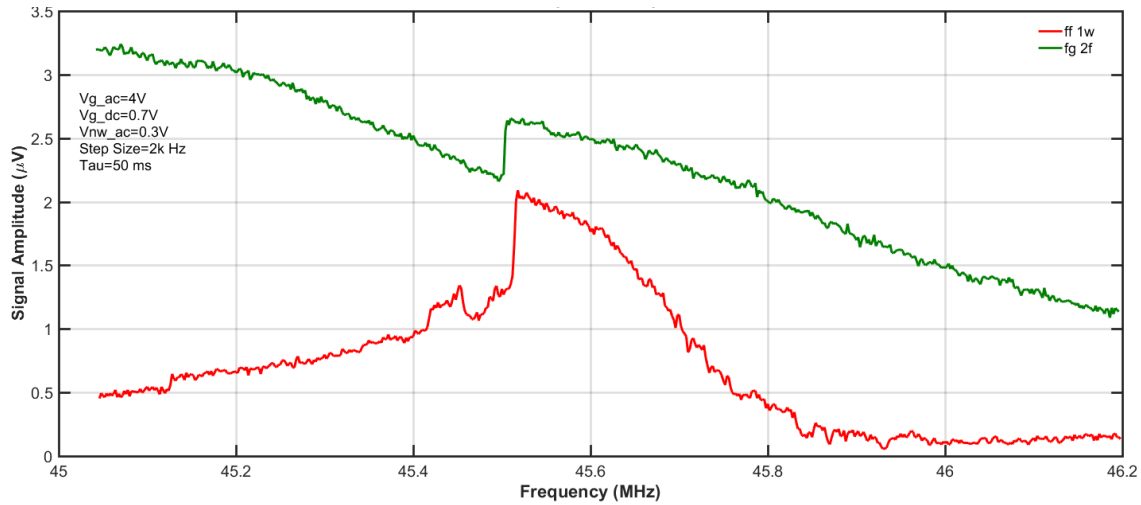


Figure 4.35: Comparison of the two detection schemes favors the two source/ 1ω technique for this coupled NW array sample in parallel with previous single NW measurements

Nonlinear drive of a mechanical resonator should result in some hysteresis characteristic for a mechanical mode. Any doubt related to the mechanical origin of the second mechanical mode at 58 MHz arising from the independence of its spectrum signal from gate DC voltages shown in Fig. 4.34 is suppressed by providing the hysteresis behavior of this mode in Fig. 4.36. Similar hysteresis characteristic is also found for the first mode at 45 MHz.

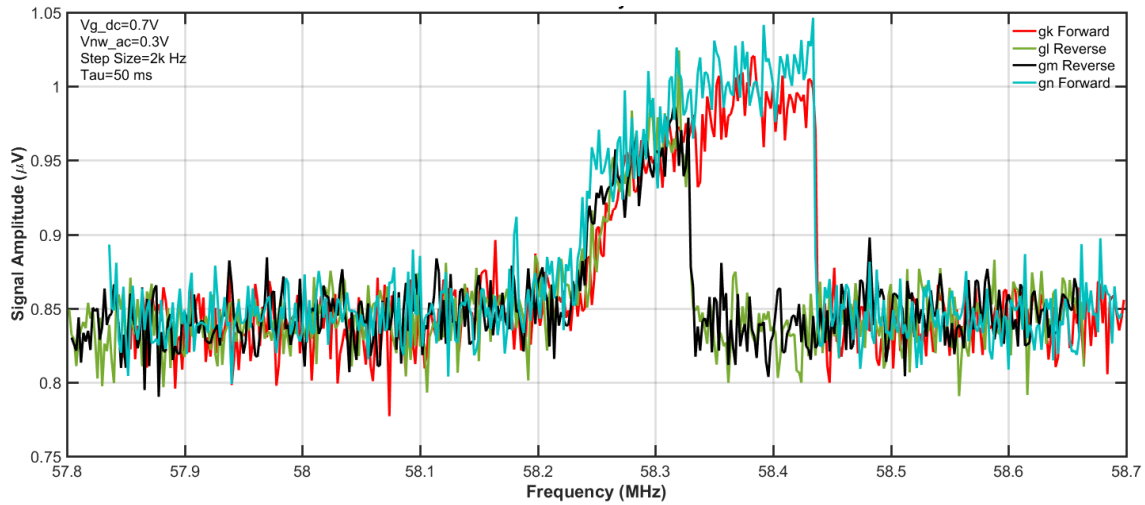


Figure 4.36: Hysteresis property of the first NW array sample is shown for the second mechanical mode

Although the frequency spectrum characterization measurements verify the mechanical origin of the spectrum peaks of 45 MHz and 58 MHz, association of these mechanical peaks to specific in-plane or out-of-plane flexural modes for the fabricated vertical NW array is not straightforward. Since there is inevitable spatial variation along each NW and between NWs in a vertical stack. Hence, this process requires significant experimental NW spatial measurements and FEM simulations.

The coupled vertical NW array on Sample 2 has the NW and CM lengths of 2 μm and 1000 nm as shown in Table 4.2. Both coupled vertical NW samples are otherwise identical. The frequency spectrum behavior of the first mechanical mode at approximately 70 MHz with respect to gate DC voltages is shown in Fig. 4.37.

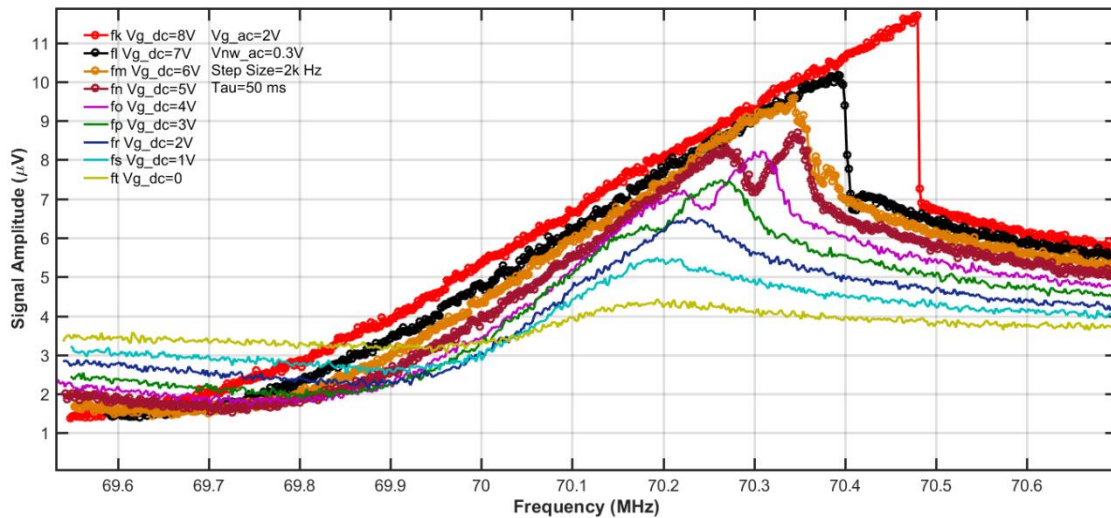


Figure 4.37: A signal response reminiscent of a bandpass filter is possible by close packing of some mechanical NW array modes

Fig. 4.37 demonstrates somewhat different spectrum characteristics. The frequency spectrum in Fig. 4.37 indicates that there are two mechanical peaks in close proximity which is reminiscent of a bandpass filter. Hence, it seems that the 70 MHz peak may actually be composed of two separate modes adjacent to each other. Transformation from linear to nonlinear oscillation and spring hardening with increasing gate voltages are evident from Fig. 4.37. Moreover, a gate AC voltage variation results in resonance signal characteristics similar to Fig. 4.37.

There is another mechanical mode at approximately 77 MHz for this vertical stack sample. Similar plots examining the effect of gate AC and DC voltages on the resonance frequency and the signal amplitude of this mode are also obtained. Figure 4.38 presents the signal dependence on gate AC voltages. These measurements indicate results parallel to the ones obtained for the 70 MHz mode in terms of spring hardening and linear signal transition to nonlinear regime.

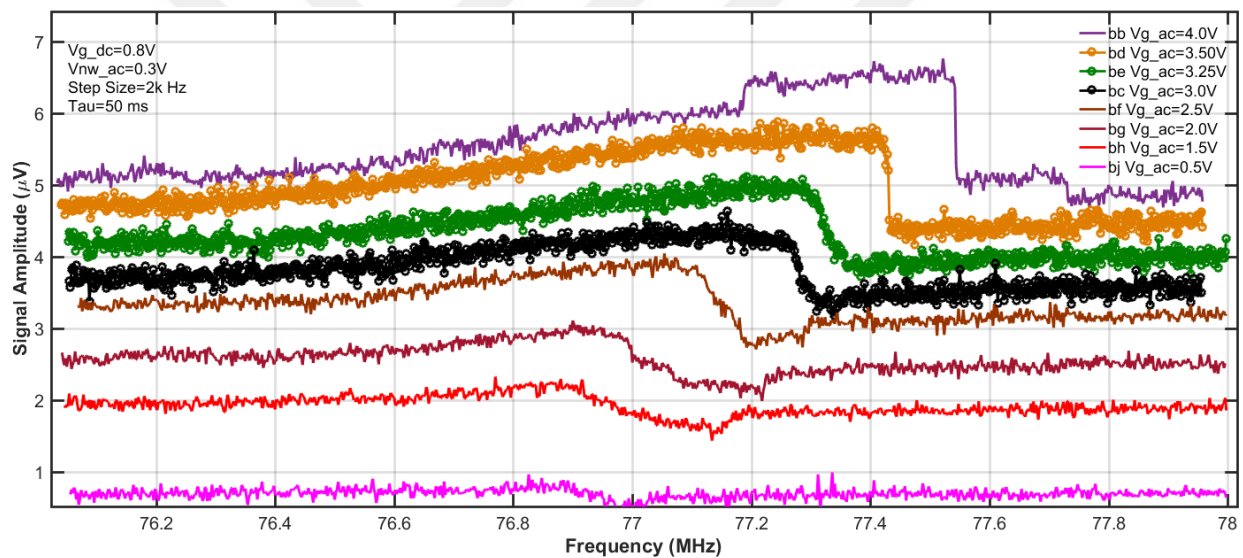


Figure 4.38: Resonance frequency relation with gate voltages for the 77 MHz mode shows spring hardening and transition to nonlinear oscillation features

Comparison of the frequency spectrum signals detected through the two-source/ 1ω and two-source/ 2ω measurement schemes for both mechanical modes is parallel to previous results in that the two-source/ 1ω technique is more efficient to resolve small mechanical vibrations as shown in Fig. 4.39 for the 77 MHz mode.

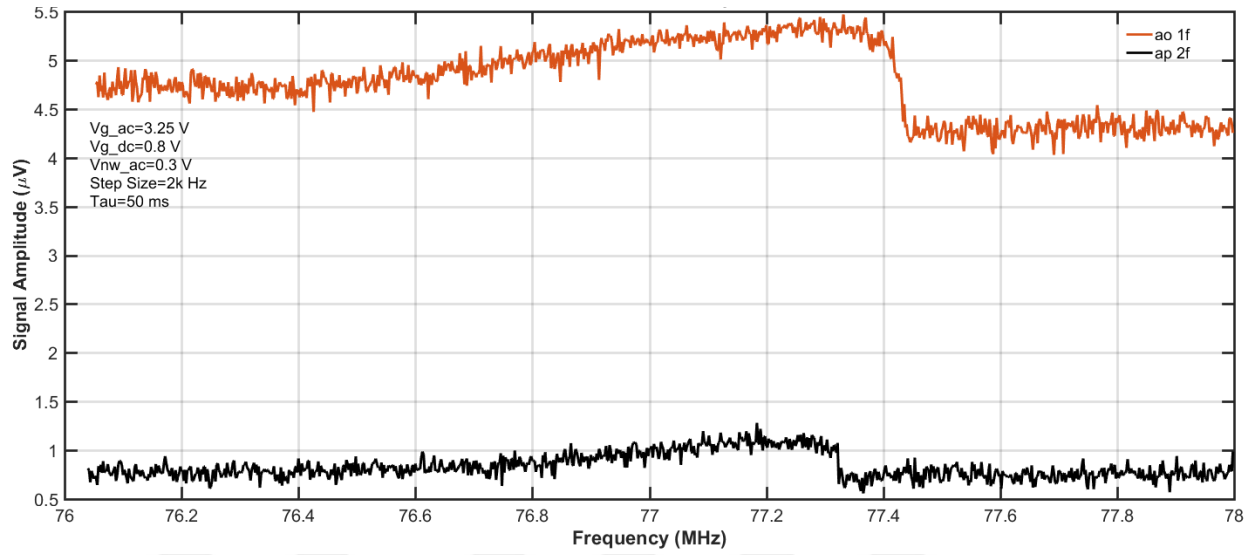


Figure 4.39: Both detection setups provide resolvable spectrum peaks for the 77 MHz mode.

Resonance signal variation with respect to gate AC voltages and transition to nonlinear drive of a resonator array are also demonstrated using the two-source/ 2ω detection as shown in Fig. 4.40 for the 77 MHz mode. Spring hardening is realized in parallel with the two-source/ 1ω scheme results for the 70 MHz and 77 MHz modes as the applied gate voltage increases.

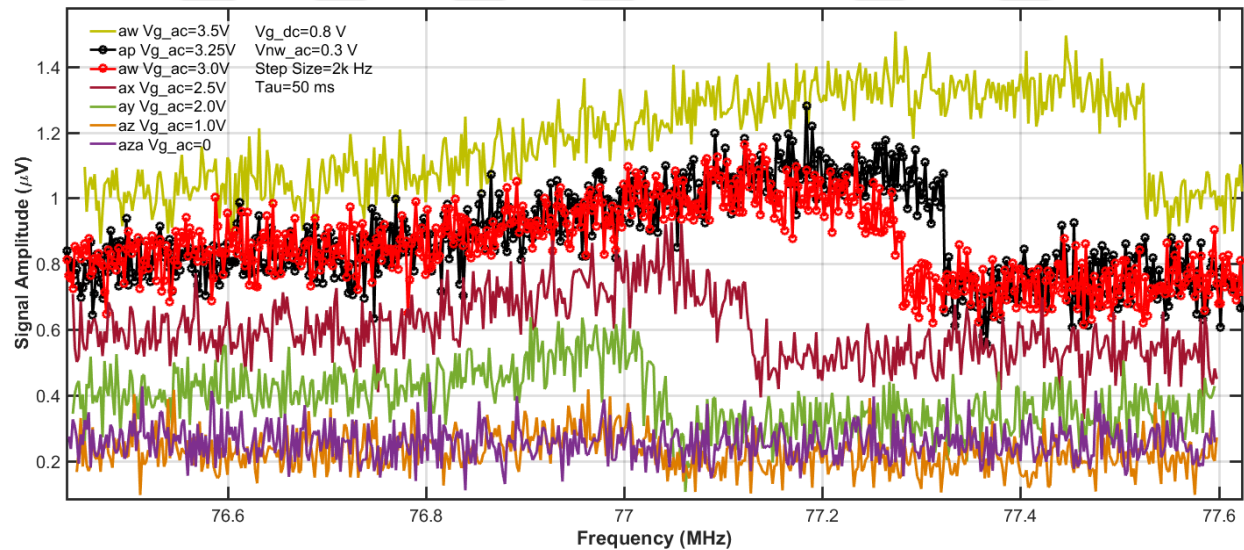


Figure 4.40: Gate voltages are able to drive the NW array in a nonlinear fashion using the two-source/ 2ω method for the 77 MHz mode.

More mechanical modes are found at higher frequencies as shown in Fig. 4.41 for the same coupled vertical NW array sample. Fig. 4.41 demonstrates the frequency spectrum measurements with respect to varying gate DC voltages. Frequency spectrum measurements are performed to confirm and then characterize the mechanical nature of each peak.

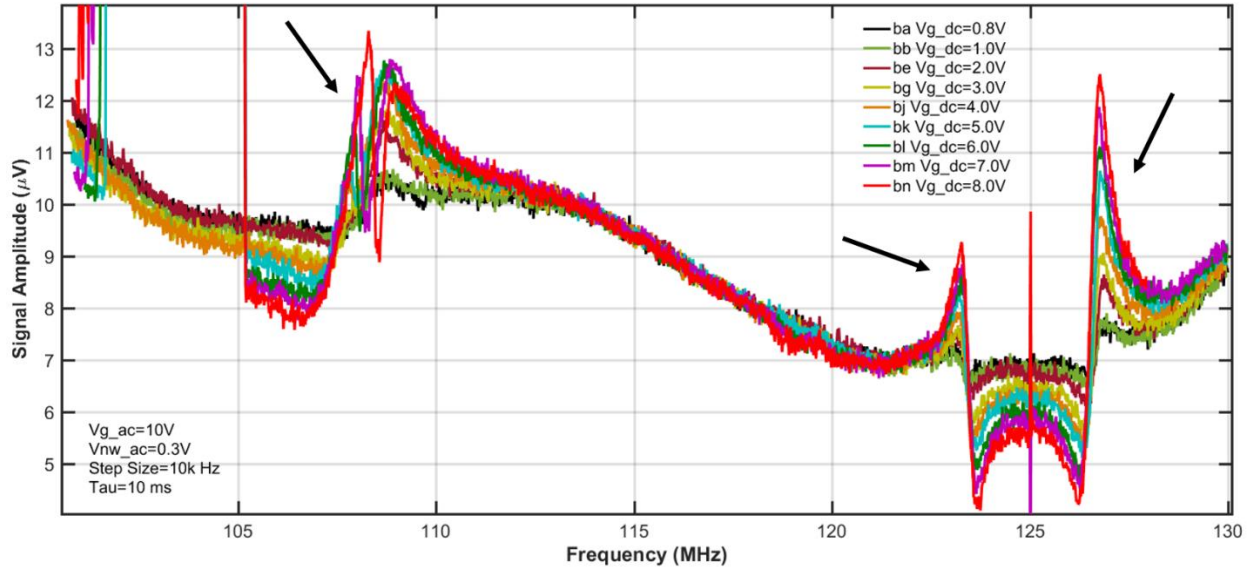


Figure 4.41: More mechanical modes at higher frequencies are detected for the same coupled NW array.

Characterization of the frequency spectrum with respect to gate DC voltages yields spring hardening for both approximately 108 MHz and 122 MHz modes as shown in Figs. 4.42 and 4.43 respectively. However, transition to any nonlinear resonator motion is not materialized for both modes in the range of employed voltages.

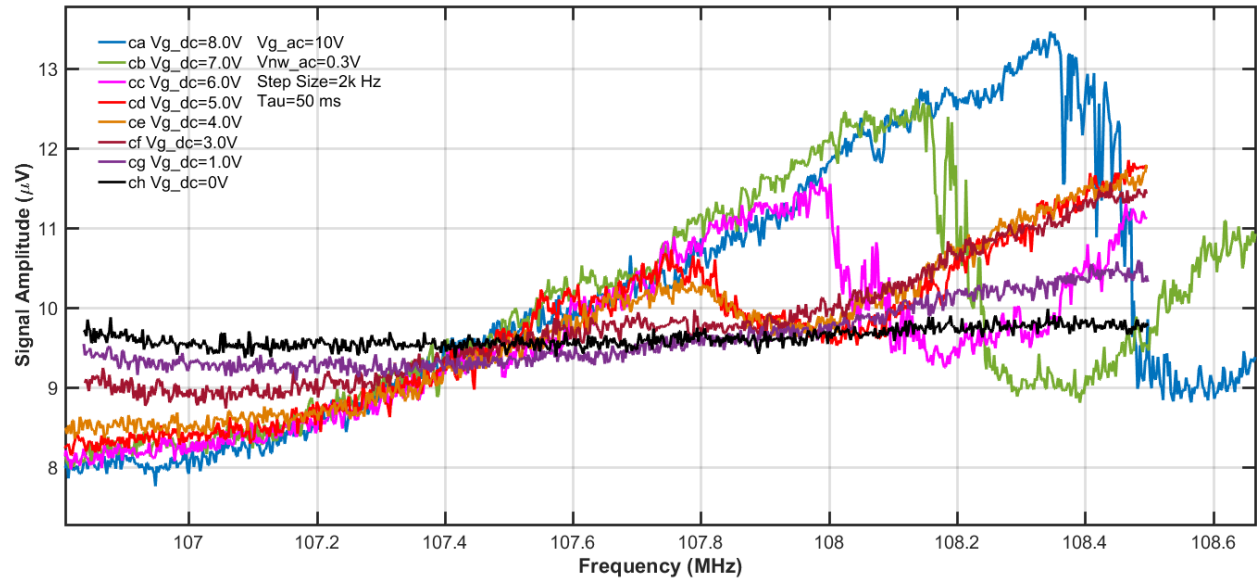


Figure 4.42: Effect of the gate DC voltage on the signal response of the 108 MHz mode

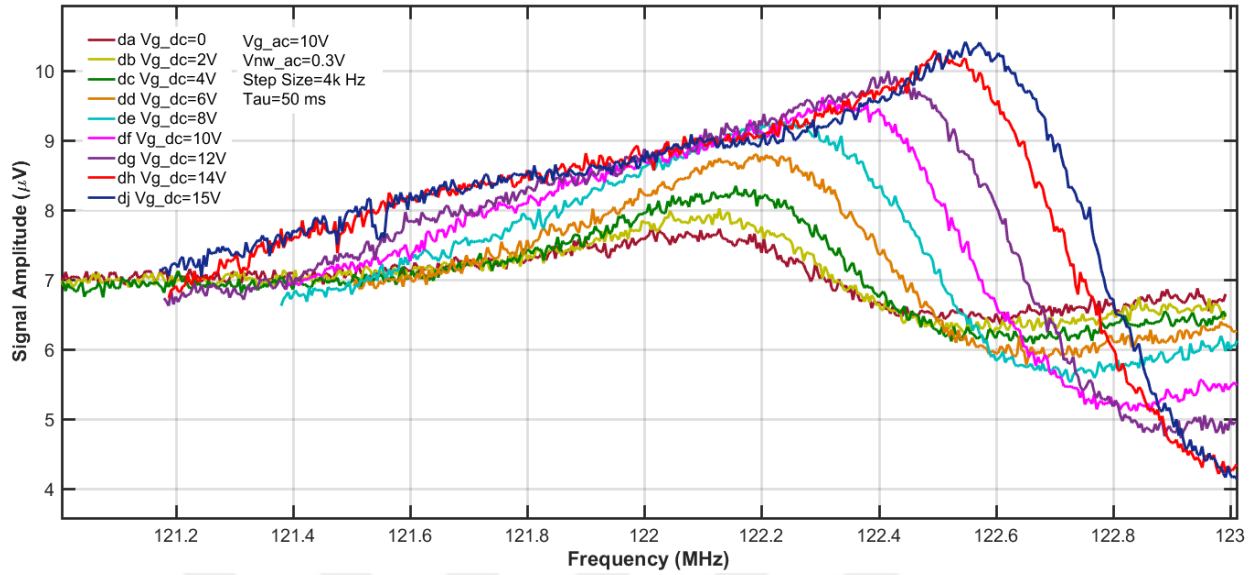


Figure 4.43: Interaction between gate DC voltages and the frequency spectrum peak at 122 MHz shows a linear relation for the considered voltage range.

Up to this point, the frequency spectrum measurements with respect to gate voltages for all of the detected mechanical modes of Sample 2 imply spring hardening using both downmixing schemes. On the other hand, spring softening is realized with an increase in a gate DC voltage for the 128 MHz mode as shown in Fig. 4.44. Thus, this coupled NW array sample features close and numerous mechanical modes having spring hardening and spring softening characteristics simultaneously for different mechanical modes on the same sample.

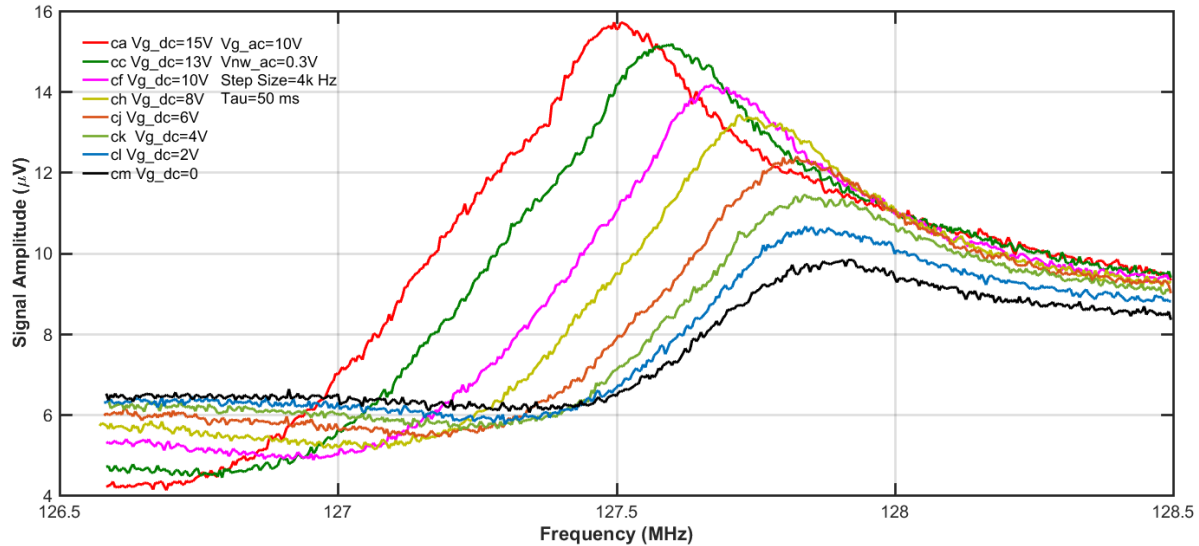


Figure 4.44: Spring softening is realized for the 128 MHz mode unlike all previous detected mechanical modes of Sample 2.

Interestingly, the frequency spectrum measurements with respect to gate AC voltages shown in Fig. 4.45 and 4.46 for the 122 MHz and 128 MHz mechanical modes demonstrate some drifting

behavior for the resonance frequency such that spring softening follows initial spring hardening in the 122 MHz mode case or vice versa in the 128 MHz mode case.

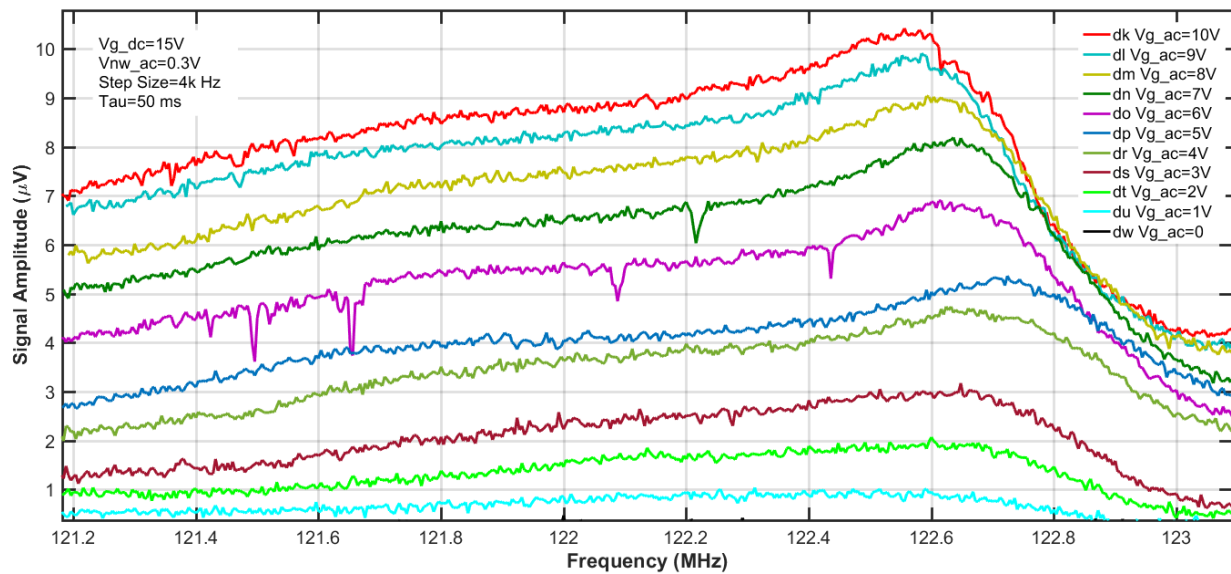


Figure 4.45: Drifting behavior of the resonance frequency of the 122 MHz mode with gate AC voltages

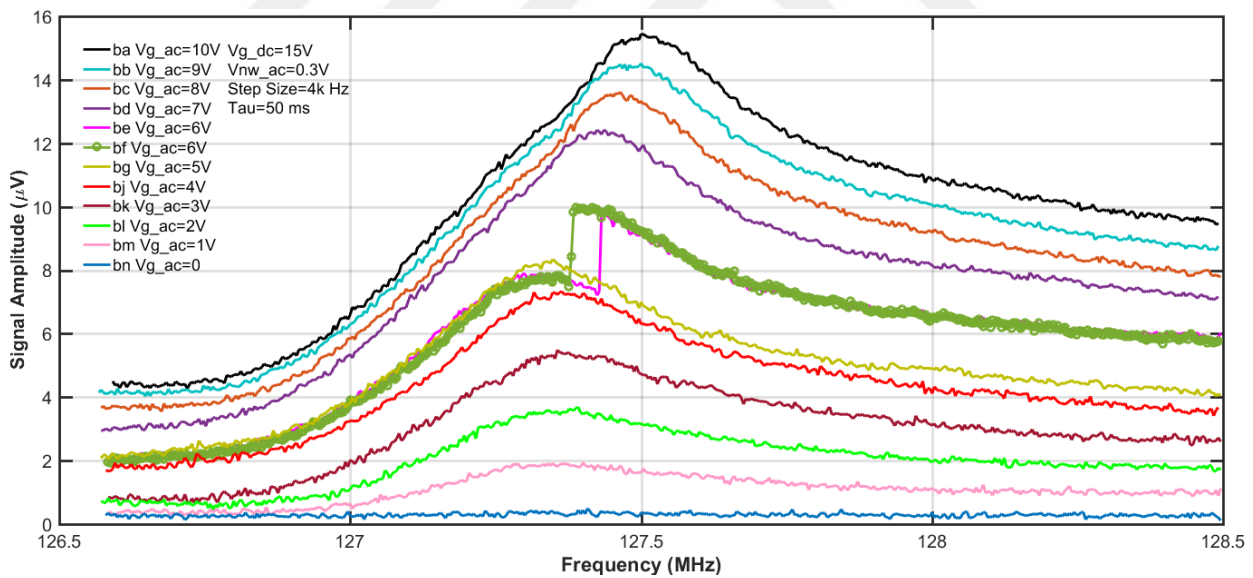


Figure 4.46: The mechanical mode at 128 MHz also exhibits the drifting resonance frequency characteristic with gate AC voltages

Comparison of spectrum measurements performed in deep vacuum and at the atmospheric pressure such as the one shown for the 122 MHz mode in Fig. 4.47 confirms the mechanical origin of these modes. As a result, five mechanical modes are detected within the frequency window from 70 MHz to 128 MHz having various frequency spectrum characteristics. Close packing of numerous mechanical modes might be beneficial in some MEMS and NEMS applications. These applications

include sensor implementations that track shifts in resonance frequencies of multiple mechanical modes or examine any interaction between multiple resonance modes etc.

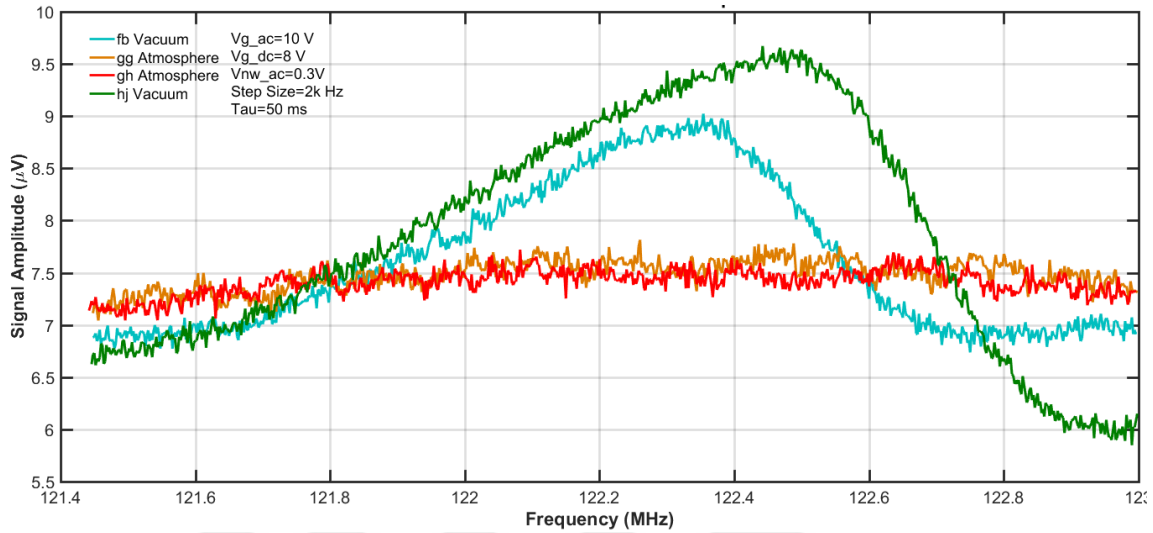


Figure 4.47: Comparison of the vacuum and atmospheric measurements for the 122 MHz mode

Sample 3 has the identical coupled NW array geometry with Sample 2 except for the new CM length of 500 nm as shown in Table 4.2. This coupled NW stack sample features a mechanical mode at 74 MHz. Resonance signal relation with varying gate AC voltages is plotted using either gate in Fig. 4.48 and 4.49 for this mode. Although both figures imply spring hardening with increasing gate voltages, different spectrum responses for each employed gate might be associated with finite overlay accuracy of the utilized fabrication flow and asymmetric static deflection profile of NWs in the array at rest.

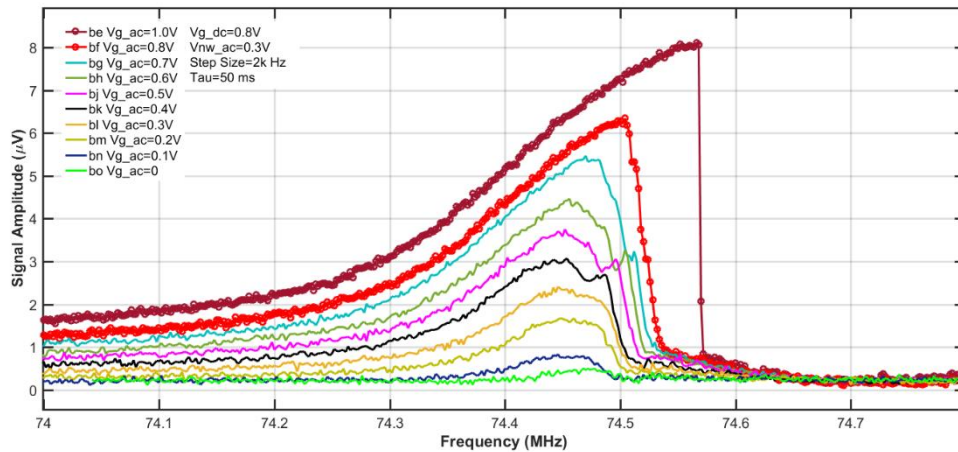


Figure 4.48: These frequency spectrum sweeps indicate a small second signal peak adjacent to the primary mode.

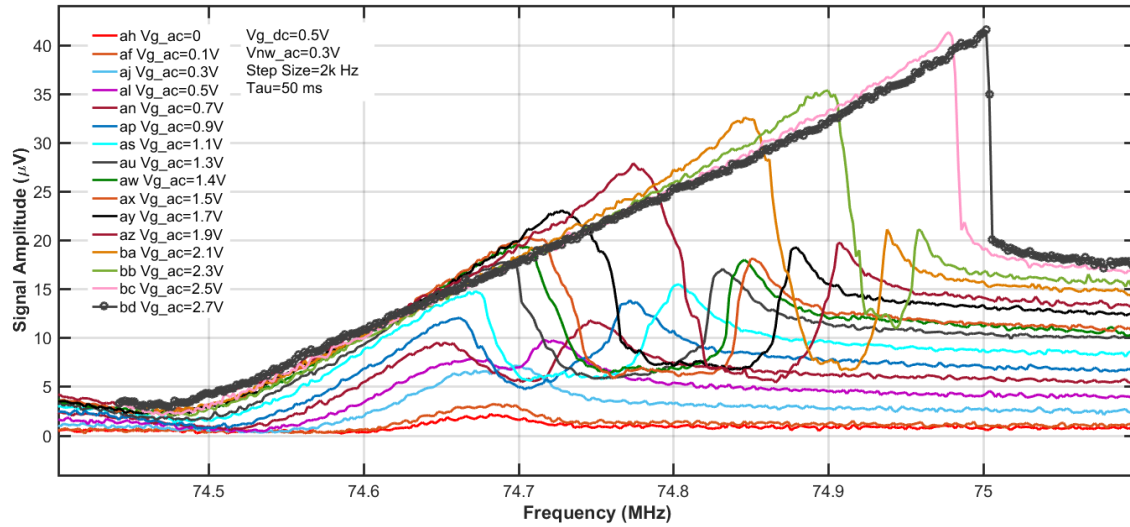


Figure 4.49: Employment of the other electrode promotes the small peak significantly such that frequency spectrum responses reminiscent of a typical bandpass filter behavior are realized.

Fig. 4.49 shows again there are two spectrum peaks in close proximity that form some kind of bandpass filter behavior. The two signal peaks seem to merge at higher voltages at the nonlinear regime transition point. Some low voltage measurement data of Fig. 4.49 are replotted in Fig. 4.50 to examine them more closely. Fig. 4.50 demonstrates clearly the twin frequency peaks around 74.7 MHz and their dependence on some gate AC voltages. Bandpass ripple variation with the applied gate voltages is in accordance with the literature.

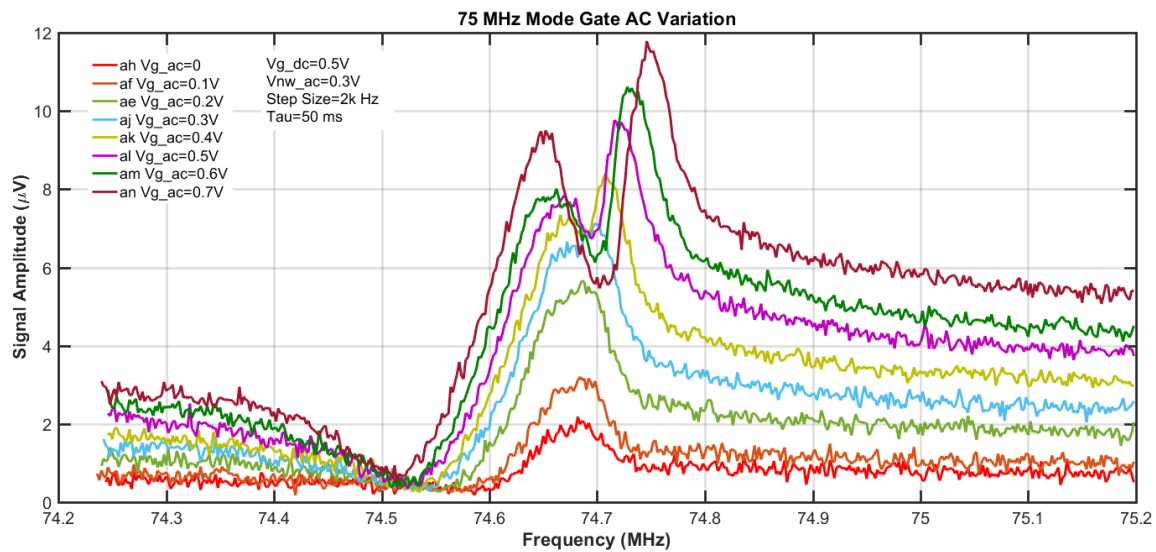


Figure 4.50: Evolution of the twin spectrum peaks with respect gate voltages is illustrated in detail.

Moreover, Figure 4.51 shows that a resolvable peak which is weaker than the signal obtained with the two-source/ 1ω detection technique is also detected using the two-source/ 2ω method for the 75 MHz mode.

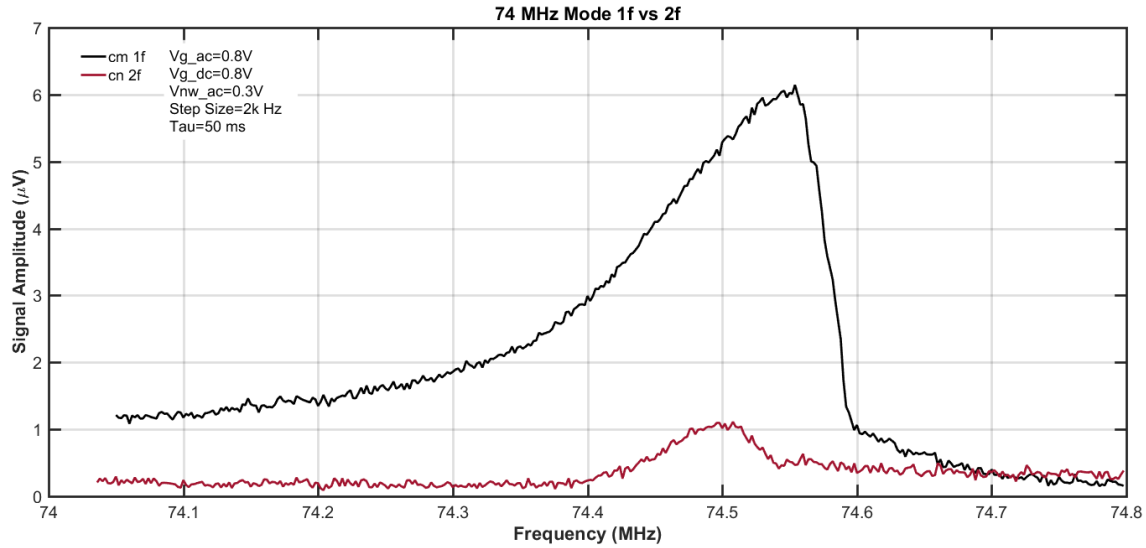


Figure 4.51: Both detection techniques result in resolvable spectrum peaks for the 74 MHz mode

Only difference of Sample 4 from Sample 2 and 3 is that the CM length of 100 nm is selected in this case for Sample 4 as shown in Table 4.2. The coupled vertical NW array on Sample 4 has a mechanical mode at 99 MHz. Mode dependence on gate AC voltages which displays spring hardening behavior is shown in Fig. 4.52. However, this rather unusual signal response seems to consist of the superposition of two adjacent spectrum peaks as well.

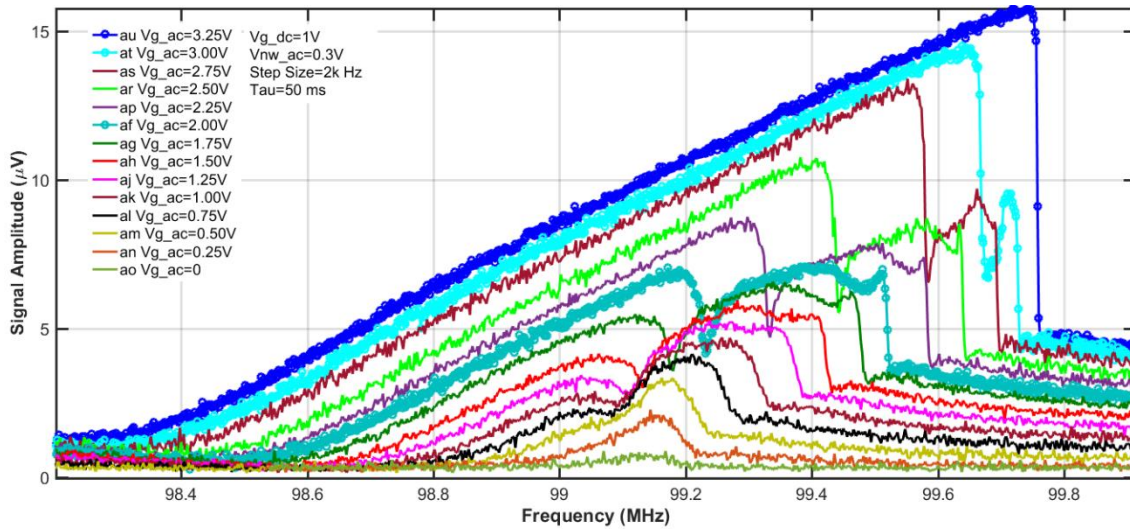


Figure 4.52: The spectrum response with respect to gate AC voltages for the 99 MHz mode of Sample 4

On the other hand, comparison of the employed detection schemes shown in Fig. 4.53 for this mode presents a distinct spectrum response for each technique. However, similar signal amplitudes are realized for both detection methods unlike all the previous cases.

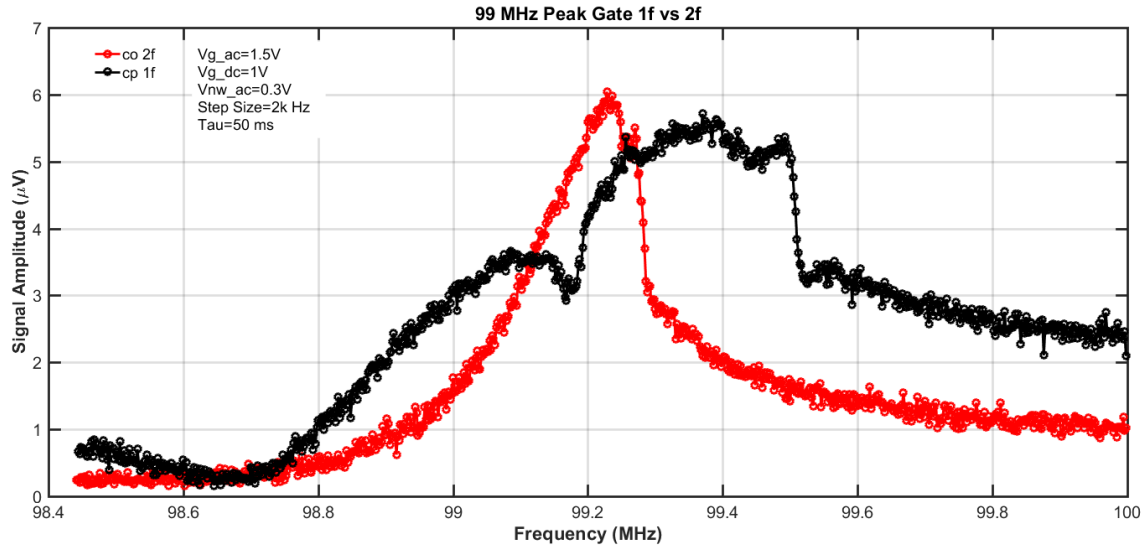


Figure 4.53: The amplitudes of the spectrum signals detected using both techniques match for the first time.

Further frequency spectrum measurements using the two-source/ 2ω scheme shown in Fig. 4.54 indicate clearly the linear to nonlinear transition and spring hardening characteristics in parallel with the two-source/ 1ω downmixed signals shown in Fig. 4.52. Some two-source/ 2ω measurements also seem to include a small second peak next to the main peak.

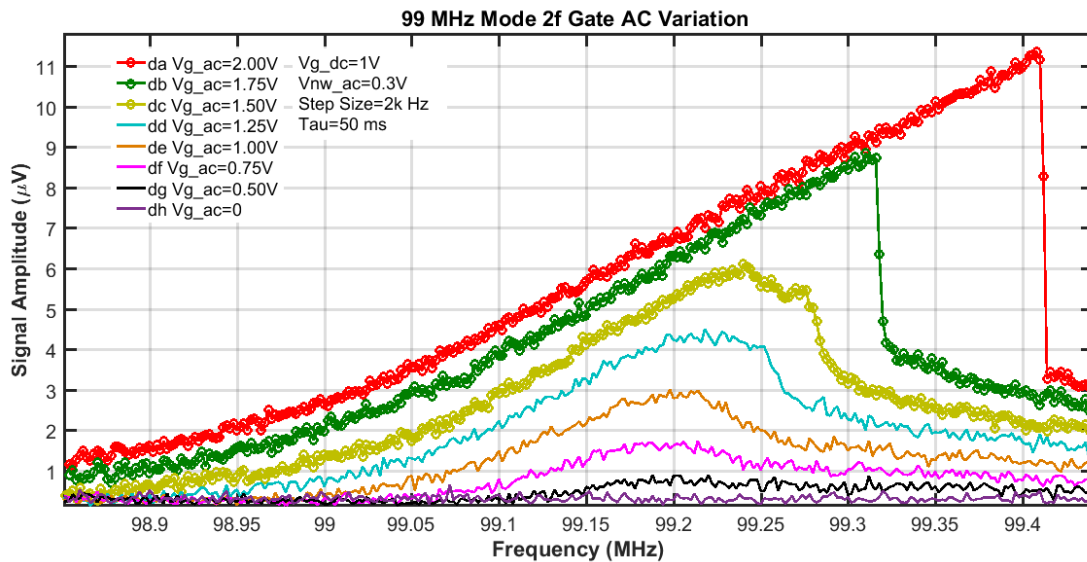


Figure 4.54: Effect of the gate AC voltage on the two-source/ 2ω detected signal response at 99 MHz.

The frequency spectrum sweeps of Fig. 4.55 at higher frequencies reveal two more mechanical modes around 129 MHz. The higher amplitude mechanical mode has the signal transition from linear to nonlinear oscillation mode and spring hardening features with increasing gate voltages. Fig. 4.55 indicates that there is also a barely noticeable mechanical mode adjacent to the obvious primary signal peak.

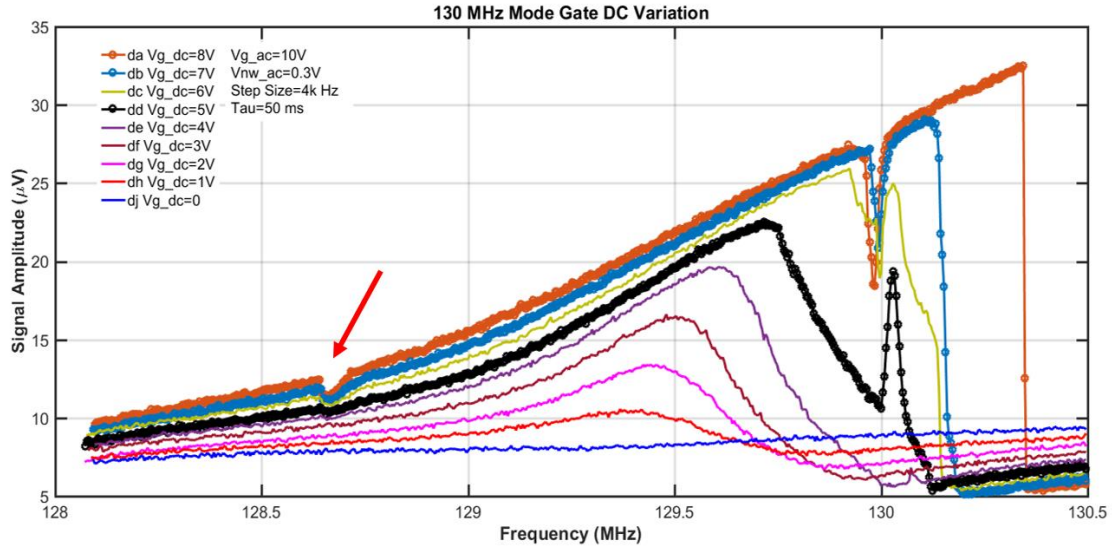


Figure 4.55: Higher frequency sweeps reveal two more mechanical modes around 129 MHz.

Sweeping the frequency spectrum in the ascending and descending frequency direction is used to reveal the hysteresis feature of mechanical modes driven in a nonlinear fashion. Existence of hysteresis for the nonlinearly driven 129 MHz mode of Sample 4 is shown in Fig. 4.56 to prove the mechanical nature of this mode. All of the measured mechanical modes having some degree of linear-to-nonlinear transition exhibit similar kind of hysteresis behavior.

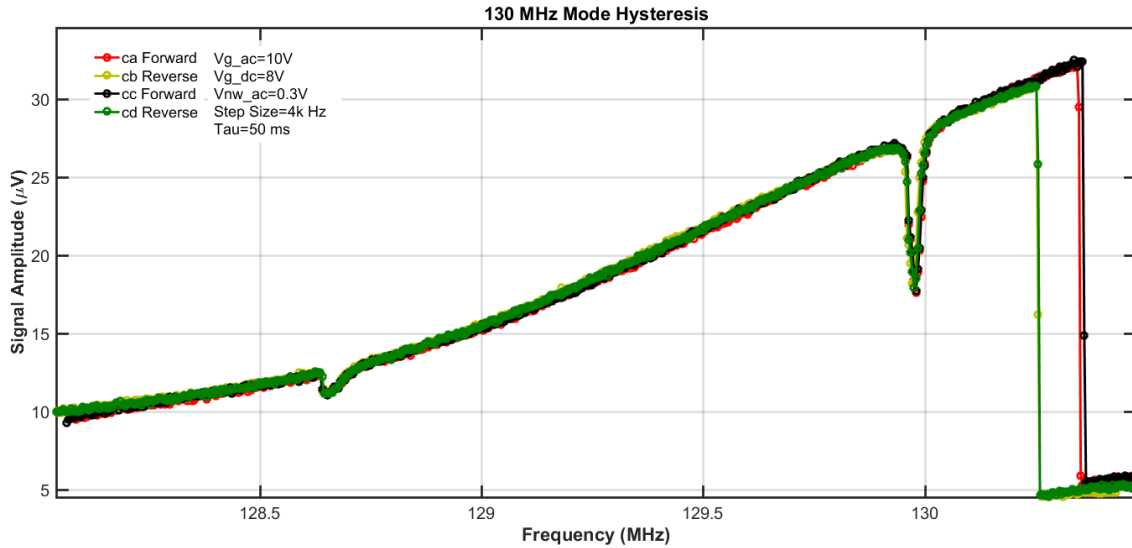


Figure 4.56: This representative hysteresis behavior is shared between the nonlinearly driven mechanical modes detected for all the coupled NW array samples.

Chapter 5: Frequency Spectrum Measurement Analysis

5.1. Analysis of Single NW Spectrum Measurement

Frequency spectrum measurement results of the three fixed-fixed single NW samples are summarized in Table 5.1. Measured NWs with the properties shown in Table 4.1 let the effect of NW orientation and length on resulting downmixed output signals be examined.

Table 5.1: Detected mechanical modes with the measured single fixed-fixed NW samples

	Mode 1 Frequency (MHz)	Mode 2 Frequency (MHz)
Sample 1	46	101
Sample 2	44	-
Sample 3	18	45

Fig. 5.1 compares the two-source/ 1ω detected output signals from the NWs oriented along $\langle 100 \rangle$ and $\langle 110 \rangle$ crystallographic directions that are otherwise identical under common measurement conditions. Although the output signal increase shown in Fig. 5.1 for the $\langle 100 \rangle$ orientation might be justified with the higher gauge factor at this direction, it also might be related to different asymmetric beam deflections at rest for each sample considering the sensitivity of the two-source/ 1ω scheme on an initial static beam profile.

Frequency sweeps for the Si NW sample having the $\langle 100 \rangle$ orientation and $5\text{ }\mu\text{m}$ length reveal two resonance peaks approximately at 44 MHz for the first mode in Fig. 4.14 and 101 MHz for the second mode in Fig. 4.15. A finite element analysis taking into account of oxide encapsulation around the Si NW and trapezoidal cross-section [71, 72] results in the resonance frequencies of 47.09 MHz and 100.98 MHz for the first in-plane and out-of-plane modes, respectively. On the other hand, frequency spectrum measurements of the similar NW except for the NW length of $8\text{ }\mu\text{m}$ indicate two resonance peaks approximately at 17.9 MHz for the first mode in Fig. 4.23 and 44.75 MHz for the second mode in Fig. 4.27. The similar ratio between the first and second modes for both samples is striking and implies that similar cross sections are obtained for both samples. Comparison of the voltages necessary to drive the first mechanical mode of these two identical except for the NW length samples in a nonlinear fashion shown in Fig. 4.13 and 4.24 confirms that it becomes increasingly difficult to excite and detect a NW motion as a beam length keeps decreasing leading to increases in both resonator stiffness and mode frequencies.

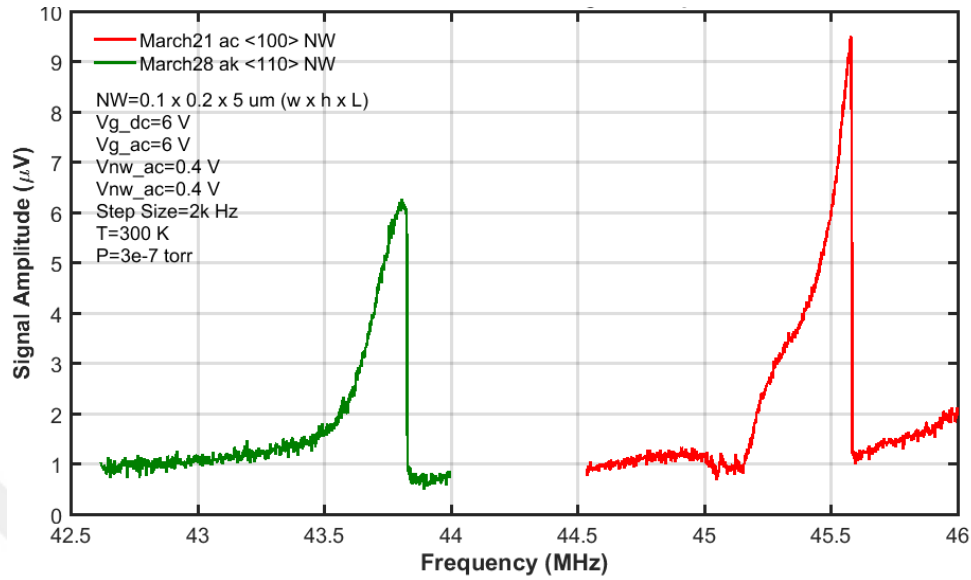


Figure 5.1: Effect of NW orientation on the amplitude of two-source/ 1ω detected output signals

Relatively low Q value of 1500 is obtained for the in-phase mode of Sample 1 in vacuum. Oxide encapsulation around each measured Si NW leads to a bilayer structure. Moreover, overhanging membrane formed at each clamping location during the employed top-down fabrication flow yields imperfect clamping. Both of these factors can be attributed to low Q values of the measured resonators.

All single NW frequency spectrum measurements indicate nonexistent or very weak output signals detected with the two-source/ 2ω scheme. According to Eq. 4.11, asymmetric NW profile at rest seems to provide significant amplification for the two source/ 1ω frequency downmixing method such that resolvable electrical signals are obtained to characterize the second mechanical mode of some NW samples. As pointed out earlier, the two-source/ 1ω scheme captures the linear component of a time-varying resistance change and thus, an output signal is proportional to a NW vibration amplitude. Fig. 5.2 depicts the output signal amplitude as a function of the gate DC voltage corroborating this linear relation [68, 69].

In order to safely associate this linear transduction to piezoresistance, the extent of a linear resistance modulation originated from capacitive coupling to a side-gate electrode is investigated by static transconductance measurements at ambient and cryogenic temperatures. However, sweeping a gate DC voltage in a large range results in no appreciable resistance change. This result in line with the literature [68, 73] can be expected considering the large nominal electrode-NW gap of 400 nm and high doping level of the measured NWs. Hence, modulated resistance of any measured NW is a direct result of a mechanical strain induced during resonance.

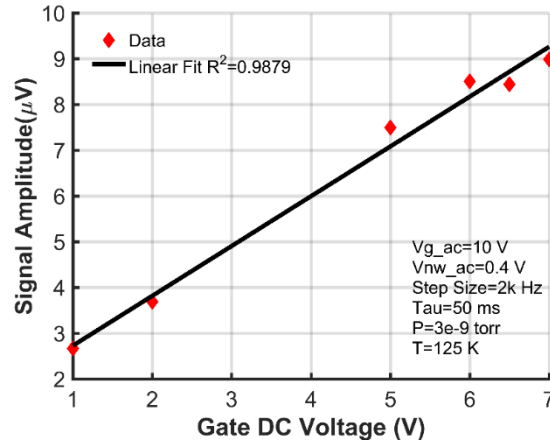


Figure 5.2: A linear relation between detected signal amplitudes and gate voltages exists for the 1ω scheme

Resonance frequency dependence of some detected mechanical modes of the measured NW samples on gate AC and DC voltages is shown in Fig.5.3. Fig. 5.3 indicates a positive linear relation between the resonance frequency of the measured first in-plane modes and gate voltages resulting in spring hardening. Linear resonance frequency tuning range (Δf) seems to be much higher for the sample with the 5 μm NW length than NW having the length of 8 μm . This result depicts the easy of nonlinear excitation of compliant NW structures corresponding to their low dynamic range characteristic.

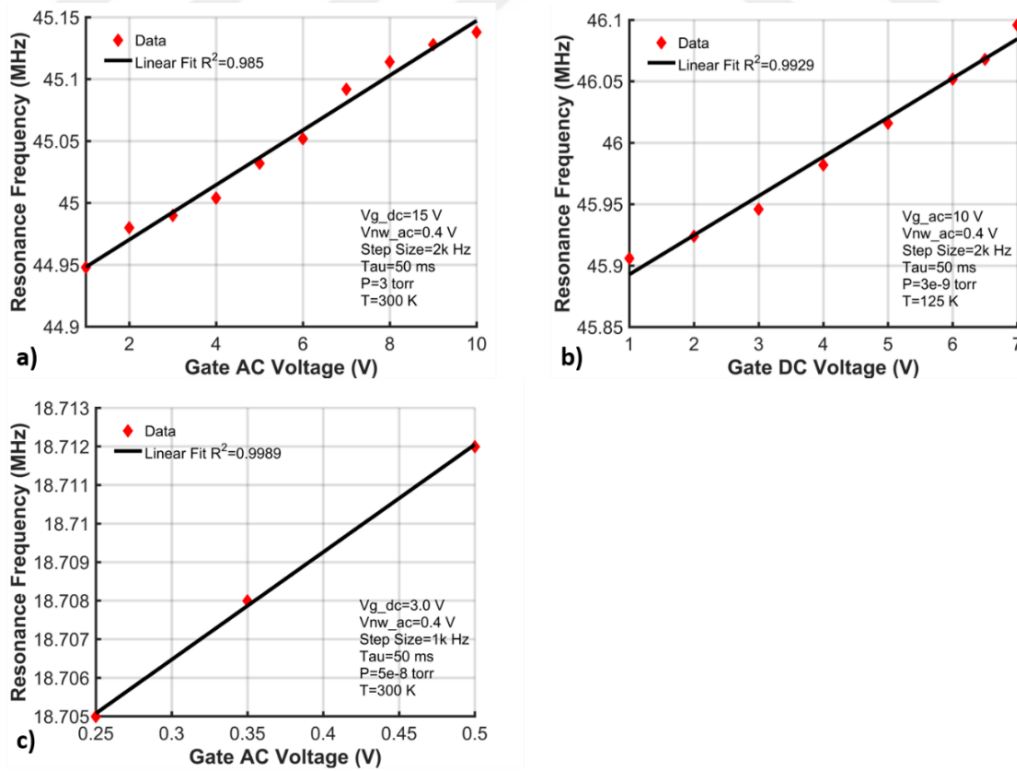


Figure 5.3: Resonance frequency of a mechanical mode can be tuned linearly with gate voltages

Resonance frequency shift of a mechanical mode before the onset of nonlinearity with respect to gate voltages is normalized using the resonance frequency and voltage difference inducing these shifts as $(\Delta f/f)/\Delta V$. Table 5.2 summarizes the calculated normalized frequency shift results for the detected mechanical modes of all NW samples. Results in Table 5.2 indicate that an increase in gate voltages is accompanied by an increase in the resonance frequency of the in-plane mode of each sample. Moreover, the frequency shift behavior of the out-of-plane mode of the NWs seem different from the in-plane modes. While there is always significant spring hardening for the in-plane modes, both spring hardening and softening although to a lesser degree are realized for the in-plane modes.

Table 5.2: Calculated normalized resonance frequency shift data for each detected mechanical mode of the measured NW samples

	Voltage Range	Δf (kHz)	$(\Delta f/f)/\Delta V$ (ppm)	Notes
Sample 1	1V-7V	200	731	First Mode, Q= 1500
Sample 2	1V-4V	30	228	First Mode, Q= 700
Sample 3	3V-7V	12	160	First Mode, Q= 1400
Sample 1	1V-15V	-48	-34	Second Mode, Q= 350
Sample 3	5V-15V	6	13	Second Mode, Q= 1100

FEM simulations are performed to understand the different frequency shift behaviors of the NW samples shown in Table 5.2 in such a way that the effect of a DC voltage applied to a side-gate electrode on NW resonance frequency is investigated. A commercial finite element software with 3D free-tetrahedral mesh elements is employed to perform electrostatic deflection and modal analysis simulations. Single crystalline isotropic silicon having the mass density and modulus of elasticity of 2329 kg/m³ and 170 GPa respectively is used as the structural material.

In the simulations, the side-gate electrode consists of a thin metal layer on top of a 1 μm thick Si base layer as shown in Fig. 5.4. Moreover, a double clamped NW having the width, thickness and length of 60 nm, 65 nm x 2000 nm respectively is used. The metal layer is higher than the top surface of the NW to better comply with the measured NW samples. In the first part of the simulation, while the NW is grounded, the gate DC voltage is swept from 0 to 15 V with 5 V intervals. Resulting electrostatically deflected NW is taken as an input for a modal analysis simulation in the second part of the simulation at each gate DC voltage value. Furthermore, a uniaxial stress is defined along the length of the NW.

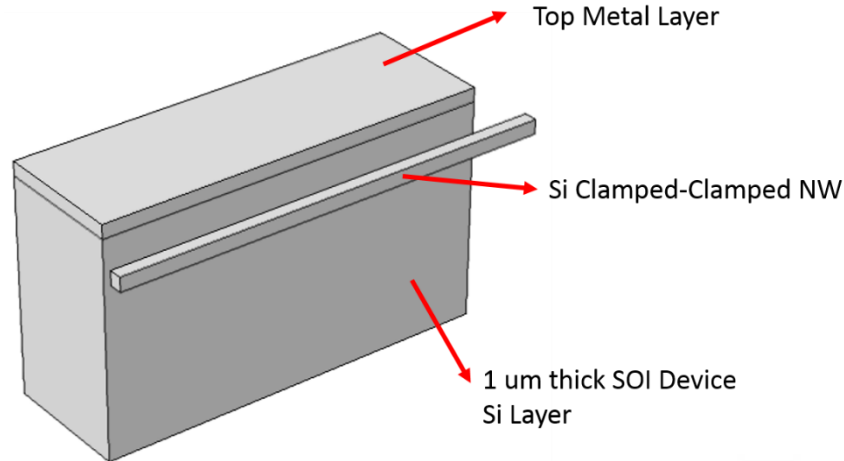


Figure 5.4: Employed simulation geometry to understand the resonance frequency shift of a NW mode with respect to gate voltages. NW:60x65x2000 nm (wxhxL)

Resulting first in-plane and out-of-plane flexural mode shapes are shown in Fig. 5.5. Thus, NW in-plane and out-of-plane resonance frequencies are determined with respect to gate voltages at a given NW uniform stress. In this way, normalized resonance frequency shifts calculated in the same manner using the simulation data are summarized in Table 5.3.

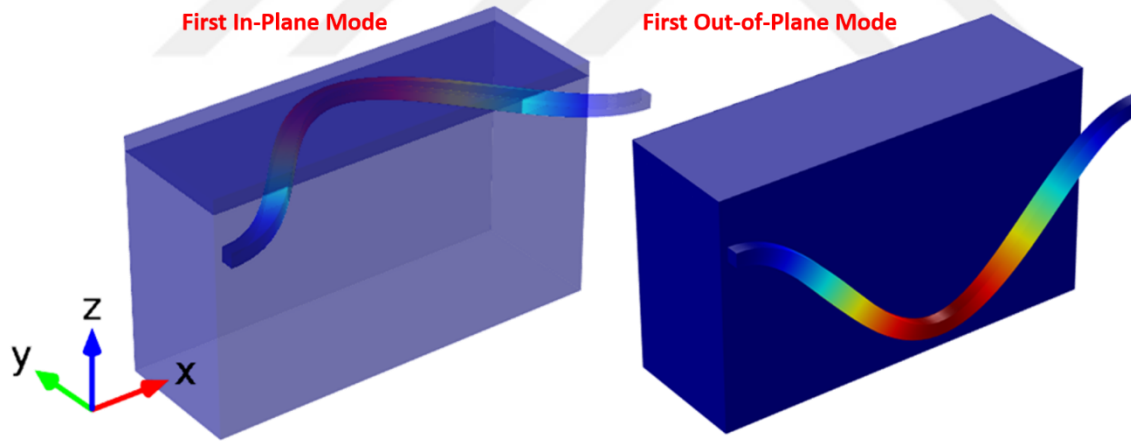


Figure 5.5: Resulting in-plane and out-of-plane first flexural modes

The normalized resonance frequency shift results in Table 5.3 indicate that an increase in a gate DC voltage results in spring softening for both first in-plane and out-of-plane flexural modes except for high uniaxial compressive stresses. Moreover, normalized frequency shifts of the out-of-plane mode are much less than shifts of the in-plane mode similar to the measurement results given in Table 5.2. Although, frequency spectrum measurements point out the existence of spring softening and hardening for the in-plane and out-of-plane modes of a same NW sample, no such result is found with the performed simulations. This inconsistency might be related to spatial nonidealities of a measured NW and imperfect clamping conditions at any anchor-NW junction.

Table 5.3: Calculated normalized resonance frequency shift results of the NW in-plane and out-of-plane first flexural modes from the performed FEM simulations

NW Uniform Stress (MPa)	In-plane Frequency Shift $\Delta f/f/V$ ppm	Out-of-plane Frequency Shift ($\Delta f/f/V$) ppm
-500	116079	7434
-450	6151	929
-400	86	67
-350	-478	-67
-300	-513	-94
-200	-420	-91
-100	-337	-79
0	-280	-69
100	-238	-60
200	-206	-53
300	-183	-48
400	-163	-44
500	-148	-40
750	-120	-33
1000	-101	-28

5.2. Analysis of Coupled Vertical NW Stack Spectrum Measurements

Frequency spectrum measurement results of the coupled vertical NW array samples are outlined in Table 5.4. Sample 1 is used to study the effect of the NW's length on frequency spectrum characteristics of a coupled vertical NW stack. On the other hand, the dependence of frequency spectrum characteristics of a coupled NW array on coupling element stiffness is examined by changing the CM length of the remaining samples for a common NW structure.

Table 5.4: Detected mechanical modes of the coupled vertical NW array samples. Any mechanical mode shown together with an asterisk symbol implies existence of another mechanical mode nearby.

	Coupling Membrane Length (nm)	NW Length (μm)	Mode 1 (MHz)	Mode 2 (MHz)	Mode 3 (MHz)	Mode 4 (MHz)	Mode 5 (MHz)
Sample1	150	3	46	58	-	-	-
Sample4	100	2	99*	129*	-	-	-
Sample3	500	2	75*	-	-	-	-
Sample2	1000	2	70*	77	108	122	128

Spectrum measurements of the detected mechanical modes reveal Q s on the order of 400 for the coupled NW array samples lower than the single NW samples. Addition of a pair of coupling elements into the overall picture and anchor like NW-CM junction increase proportional to number of resonators in an array cause more energy sinking. Thus, energy dissipation in a CM should be suppressed to get higher Q s. Release of a CM from an underlying substrate and resulting higher mechanical coupling between NWs in an array can deliver higher Q s at least for the in-phase mode.

Similar to the single NW samples, the two-source/ 2ω scheme results in signal amplitudes considerably lower than the two-source/ 1ω method except for the 99 MHz peak of Sample 4. Signal amplitudes detected through the two-source/ 1ω and two-source/ 2ω schemes as a function of a side-gate voltage are depicted in Fig. 5.6. Fig. 5.6 indicates a linear and quadratic dependence of a signal output on gate voltages for the two-source/ 1ω and two-source/ 2ω schemes respectively. Hence Fig. 5.6 validates targeting of these two-source/ 1ω and two-source/ 2ω downmixing techniques only to time-varying linear and quadratic resistance components respectively.

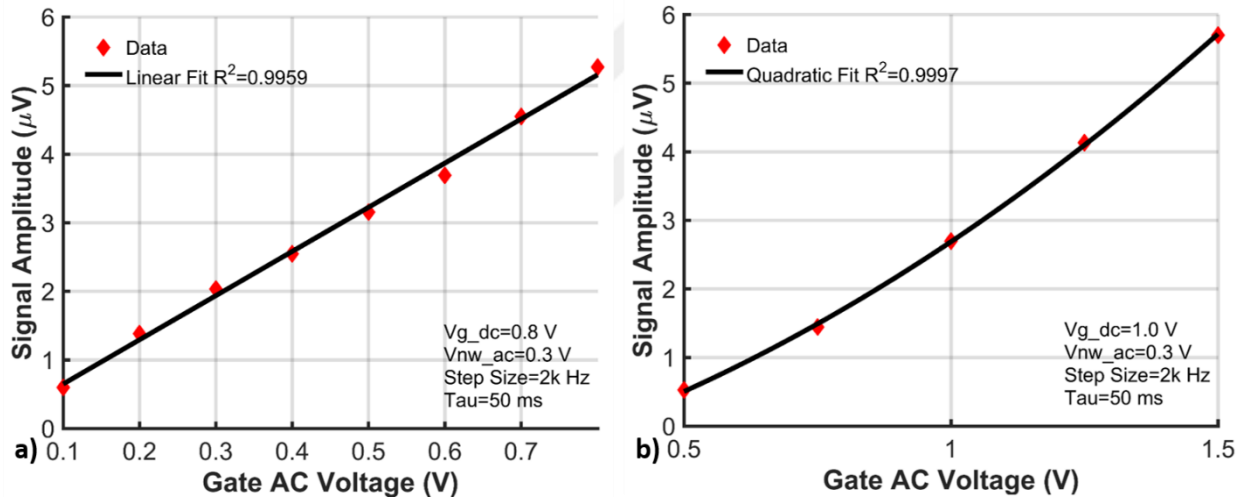


Figure 5.6: Signal amplitude relation with gate voltages exhibits a linear in (a) and quadratic in (b) characteristic for the two-source/ 1ω and two-source/ 2ω downmixing schemes respectively.

On the other hand, resonance frequency dependence on gate voltages is quite complicated unlike a simple linear relation obtained for all of the detected mechanical modes of the single NW samples as shown in Fig. 5.3. In some cases, resonance frequency of a mechanical mode drifts with respect to gate voltages as shown in Fig. 4.45-4.46.

Normalized frequency shift results shown in Table 5.5 for some detected spectrum peaks indicate that both spring hardening and softening are realized for Sample 2 which has the highest mechanical coupling between NWs in the fabricated array due to its long CM of 1000 nm. Comparison of the Q s of Sample 2,3 and 4 validates the prediction of the detrimental effect of a CM itself on array Q leading to the lowest Q s for the longest CM length device of Sample 2.

Table 5.5: Normalized frequency shift results for the detected mechanical modes of the coupled vertical NW array samples using frequency spectrum measurements

	Voltage Range	f (MHz)	Δf (kHz)	$(\Delta f/f)/\Delta V$ (ppm)	Notes
Sample 1	0.5-2 V	46	-62	-904	First Mode, Q=360
Sample 2	1-7V	70	190	451	First Mode, Q=400
Sample 2	0.5-0.6 V	76	500	65789	Second Mode, Q=200
Sample 2	4-8 V	108	580	1343	Third Mode, Q=360
Sample 2	2-15 V	122	400	252	Fourth Mode, Q=300
Sample 2	2-15 V	128	-350	-210	Fifth Mode, Q=500
Sample 3	0.1-0.8 V	75	58	1112	First Mode, Q=770
Sample 4	0.5-1.5 V	99	44	444	First Mode, Q=1008
Sample 4	1-7 V	129	628	808	Second Mode, Q=416

Impossibility of direct comparison of frequency spectrum measurements of the single fixed-fixed NW and coupled vertical NW array samples are two-fold. First, different device layout parameters such as resonator dimensions and resonator-to-electrode gaps pose significant challenges. Second, the fabrication flow [72] used to fabricate the single NW samples includes a low temperature oxidation (LTO) step approximately at 425 °C resulting in NW oxide encapsulation and a residual stress in fabricated NWs different than that of NWs in an array. These issues obstruct easy qualitative assessments about inclusion of a CM and employment of multiple resonators in an array structure on frequency spectrum characteristics. As a result, FEM simulations are conducted to determine conclusively whether any detected mechanical mode is a collective array mode or an individual NW resonance. In other words, existence of mechanical coupling between NWs in a stack is investigated.

FEM analyses implemented to understand the nature of mechanical modes for the Si NW samples are repeated for the coupled NW stack samples. One might expect to get 8 in-plane and out-plane resonance modes from a vertical NW array consisting of 8 NWs. However, inevitable spatial non-uniformity of a NW along its length and between NWs in a vertical array and absence of accurate NW spatial measurements complicate implementation of precise FEM simulations at the moment. Thus, FEM simulations cannot be used to model a fabricated coupled vertical NW array such that its measured frequency spectrum peaks are matched to specific FEM modes conclusively. Moreover, since measured and simulated resonance frequencies of a NW stack cannot be compared directly, uniaxial residual stress in resonators cannot be estimated. However, FEM simulations are performed to analyze various resonance frequency shift conducts of the measured NW arrays shown in Table 5.5 with respect to gate DC voltages. Simulations consisting of a vertical NW array of four resonators and a couple of CMs as shown in Fig. 5.7 that are otherwise

identical to those simulations performed for the single NW samples are carried out. Four identical NWs in the array are employed to follow each in-plane and out-of-plane resonance mode with respect to gate voltages easily.

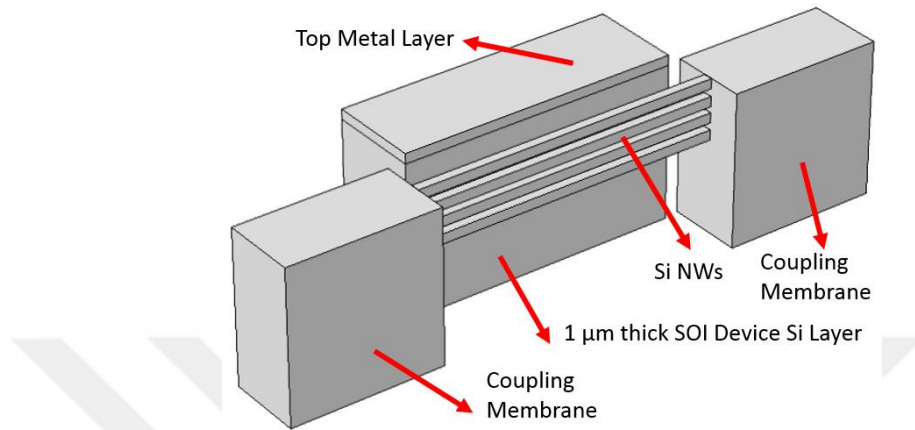


Figure 5.7: Resonance frequency relation with varying gate DC voltages is examined for each mode using a simulation geometry consisting of four identical NWs. NW:60x65x2000 nm, CM:500x1000x1000 nm (wxhxD),

Fig. 5.8 depicts some resulting in-plane and out-of-plane mode shapes of the simulated coupled vertical NW array. An in-phase and three out-of-phase mode shapes are obtained for both in-plane and out-of-plane resonances. Tracking of simulated NW array in-plane and out-of-plane resonance frequencies with respect to gate voltages at a given NW uniform stress leads to normalized frequency shifts summarized in Table 5.6.

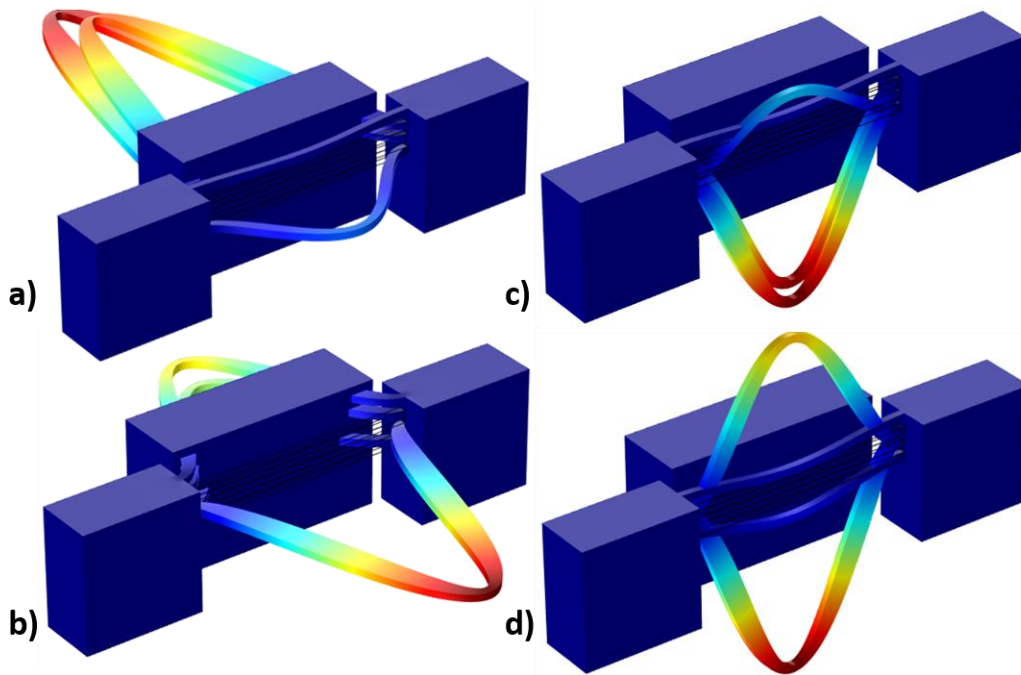


Figure 5.8: Some resulting in-plane in (a,b) and out-of-plane in (c,d) modes from the FEM modal analysis of the considered coupled vertical NW array

Resonance frequencies of in-plane and out-of-plane modes of the simulated array are in close proximity to each other and the resonance frequencies shown in Table 5.6 at each applied uniform stress are given to depict the approximate level of them. Resonance frequency relation of the coupled NW array with the applied uniaxial stress are in line with the analytical relation for a clamped-clamped NW such that an increase in a tensile stress corresponds to a higher resonance frequency.

Table 5.6: Normalized frequency shift results of the simulated coupled NW array show a clear distinction between in-plane and out-of-plane modes.

Stress (MPa)	f (MHz)	In-plane Modes				Out-of-plane Modes			
		Mode1	Mode2	Mode3	Mode4	Mode1	Mode2	Mode3	Mode4
		$\Delta f/f/\Delta V$ (ppm)	$\Delta f/f/\Delta V$ (ppm)	$\Delta f/f/\Delta V$ (ppm)	$\Delta f/f/\Delta V$ (ppm)	$\Delta f/f/\Delta V$ (ppm)	$\Delta f/f/\Delta V$ (ppm)	$\Delta f/f/\Delta V$ (ppm)	$\Delta f/f/\Delta V$ (ppm)
750	240	-71	-205	-118	-160	9	-5	7	6
400	197	-128	-291	-169	-236	14	12	-8	8
200	167	-248	-339	-234	-327	21	19	-11	10
100	149	-355	-315	-441	-331	28	24	8	-8
0	128	-163	-27	-546	-475	43	34	13	-10
-100	103	-279	-778	-1138	-677	87	59	19	3
-200	66	-326	-	-	-916	428	161	137	178

Comparison of the normalized resonance frequency shift results of the single NW and coupled NW array simulations, and measurements depicts a complex picture. In simulations, spring softening is realized for in-plane modes regardless of applied uniform stress similar to the single NW case. On the contrary, measurements demonstrate spring hardening for all in-plane modes of the employed single NW samples and most of the detected mechanical modes of the coupled NW arrays. Sansa *et al.* [68] found a spring hardening and softening behavior with respect to gate DC voltages for their bottom-up and top-down single Si NW samples respectively. These different characteristics might be related to spatial nonidealities along a fabricated NW, imperfect clamping conditions at any anchor-NW junction or an initial resonator profile at rest exhibiting static deflections.

The most striking feature of Table 5.6 is the clear distinction between in-plane and out-plane mechanical modes in terms of the magnitude of normalized frequency shifts. Normalized frequency shifts of the out-of-plane modes are much less than those of the in-plane modes similar to the single NW simulation results given in Table 5.3. Both simulations and measurements share this distinct nature of the resonance frequency dependence on gate voltages for in-plane and out-of-plane mechanical modes.

Moreover, there is a contrast between the frequency shift behavior of the mechanical modes of the single NW and coupled NW array simulations. On the one hand, either spring hardening or softening is realized for both mechanical modes of a single NW depending on an applied uniaxial stress as in Table 5.3. In contrast, the only coupled NW array simulations demonstrate both resonance shifting characteristics for in-plane and out-of-plane modes of a NW array simultaneously at all stresses in accordance with the spectrum measurements of Sample 2. Moreover, the coupled NW array simulations also show both resonance shifting characteristics for different out-of-plane modes simultaneously for a same sample at zero or tensile uniaxial stresses.

The resonance frequency raw data of the simulated coupled NW array with respect to gate voltages for the uniaxial compressive stress of 100 MPa is given in Table 5.7. Interestingly, Table 5.7 depicts a drifting resonance frequency behavior for one of the out-plane modes reminiscent of the measured frequency spectrums of the 122 MHz and 128 MHz modes of the coupled NW array of Sample 2 shown in Figs. 4.45-4.46.

Table 5.7: Resonance frequency of the simulated coupled NW array with respect to gate voltages is given for each mode at the compressive uniaxial stress of 100 MPa.

Voltage (V)	In-plane Modes				Out-of-plane Modes			
	Mode 1 (MHz)	Mode 2 (MHz)	Mode 3 (MHz)	Mode 4 (MHz)	Mode1 (MHz)	Mode 2 (MHz)	Mode 3 (MHz)	Mode 4 (MHz)
5	102.637	103.093	103.323	104.726	114.779	116.033	116.433	117.788
10	102.501	102.88	102.995	104.478	114.803	116.051	116.437	117.782
15	102.426	102.58	102.426	104.105	114.85	116.084	116.447	117.78
20	102.208	101.89	101.56	103.663	114.929	116.135	116.466	117.794
$\Delta f/f/\Delta V$ (ppm)	-279	-778	-1138	-677	87	59	19	3

Effect of the mechanical coupling between NWs in a vertical array on frequency spectrum properties is investigated by performing similar FEM simulations using the two resonator geometries shown in Fig. 5.9. In one case, elimination of employed CMs corresponds to zero mechanical coupling between the NWs in the array. On the other hand, reducing the width of CMs to on the order of an associated NW width results in very compliant coupling elements and thus, significant mechanical coupling is achieved.

Table 5.8 and 5.9 present resonance frequencies with respect to gate DC voltages and calculated normalized frequency shift data for some in-plane and out-of-plane modes of each simulated geometry at the zero residual stress. Frequency shift responses indicate a similar kind of behavior

for the considered in-plane and out-of-plane modes for each resonator architecture. On the contrary, a mode frequency range from the lowest to highest mode is proportional to mechanical coupling for both in-plane and out-of-plane modes. Thus, mode frequencies diverge from each other with increasing mechanical coupling as expected. Moreover, the frequency spectrum measurement results of Sample 2,3 and 4 in Table 5.4 which have a common composite resonator configuration except for the different CM lengths, depict that the resonance frequency of an in-plane or out-of-plane mode decreases with an increase in the CM length in parallel with the simulation results.

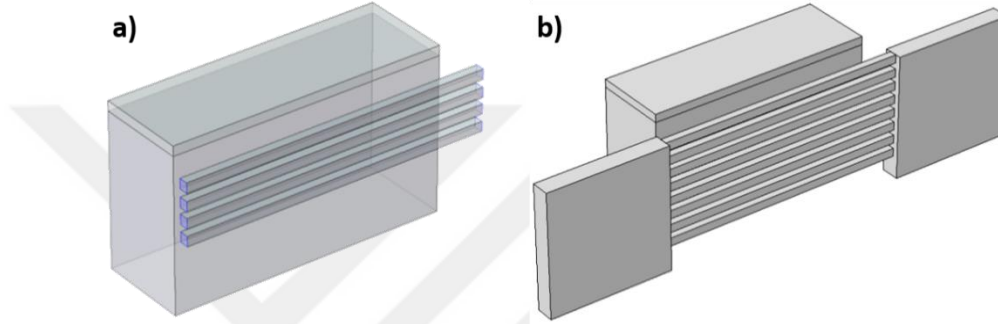


Figure 5.9: Effect of mechanical coupling on resonance frequency shift characteristic of a mechanical mode is investigated by FEM simulations considering no coupling in (a) and compliant coupling in (b).

Table 5.8: Mode frequencies of the simulated vertical NW array having no CM with respect to gate voltages.

Voltage (V)	In-plane Modes				Out-of-plane Modes			
	Mode 1 (MHz)	Mode 2 (MHz)	Mode 3 (MHz)	Mode 4 (MHz)	Mode1 (MHz)	Mode 2 (MHz)	Mode 3 (MHz)	Mode 4 (MHz)
0	131.779	131.934	132.428	132.533	142.6	142.857	143.305	143.421
5	131.704	131.869	132.371	132.475	142.605	142.862	143.302	143.419
10	131.448	131.687	132.214	132.31	142.618	142.877	143.295	143.414
15	130.979	131.371	131.977	132.074	142.641	142.904	143.287	143.411
20	130.297	130.888	131.648	131.829	142.671	142.945	143.285	143.414
$\Delta f/f/\Delta V$ (ppm)	-562	-396	-294	-266	25	31	-7	-2

Table 5.9: Mode frequencies of the simulated NW array having a compliant CM with respect to gate voltages.

Voltage (V)	In-plane Modes				Out-of-plane Modes			
	Mode 1 (MHz)	Mode 2 (MHz)	Mode 3 (MHz)	Mode 4 (MHz)	Mode1 (MHz)	Mode 2 (MHz)	Mode 3 (MHz)	Mode 4 (MHz)
0	116.419	126.538	128.89	129.459	137.125	139.173	139.421	140.094
5	116.391	126.504	128.807	129.362	137.129	139.179	139.424	140.092
10	116.306	126.4	128.554	129.088	137.142	139.198	139.432	140.089
15	116.167	126.229	128.13	128.698	137.166	139.23	139.446	140.086
20	115.976	125.991	127.595	128.233	137.205	139.278	139.468	140.085
$\Delta f/f/\Delta V$ (ppm)	-190	-216	-502	-474	29	38	17	-3

Chapter 6: Conclusions

Development of sophisticated oscillator and filter architectures at the nanoscale based on Si NWs depends on the ability to realize novel design, fabrication and measurement schemes. This study is performed to address these fronts.

- A new composite resonator architecture is developed at the nanoscale by stacking NWs perpendicular to the surface of a substrate and coupling the NWs in the resulting vertical array mechanically by means of a membrane-type coupling element called CM.
- Employment of CMs corresponds to a significant expansion to rather limited mechanical coupling toolkit at the nanoscale due to connections even between non-adjacent resonators. Ability to deliver desired level of mechanical coupling by varying the in-plane CM length together with compactness of the structure accentuated at the nanoscale by employing a common actuation electrode are demonstrated.
- Coupled NW arrays consisting of 8 NWs designed based on finite element modeling (FEM) modal analysis simulations are fabricated using the developed top-down fabrication flow from the 1 μm thick device layer of a silicon-on-insulator (SOI) wafer.
- Electromechanical characterization of piezoresistive single Si NW samples fabricated in the 10 μm thick device layer of a SOI substrate is demonstrated for the first time in the literature. Detected mechanical modes from 18 MHz to 101 MHz for single NW samples are successfully associated to the first flexural in-plane and out-of-plane modes using FEM simulations thanks to the determination of an actual NW cross section by TEM measurements.
- NW array measurements result in multiple mechanical modes both dispersed in a wide frequency range and in close proximity such that being reminiscent of typical spectrum response of a bandpass filter.

Other main findings can be summarized as follows. Employed two piezoresistive frequency downmixing techniques namely the two-source/ 1ω and two-source/ 2ω detection schemes demonstrate a linear or quadratic dependence of a signal amplitude on gate voltages respectively. On the other hand, while resonance frequency dependence on gate voltages is found linear for all the detected mechanical modes of the single NW samples, coupled NW array samples exhibit quite complicated variations. In some cases, resonance frequency of a mechanical mode even drifts with respect to gate voltages. Sensitivity of the two-source/ 1ω scheme to an initial static beam profile hinders direct comparison of any two NW samples following different crystal orientations. The

two-source/ 2ω scheme results in signal amplitudes considerably lower than the two-source/ 1ω method for all measured samples in general. Easy of nonlinear excitation of the relatively compliant samples underlines low dynamic range characteristic of nanoresonators. Since transconductance measurements at ambient and cryogenic temperatures yield no appreciable resistance change in parallel with the literature, any time-varying linear resistance change is associated with the piezoresistance mechanism.

Relatively low Q s of the measured fixed-fixed NWs are related to oxide encapsulation around each NW leading to a bilayer structure and imperfect clamping originated from an overhanging membrane formed at each NW-anchor junction. Spectrum measurements of the coupled NW arrays reveal Q s in the order of 400 which is lower than those of the single NW samples. This further reduction in Q is associated with the addition of a pair of coupling elements and numerous anchor like NW-CM junctions into the overall picture. So, it is not surprising to get the lowest Q s for the mechanical modes of the longest CM length device.

Unlike single NW samples, inevitable non-uniformity of NWs in an array and absence of accurate spatial measurements complicate implementation of FEM simulations to relate detected modes of a NW array to specific array modes and to determine a uniaxial residual stress along NWs. Thus, other FEM simulations are conducted to investigate more fundamental issues such as existence of mechanical coupling between NWs in a stack and distinguishing collective array modes from an individual NW resonance.

To this end, experimental resonance frequency shifts of single NW and NW array samples with respect to electrode voltages are compared between each other and with FEM results. This comparison between simulations and measurements reveals similar and distinct characteristics simultaneously. For example, simulations and measurements indicate spring softening and hardening characteristics respectively with respect to gate voltages for in-plane modes. These different characteristics might be related to spatial nonidealities along a fabricated NW, imperfect clamping conditions at any anchor-NW junction or an initial resonator profile at rest exhibiting asymmetric static deflections. On the other hand, much less normalized frequency shift results of out-of-plane modes than those of in-plane modes are shared between both simulations and measurements. Interestingly, comparison of frequency shift behaviors of the simulated single NW and coupled NW array lets out-of-plane modes of a single NW and a coupled NW array be distinguished. Since some in-plane and out-of-plane modes exhibit spring softening and hardening characteristics simultaneously only for the same simulated coupled NW array similar to some spectrum measurements.

The coupled NW array simulation provides a drifting resonance frequency behavior with respect to gate voltages for some out-of-plane modes similar to some measurement results. Moreover,

while simulated frequency shift responses indicate a similar kind of behavior regardless of the degree of mechanical coupling, mode frequencies diverge from each other with increasing mechanical coupling as expected. Also, a decrease in the resonance frequency of an in-plane or out-of-plane mode is realized in the simulation with an increase in the CM length in parallel with measurements.

As a future work, release of the fabricated CMs from the underlying substrate can be implemented to increase mechanical coupling between NWs in a vertical array and Q at least for the in-phase mode simultaneously. Although oxidation and subsequent oxide dry etching of NWs are utilized to enhance spatial uniformity of NWs in a vertical stack for same samples, existence of thin membranes between vertical stacks and side gate electrodes hinders employments of these samples in coupled array measurements. This issue clearly deserves more study to attain a higher degree of NW uniformity in a stack. Issues related to spatial nonidealities of NWs in a vertical array and actual cross section structure should be addressed by TEM measurements to associate detected mechanical modes of a NW array to specific array modes by FEM simulations. Moreover, laying of multiple coupled vertical arrays in a series configuration as shown in Fig. 6.1 can be performed to realize a series electromechanical filter at the nanoscale. In this way, filter characteristics such as BW can be adjusted reliably by means of a coupling element connecting sequential arrays. Furthermore, a coupled vertical NW array can be based on other beam types such as a free-free beam to increase Q of the overall array.

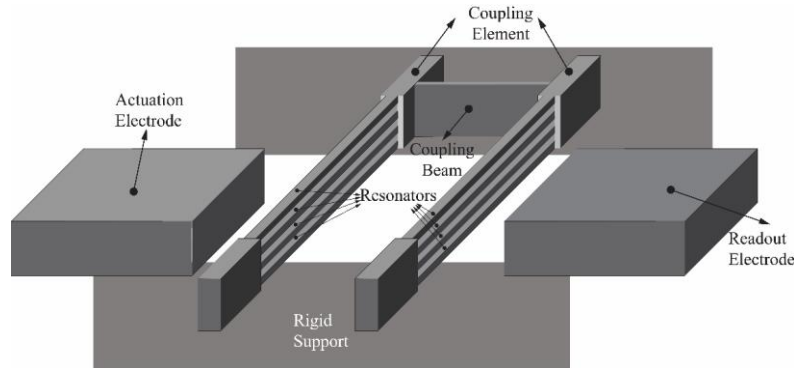


Figure 6. 1: A series electromechanical filter consists of a pair of coupled vertical NW arrays

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APPENDIX A: OUT-OF-PLANE NUMERICAL COUPLING MODELING

Electromechanical Filters Based on Coupled Nanowire Resonators: Modeling Aspects

Y. Kilinc ^{a,1}, B. E. Alaca ^{a,b}

^a Dept. of Mechanical Engineering, Koc University, Rumelifeneri Yolu, Sariyer 34450 Istanbul, Turkey

^b Surface Science and Technology Center (KUYTAM), Koc University, Rumelifeneri Yolu, Sariyer 34450 Istanbul, Turkey

ABSTRACT

Mechanical coupling is exploited extensively for resonators in microelectromechanical systems (MEMS). In instances where the use of very compliant coupling beams is required, direct scaling of existing mechanically-coupled MEMS filter structures into the nanoscale seems challenging due to very thin coupling beams. To this end, a flexible and compact mechanical coupling method is developed at the nanoscale using coupling membranes. Switching from the conventional coupling beam to the coupling membrane of this work also leads to mechanical coupling even between non-adjacent resonators to presumably get more favorable filter characteristics. However, the challenges associated with coupling modeling of this unorthodox approach involve changing filter mode shapes and filter center frequency with respect to coupling membrane dimensions. To address this problem, a generic second-order filter architecture is used to illuminate limitations of the frequently employed analytical quarter-wavelength approach for coupling beam modeling in MEMS filters. A numerical filter modeling methodology is developed to have the filter center frequency and bandwidth as a function of coupling dimensions directly from modal analysis in finite element modeling. The developed numerical methodology is used to model electromechanical filters consisting of coupling membranes at the nanoscale.

Keywords: Nanoelectromechanical systems (NEMS), mechanical coupling, electromechanical filter, numerical modeling, nanowire

¹ Corresponding author. Tel.: +90 212 338 1727; fax: +90 212 338 1548.
E-mail addresses: ykilinc@ku.edu.tr (Y. Kilinc), ealaca@ku.edu.tr (B. E. Alaca).

1. INTRODUCTION

Resonators based on micro/nano electromechanical systems (MEMS/NEMS) are utilized widely in on-chip, high quality-factor (Q) and low insertion-loss oscillators [1-4]. MEMS oscillators are already engaged in head-on competition with 32 kHz crystal counterparts in the timing market with less than 1 μA power consumption and ± 5 ppm frequency stability for mobile and wearable electronics [5]. For example, a 524-kHz silicon double tuning fork design featuring ± 100 ppm frequency stability and with an approximately 100- μA power consumption can provide oscillator frequencies up to 26 MHz [6].

The use of coupling in resonant systems represents a variety of advantages. These include providing improvements in device properties such as increased sensitivity to perturbations [7] and enabling completely new functionalities such as signal filtering [8] and mixing [9]. Sensitivity improvements are even accentuated by switching from micro to nano structures [10].

An electromechanical filter is effectively a signal engineering device composed of mechanical resonators and coupling elements [11]. They are used in multi-band, multi-mode wireless applications such as wireless receivers as RF channel select filter banks [8, 12]. With reduced size scale, coupling can be delivered either by employing various mechanical components such as U- [13] and V- [14] shaped coupling beams, CBs, or altering resonator anchor characteristics by undercutting ledges of suspended arrays [15, 16], the latter being about the only reported mechanical coupling technique at the nanoscale. The simplest series, out-of-plane, second-order electromechanical filter structure is depicted in Fig. 1.a. It consists of two identical clamped-clamped beam resonators with the width, height and length of w_r , h_r , L_r respectively. The resonators marked by R_1 and R_2 are coupled through a flexural-mode CB at a certain point along the resonator length. At the filter input port, an electrical input signal is converted to a mechanical signal to be engineered in the mechanical domain. Then, the processed mechanical signal is converted back to an electrical output signal at the filter output port. Electrostatic transduction between a resonator and an underlying actuation electrode induces the out-of-plane filter modes. Connecting resonator pairs with a network of CBs results in filter modes proportional to the number of resonators in a filter. Lowest frequency filter mode consisting of resonators vibrating in the same direction together is called the in-phase filter mode. Besides, each resonator moves in the opposite direction of neighboring resonators in case of the out-of-phase mode.

Further miniaturization of MEMS filters down to the nanoscale is a straightforward way to increase their operation frequencies. However, considering cases where utilization of very compliant *i.e.* very thin CBs is required even for microscale systems, direct scaling of existing mechanically-coupled MEMS filter structures into the nanoscale seems impractical. Moreover, scaling-induced limitations emphasized at the nanoscale such as adsorption-desorption noise, temperature fluctuation noise and insufficient power handling may enforce employment of multiple sensors. Resonator coupling represents more than frequency selective on-chip components. For example,

amplification in sensor sensitivity to perturbations can be achieved as a result of coupling [7]. Thus, delivering desired level of mechanical coupling at the nanoscale is highly crucial.

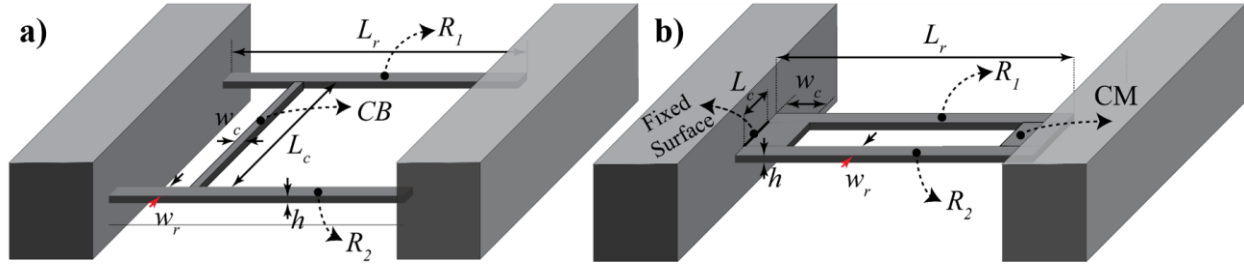


Figure A.1: a) Schematic of a second-order electromechanical filter together with resonator and CB design parameters, b) Proposed filter structure employing coupling membranes to deliver the desired level of mechanical coupling at the nanoscale.

Furthermore, the conventional CB of Fig. A.1.a can only be used to connect sequential resonators in the series filter architecture [8, 12, 17]. Sophisticated mechanical coupling schemes providing coupling of non-adjacent resonators using extra CBs were shown to improve frequency spectrum characteristics with sharper roll-offs and improved stopband rejections [18]. However, the capacity to provide mechanical coupling between non-adjacent resonators using CBs is limited even with an innovative filter layout. Thus, a coupling scheme delivering mechanical coupling for any resonator pair irrespective of resonator number for any beam-based filter configuration would be a significant improvement. In this respect, employment of coupling membranes (CMs) of Fig. A.1.b as a new and useful coupling scheme is proposed to expand mechanical coupling toolkit. The compactness of this filter structure thanks to short coupling membranes becomes even more advantageous considering the downscaling from the micro to the nanoscale.

Although the idea of mechanical coupling and the associated introduction of collective modes are interesting, the addition of a CB into the overall picture necessitates a proper CB design for a successful device implementation. When the CB mass is on the same order of the resonator mass as in the case of micro/nanoscale filters, this mass has to be taken into consideration, complicating further CB design [19].

Electromechanical modeling of a single MEMS/NEMS resonator is based on well-established analytical techniques [19-21]. However, these techniques cannot be borrowed to model coupling and support beams directly. In the literature, an analytical approach known as quarter-wavelength ($\lambda/4$) modeling is employed to design CBs and support beams [22, 23]. The $\lambda/4$ model imposes certain CB lengths for a given resonator geometry to maximize Q. Moreover, analytical solutions are only available for a limited number of CB designs having specific boundary conditions. Furthermore, as demonstrated later the $\lambda/4$ model loses its accuracy to predict the lumped stiffness of a CB, when the CB's width becomes comparable to that of attached resonators. These inaccuracies lead to significant deviations between designed and realized filter center frequency (f_0) and bandwidth (BW) parameters. Alternatively, numerical coupling modeling presents the opportunity to employ an extended set of available CB designs together with less strict design constraints, while providing improved accuracy for CB mass and stiffness parameters.

In the remainder of the manuscript, the conventional $\lambda/4$ -based analytical modeling approach will be introduced first. Then, a benchmark study will be presented to demonstrate shortcomings of the analytical model together with numerical modeling results. Later, the developed numerical modeling methodology will be applied to a specific coupling geometry, *i.e.* the CM. Lithographically-defined in-plane dimensions of the CM will ensure a flexible and compact mechanical coupling scheme especially suitable at the nanoscale.

2. COUPLING BEAM MODELING

Let us consider any electromechanical filter consisting of an arbitrary number of identical resonators. While the filter BW is centered around common resonance frequency of resonators (f_0), BW is determined by CB stiffness (k_c) according to Eq. A.1.

$$BW = f_0 \frac{k_c}{k_{rc}k_{12}} \quad (\text{A.1})$$

where k_{rc} and k_{12} are resonator stiffness at a coupling location and normalized coupling coefficient for a given filter type, respectively [22]. Thus, it seems that coupling stiffness is the only parameter that can be set to get a desired BW for a given resonator and filter architecture.

The CB of Fig. A.1.a is modeled with the $\lambda/4$ modeling as shown in Fig. A.2.a. Fig. A.2.a depicts a CB of the length, width and height of L_c , w_c and h_c , respectively, with guided boundary conditions. It is subject to mechanical forces of f_i resulting in velocity responses of $\dot{x}_i$. A general acoustic transmission line model consisting of a T network of mechanical impedances given in Fig. A.2.b. was suggested to model mass and stiffness of the CB of Fig. A.2.a. [22]. CB dimensions and filter operation frequency (ω) are used to calculate mechanical impedances, Z_{c1} and Z_{c2} , for the CB [19, 24] using Eqs. A.2-3.

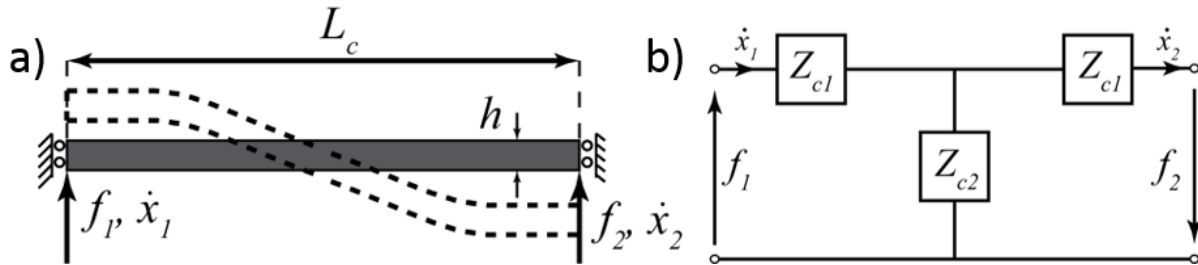


Figure A.2: a) CB with guided boundary conditions, b) T network of three mechanical impedances represents the CB in Fig. A.1.a

$$Z_{c1} = \frac{EI\alpha^3(H_6 - H_7)}{L_c^3 H_3} \quad (\text{A.2})$$

$$Z_{c2} = \frac{EI\alpha^3 H_7}{L_c^3 H_3} \quad (\text{A.3})$$

where $H_3 = \cosh \alpha \cos \alpha - 1$, $H_6 = \sinh \alpha \cos \alpha + \cosh \alpha \sin \alpha$, $H_7 = \sin \alpha + \sinh \alpha$, $\alpha = L_c(\rho w_c h \omega^2 / (EI))^{0.25}$, $I = w_c h^3 / 12$. ρ and E are the mass density and modulus of elasticity of a filter material, respectively. Thus, CB mechanical impedances are extracted directly from CB physical and geometrical properties, and filter architecture. On the other hand, the resonator

lumped parameters of equivalent mass (m_r), stiffness (k_r) and damping (c_r) can be derived with well-established electromechanical models for clamped-clamped resonators while considering the first flexural out-of-plane mode shape [19]. As a result, the second-order electromechanical filter of Fig. A.1.a can be represented by the equivalent mechanical circuit of Fig. A.3.a. This equivalent circuit can be simulated via a circuit simulator to obtain a filter frequency spectrum for any resonator and CB design. Then, the filter frequency spectrum characteristics of BW and f_0 taken from a circuit simulation of the equivalent circuit of Fig. A.3.a can be compared with those obtained from a finite element modeling (FEM) simulation using the same resonator and CB configuration. By this way, light can be shed on the limitations of the CB modeling with the $\lambda/4$ approach.

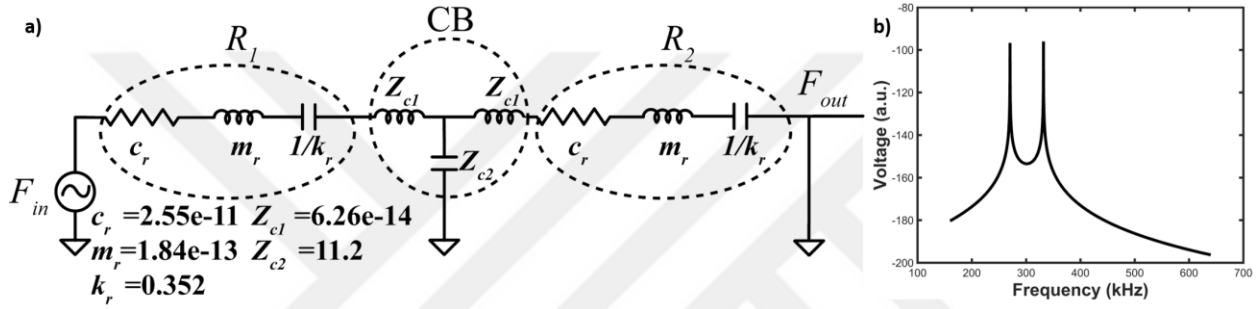


Figure A.3: a) Lumped-parameter equivalent mechanical circuit of the filter of Fig. 1.a, b) Simulated filter frequency spectrum obtained using the proposed numerical modeling methodology. Resonator: $1 \times 1 \times 200 \mu\text{m}$ ($w_r \times h_r \times L_r$), CB: $4 \times 1 \times 20 \mu\text{m}$ ($w_c \times h_c \times L_c$).

A resonator of w_r and L_r of $1 \mu\text{m}$ and $50 \mu\text{m}$, respectively, is selected to conduct the study. The CB length (L_c) is determined using the $\lambda/4$ condition [19]. The resonator (h_r) and CB heights (h_c) are set equal to each other and to the resonator width (w_r). All resonator and CB dimensions are kept constant except for the CB width (w_c). A commercial finite element software with 3D free-tetrahedral mesh elements is employed to perform modal analysis simulations. Polycrystalline silicon with ρ and E of 2329 kg/m^3 and 170 GPa , respectively, is employed as the filter structural material.

In Fig. A.4.a, filter BW is plotted as a function of the normalized CB width (w_c/w_r) for various normalized CB attachment locations (L_a/L_r). Lines are obtained by implementing the $\lambda/4$ model for the aforementioned out-of-plane filter of Fig. A.1.a, whereas discrete points represent FEM predictions. An important observation from Fig. A.4 is that the analytical model produces BW results matching with FEM predictions for small CB widths ($w_c/w_r < 0.5$) and CBs attached closer to anchors ($L_a/L_r \leq 0.2$). On the other hand, there are significant filter BW deviations between the analytical model and FEM results for wider CBs attached closer to the midpoint of resonators.

In an effort to understand this inconsistency, the resonator and CB mode shapes are examined. The normalized CB width is changed from 0.1 to 2 and corresponding evolution of filter modes is tracked. The CB mode shape for the filter in-phase mode are depicted in Fig. A.4.b. Interestingly, the CB mode shape has a strong dependence on the normalized CB width. Fig. A.4.b shows gradual deviation of the CB mode shape from the analytically-assumed shape of Fig. A.2.a with increasing

CB widths. Gradually differentiating BW results between the analytical and FEM results in Fig. A.4.a and corresponding CB mode shape change from the analytical shape of Fig. A.2.a suggest some correlation between them. Mode shape of Fig. A.2.a is assumed implicitly in analytical effective stiffness calculations in Eqs. A.2-3. Thus, deviations of resonator or CB mode shapes in simulations from their assumed analytical counterparts lead to inconsistencies in terms of filter BW results. Again, CB mode shape shown in Fig. A.4.b clearly shows progressive change from the mode shape of Fig. A.2.a for increasing CB widths. Hence, the most consistent filter BW results between the analytical model and FEM estimates are obtained with thin CBs in which considerable similarity of resonator and CB mode shapes exists. Thus, resonator and CB mode shapes should also be taken as design parameters in addition to the conventional set of parameters given in Eqs. A.2-3. Furthermore, Eqs. A.2-3 become even less applicable for CB modeling when the length of a CB attains the same order as that of the resonator width. Thus, the CB analytical model given by Eqs. A.2-3 is only valid for very thin CBs ($w_c/w_r < 0.5$), whose lengths are only determined by the $\lambda/4$ condition.

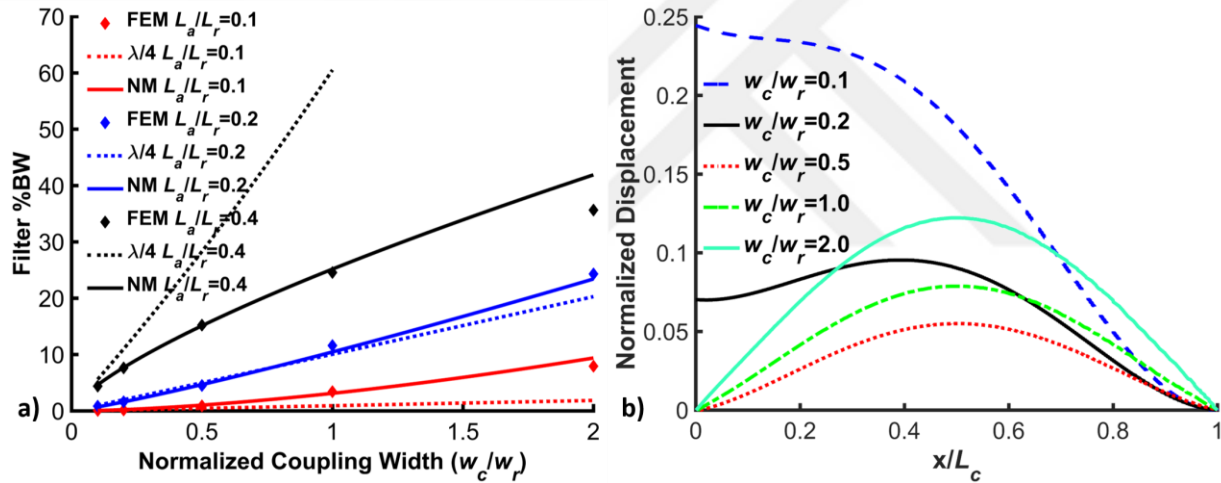


Figure A.4: Parameter space consisting of $0.1 < w_c/w_r < 2$, $0.1 < L_a/L_r < 0.4$ and $50 < L_r/w_r < 200$ is employed to build the numerical model for the benchmark study. Resonator: $1 \times 1 \times 50 \mu\text{m}$, CB: $w_c \times 1 \times 25 \mu\text{m}$. b) Evolution of the CB mode shape from shown in Fig. 2.a with respect to w_c provides an explanation for the limitation of the analytical model.

A proper analytical model is available only for a limited number of CBs with specific boundary conditions in the literature. Moreover, strict design window such as certain CB lengths also imposes limitations on resulting filter characteristics. Thus, more flexibility in filter design parameters provided by numerical CB modeling results in a significantly wider range of filter characteristics.

Alternative to the $\lambda/4$ model, a much more accurate description of a filter response such as filter f_0 and BW for any given resonator and CB can be obtained from simple numerical models. Numerical model developed using the following approach can increase the accuracy of existing analytical filter models in the literature. It can also be applied to complicated resonator-CB configurations whose analytical filter models are missing or too complicated to derive analytically. Thus, the main

contribution of this numerical filter design methodology is to link CB lumped parameters directly with CB and resonator dimensions for any filter configuration based only on FEM simulations.

The proposed numerical electromechanical filter design procedure can be itemized as follows:

1. Determine filter design parameters' range to form a parameter space. To this end, one needs to observe CB and resonator mode shapes with respect to investigated parameters by FEM modal analysis simulations. Simple numerical models can be built for a parameter space where moderate mode shape change for both filter components is observed.
2. Perform systematic FEM simulations in accordance with the established parameter space to collect filter f_0 and BW raw data with respect to filter dimensional parameters.
3. Construct a numerical model using filter raw data. The numerical model should provide f_0 and BW characteristics as a function of filter geometrical properties.
4. Derive the mechanical equivalent circuit of Fig. A.3.a for the overall filter. To this end, known resonator lumped parameters obtained through resonator modeling methodologies should be used together with outputs from the constructed numerical model.

As a benchmark study, the $\lambda/4$ -based analytical modeling is compared in Fig. A.4.a with the proposed FEM-based numerical model for second-order electromechanical filters of Fig. A.1.a. In accordance with the proposed numerical modeling approach, the parameter space is formed as follows: $w_c/w_r = 0.1-2$, $L_d/L_r = 0.1-0.4$, $L_r/w_r = 50-200$. CB lengths and heights are borrowed from previous values in the analytical modeling case. Next, systematic FEM simulations provide filter f_0 and BW raw data identical to discrete points representing FEM BW predictions in Fig. A.4.a. Simple linear relation of filter BW as a function of filter geometrical parameters is obtained as shown in Fig. A.4.a. The developed numerical model follows FEM BW and f_0 estimates closely even in the case of wider CBs attached closer to the resonator midpoint.

In the next section, we will apply the proposed numerical filter modeling approach to a specific filter architecture, which cannot be addressed by any analytical model available in the literature. This filter configuration includes CMs to provide mechanical coupling between resonators. Ability to deliver desired level of mechanical coupling by varying in-plane CM dimensions together with compactness of the structure accentuated at the nanoscale are the most appealing features of CMs.

3. A CASE STUDY: COUPLING MEMBRANE

The methodology outlined in the previous section will be applied to develop a numerical model for a filter consisting of CMs as shown in Fig. A.1.b. The use of a CM represents a significant expansion to the rather limited mechanical coupling toolkit at the nanoscale. Contrary to usual CBs of Fig. A.1.a, one of the side surfaces of each CM is fixed as in Fig. A.1.b. Thus, this boundary condition modification effectively sets the attachment location of a CM fixed at the end of resonators. Hence, for the development of a numerical model for this filter, the design parameter set is reduced to CM dimensions of w_c , h_c and L_c and resonator length of L_r as defined in Fig.

A.1.b. Almost all dimensional parameters are normalized by the resonator width, *i.e.* h_c/w_r , L_c/w_r and aspect ratio, $AR=L_r/w_r$. On the other hand, the CM width is normalized by the resonator length, *i.e.* w_c/L_r .

In this study, numerical modeling of second-order filters with CMs having length and width on the same order of its thickness as in Fig. A.1.b is targeted. Thus, as a first step of the modeling methodology, the parameter space is formed by considering effects of the model input parameters on CM and resonator mode shapes. Both in-phase and out-of-phase filter mode shapes are tracked. In FEM simulations, resonators with the size of $1 \times 1 \times AR$ ($w_r \times h_r \times L_r$) units are employed. Moreover, all filter dimensions can be scaled freely without any effect on filter characteristics.

In Fig. A.5.a, the resonator mode shape is plotted along its length with respect to the normalized CM width (w_c/L_r) for the filter out-of-phase mode. As the CM gets wider, the effect of the CM on the mode shape of the resonator becomes considerable. On the other hand, the CM mode shape is shown with respect to the normalized CM length (L_c/w_r) in Fig. A.5.b for the filter in-phase mode. There is a progressive change in the CM mode shape in Fig. A.5.b from the corresponding shape for the shortest CM as the length of the CM increases gradually. Remaining mode shapes of the CM and resonator such as resonator mode shape for the filter in-phase mode have lower sensitivity to investigated model parameter variations. As mentioned in the modeling methodology section, the reason behind extracting mode shapes of the filter components with respect to design parameters is to determine a proper parameter space that allows construction of simple numerical models by suppressing considerable mode shape changes. Thus, a parameter space should be optimized such that mode shape changes for the filter components lead to sufficiently accurate and simple numerical equations. According to these results, the width and length of the CM are chosen within the range of $w_c/L_r \leq 0.1$ and $L_c/w_r \leq 4$, respectively, to make the resulting equations simpler.

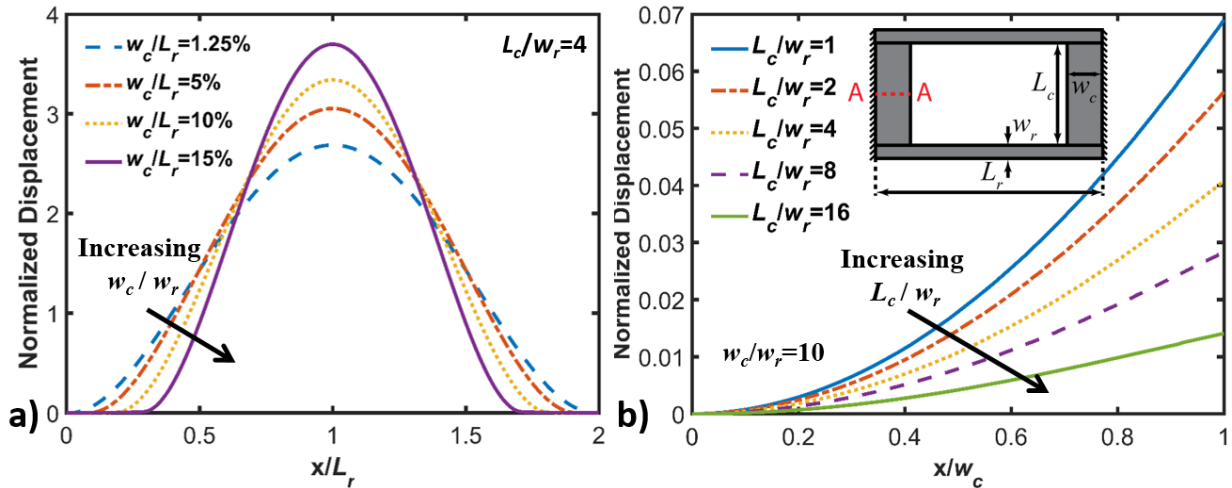


Figure A.5: Gradual increase in the CM width and length leads to progressive change for the mode shapes of (a) the resonator along its length and (b) CM along the A-A axis in the inset. Resonator: $1 \times 1 \times 200$, Membrane: $w_c \times 1 \times L_c$ units.

In order to simplify the derivation of the numerical model for the filter BW, the first part of the study assumes that CM height (h_c) is equal to resonator width (w_r). In compliance with the proposed modeling methodology, systematic FEM simulations are performed using the established parameter space to collect filter f_0 and BW raw data. Fig. A.6.a presents a representative result obtained from FEM modal analysis simulations. It demonstrates a linear relation between filter BW and normalized coupling width for different resonators lengths. Such linear relations are systematically obtained for different CM lengths within the parameter space of interest. FEM f_0 and BW raw data are used to build a numerical model that provides filter f_0 and BW as a function of filter geometrical parameters. Then, the coefficients of the general all-encompassing linear equation of Eq. A.4.a are determined from the extracted linear relations by a numerical fitting process.

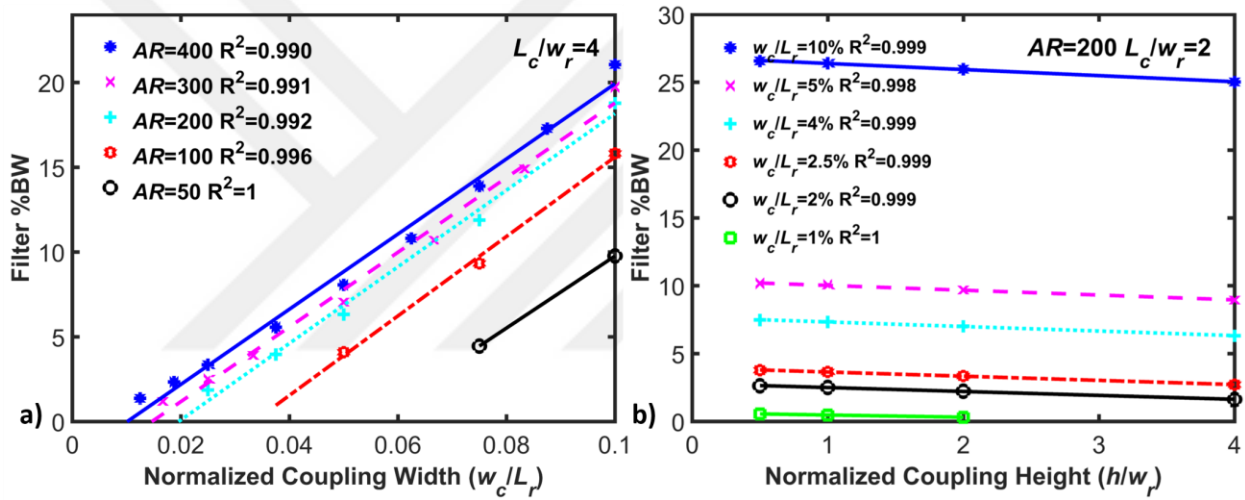


Figure A.6: Linear relations exist for the filter BW with respect to (a) normalized coupling width for various resonator ARs and (b) normalized coupling height for various normalized coupling widths according to FEM simulations.

$$\%BW = f(L_c/w_r, w_c/L_r, AR) = A_1(w_c/L_r) - B_1 \quad (A.4.a)$$

$$A_1 = 572AR^{-0.057}e^{-0.158L_c/w_r} \quad (A.4.b)$$

$$B_1 = -37(L_c/w_r)^2/AR + 194(L_c/w_r)/AR + 188AR^{-0.755} \quad (A.4.c)$$

BW values obtained through Eq. A.4 diverge from FEM results by less than 10% for the most part of the covered range. Inspection of Fig. A.6.a shows that the linear range becomes increasingly confined with decreasing resonator AR. Selection of smaller widths and longer lengths for the CM of Fig. A.1.b corresponds to an almost rigid CM especially for low AR resonators. In turn, such a membrane leads to effectively zero mechanical coupling between two adjacent resonators *i.e.* zero BW. In effect, the fixed surface of the CM shown in Fig. A.1.b seems to dominate the dynamic CM behavior. This phenomenon manifests itself as a significant deviation from the linear BW behavior shown in Fig. A.6.a resulting in increased BW errors between developed numerical model and FEM results. Thus, Eq. A.4 seems to be best applicable to filters comprising of resonators having ARs greater than 50.

From the fabrication perspective, it is practical to set the thicknesses of the CM (h_c) and of the resonator (h_r) identical to, such as the device layer thickness (h) of a silicon-on-insulator (SOI) wafer. However, the introduction of the overall filter thickness (h) as a filter design parameter can turn the numerical fitting process slightly more complicated. The dependence of the BW on the normalized thickness is also found linear as shown in Fig. A.6.b. Thus, the BW expression takes the form given in Eq. A.5 with the addition of the overall filter thickness parameter (h).

$$\%BW = f(L_c/w_r, w_c/L_r, AR, h/w_r) = -A_2(h/w_r) + B_2 \quad (\text{A.5.a})$$

$$A_2 = -12.2(L_c/w_r)/AR + 150.7AR^{-1.1} + 1917AR^{-2.28}(w_c/w_r - 5) \quad (\text{A.5.b})$$

The constant value (B_2) in Eq. A.5.a also depends on the model input parameters. However, it is far easier to extract B_2 using $h/w_r=1$ in Eq. A.4 rather than deriving an explicit relation for it. Thus, BW values are obtained through Eq. A.5 using B_2 values determined from Eq. A.4. The standard deviation of BW results from corresponding FEM data is less than 15%.

Integration of an electromechanical filter with the rest of electrical components in a system such as actuation/readout components and subsequent signal post-processing stages, and determination of the collective frequency spectrum can also be quite desirable. This can be achieved by using the mechanical equivalent circuit shown in Fig. A.3.a. In Fig. A.3.a, the CB is represented by the two independent impedance parameters of Z_{c1} and Z_{c2} . These two coupling element parameters representing all unknown parameters in Fig. A.3.a can be determined uniquely using two filter characteristics such as BW and f_0 for any filter design. Since the numerical equations are already established for the filter BW, the next key objective should be the determination of filter f_0 . Due to finite mass of CMs, the f_0 of the considered electromechanical filter of Fig. A.1.b depends on CM and resonator dimensions as set forth in Eq. A.6.

$$f_0 = f(L_c/w_r, w_c/L_r, AR) = A_3(w_c/L_r) + B_3 \quad (\text{A.6.a})$$

$$A_3 = 3e6 AR^{-2}(L_c/w_r)^{0.088AR^{0.1}} \quad (\text{A.6.b})$$

$$B_3 = 7.9e5 e^{-0.041(L_c/w_r)} AR^{0.007(L_c/w_r)-1.983} \quad (\text{A.6.c})$$

The shift in filter f_0 from the resonance frequency of identical resonators in a filter through finite-mass of a coupling element is ignored by the existing analytical filter modeling methodologies. However, Eq. A.6 is quite successful to predict the filter f_0 with errors less than 5% of FEM data within the parameter space of interest as shown in Fig. A.7. Progressive errors for filter f_0 with increasing AR is just an incidental result at the normalized CM length (L_c/w_r) plotted and not representative for remaining results at different CM lengths.

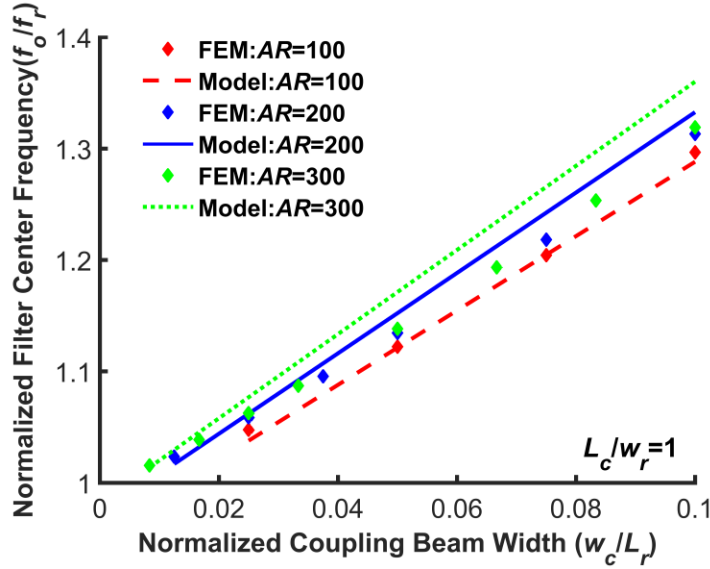


Figure A.7: Change in filter f_0 normalized to the standalone resonator resonance frequency with CM dimensions proves the necessity to model it in the examined CM case. CM: $w_c \times 1 \times 1$, Resonators: $1 \times 1 \times L_r$ units.

Thus, it is possible to predict filter f_0 and BW properties numerically based solely on filter geometry for an electromechanical filter. On the other hand, appropriate filter geometries can also be extracted for a desired combination of filter f_0 and BW. The proposed numerical modeling methodology is fulfilled by getting CM impedance parameters. The knowledge of filter f_0 and BW together with resonator lumped parameters can be converted to CM impedance parameters using the equivalent circuit in Fig. A.3.a. For example, the calculated mechanical impedance parameters of a CM are shown in Fig. A.3.a. Then, the equivalent mechanical circuit can be simulated with a circuit simulator to get the frequency spectrum of the filter as in Fig. A.3.b. Thus, determination of the transfer function of the filter enables a further system-level modeling, in which the rest of the actuation, readout and signal processing components are taken into account.

4. DISCUSSION

Number of resonators in any filter architecture can be increased at will. However, CMs modeled in this work with lengths of only a fraction of adjoined resonator length enable very large resonator density. Switching from horizontal to vertical stacks of resonators as shown in Fig. A.8.a seems instrumental to reach even higher resonator densities. In Fig. A.8.a, a vertical stack of three nanowires with w_r , h_r and L_r of 60 nm, 60 nm and 2 μm is shown. They are fabricated with CMs at their ends between two side electrodes. A gap of 500 nm between the Si NWs and electrodes is established. Nanowires are etched in a $\langle 100 \rangle$ Si wafer by employing a fabrication flow similar to the one described elsewhere [25]. The number of independent equations required to describe filter frequency spectrum characteristics increases proportionally with the number of resonators in a filter. The equivalent mechanical circuit of a series filter consisting of three identical resonators is shown in Fig. A.8.b. Presented numerical modeling methodology can be exploited to derive numerical equations for CM lumped-parameters.

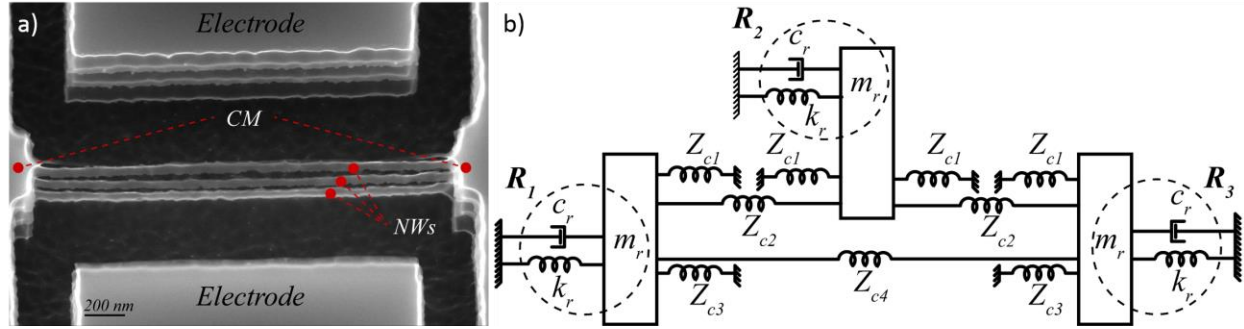


Figure A.8: a) A vertical stack of three resonators with CMs is used to constitute a filter. b) Each mechanical coupling for any resonator pair is modeled with three mechanical impedances in the equivalent mechanical circuit such as the one in Fig. A.3.a.

In FEM simulations, the effect of electrostatic spring softening by capacitive coupling to a side electrode and the effect of the residual stress on the resonance frequency are ignored, while they can be implemented easily for more rigorous analysis.

5. CONCLUSIONS

A numerical filter design methodology based on FEM modal analysis simulations is developed. Proposed numerical approach might be beneficial for electromechanical filters whose analytical models are either missing, too complex to derive or misleading in terms of filter characteristics such as filter f_0 or BW. This design methodology is applied to a specific second order filter where a CM is fixed at each end of resonators. Contrary to the conventional $\lambda/4$ or stiff CB models, filter BW and f_0 equations extracted through numerical fitting to FEM modal analysis simulation data are quite satisfactory within the parameter space of interest with errors less than 15%. Thanks to lithographically-defined in-plane CM dimensions, CM provides a flexible mechanical coupling scheme. The compactness of this filter structure due to short CMs together with connecting all adjacent or non-adjacent resonators by common CMs at their ends represent the innovative aspect of utilizing CMs. Considering limited mechanical coupling options at the nanoscale, employment of CMs enables high-density resonator stacks having desired level of mechanical coupling at the nanoscale.

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APPENDIX B: IN-PLANE NUMERICAL COUPLING MODELING

In-plane Electromechanical Filter Numerical Modeling

Y. Kilinc ^{a, 2}, B. E. Alaca ^{a,b}

^a Dept. of Mechanical Engineering, Koc University, Rumelifeneri Yolu, Sariyer 34450 Istanbul, Turkey

^b Surface Science and Technology Center (KUYTAM), Koc University, Rumelifeneri Yolu, Sariyer 34450 Istanbul, Turkey

Abstract

Modeling of in-plane electromechanical filters is investigated by drawing contrast between filters featuring in-plane or out-of-plane flexural mode resonators. Analytical coupling beam modeling used to calculate its lumped parameters in case of out-of-plane filters is found inapplicable for in-plane filters. However, coupling beam is still modeled with a general T network of mechanical impedances numerically. Numerical modeling is implemented by exploiting filter equivalent circuit and finite element modeling (FEM) modal analysis. In the mechanical circuit of a generic second-order in-plane filter, transformer turn ratio and filter bandwidth are used to model coupling beam equivalent stiffness with respect to resonator aspect ratio and coupling beam width. Resonator mode shape change with respect to coupling location is addressed by adopting rigid anchor assumption at a coupling location. Moreover, the first flexural mode shape is assumed for either segment of constituent resonators split at the coupling location. Thus, in-plane electromechanical filters are successfully modeled with the knowledge of bandwidth and transformer turn ratio parameters without any need for further FEM simulations. Thanks to ease of fabrication of in-plane filters at a common lithography level with actuation/readout electrodes, it is shown that in-plane coupling seems to be best suited for realizing filters having high bandwidths.

² Corresponding author. Tel.: +90 212 338 1727; fax: +90 212 338 1548.
E-mail addresses: ykilinc@ku.edu.tr (Y. Kilinc), ealaca@ku.edu.tr (B. E. Alaca).

1. Introduction

Introduction of micro/nanoelectromechanical systems (MEMS/NEMS) resonators as a compromise between crystal and all-electrical counterparts paved the way to on-chip, miniaturized, high quality factor (Q) and high-frequency applications with CMOS compatible batch processing capability. Their resonance behavior has been subject to a variety of characterization studies regarding resonator geometry [1], actuation/readout methods [2], mode shapes and materials [3].

Resonance coupling is investigated rigorously in the literature for MEMS resonators [4]. Resonator coupling represents a variety of advantages including improvements in device properties such as increased sensitivity to perturbations [5] and reliability [6]. Moreover, completely new functionalities such as signal filtering [7] and mixing [8] can be realized by employment of interconnected resonators together.

An electromechanical filter is effectively a signal engineering device composed of mechanical resonators and coupling elements [9]. The simplest series, out-of-plane, second-order electromechanical filter structure is depicted in Fig. B.1.a. Two identical fixed-fixed beam resonators with the width, height and length of w_r , h_r , L_r respectively are coupled mechanically through a flexural-mode coupling beam (CB). Connecting resonator pairs with a network of CBs results in filter modes proportional to number of resonators in a filter. Electrostatic transduction between the resonators and electrodes in Fig. B.1.a is used to induce and sense mechanical vibrations. Resulting mode shapes of the electromechanical filter of Fig. B.1.a is shown in Fig. B.1.b. Lowest frequency filter mode consisting of resonators vibrating in the same direction together is called in-phase filter mode. Besides, each resonator moves in the opposite direction of neighboring resonators in case of the out-of-phase mode. These modes correspond to distinct peaks in the associated filter frequency spectrum.

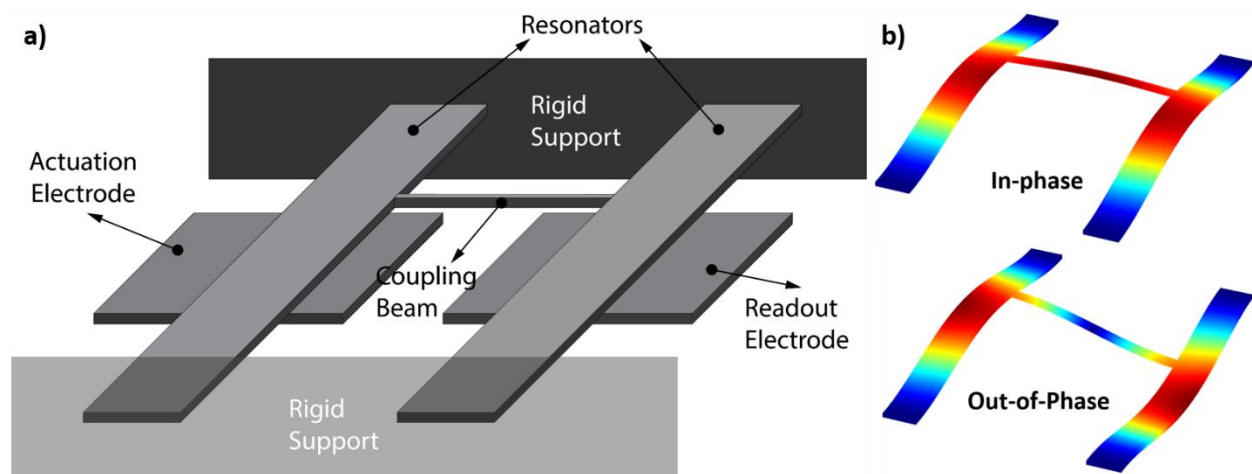


Figure B.9: a) Second-order out-of-plane electromechanical filter together with transduction electrodes b) associated in-phase and out-of-phase filter mode shapes

Let us consider any electromechanical filter consisting of an arbitrary number of identical resonators. While the filter bandwidth (BW) is centered around the common resonance frequency of resonators (f_0), BW is determined by CB equivalent stiffness (k_c) according to Eq. 1.

$$BW = f_0 \frac{k_c}{k_{rc}k_{12}} \quad (1)$$

where k_{rc} and k_{12} are resonator stiffness at a coupling location and normalized coupling coefficient for a given filter type, respectively [10]. Thus, it seems that coupling stiffness is the only parameter that can be set to get a desired BW for a given filter architecture and CB attachment location. However, further insight can be acquired by realizing that a certain mode shape is always assumed implicitly in any analytical effective stiffness calculations. Deviations of actual resonator or CB mode shapes from analytically assumed counterparts correspond to inconsistencies in terms of calculated and realized filter BW results. Thus, in cases where significant filter mode shape dependence on filter architecture exists, actual resonator and CB mode shapes should be taken into account as filter design parameters as well. Furthermore, any analytical CB modeling scheme is only valid for a parameter design space leading to relatively fixed filter mode shapes. Fortunately, variation of filter in-phase and out-of-phase mode shapes seems considerably limited in case of out-of-plane filter flexural modes of Fig. B.1.b. This is especially true when a thin CB is employed.

Although the most common resonance mode in the literature for resonators in an electromechanical filter is the first out-of-plane flexural mode, in fact any resonance mode can be accentuated by proper selection of transduction mechanism, electrode placement and signal phasing [11]. For example, simple displacement of the electrodes from underneath the resonators as in Fig. B.1.a to the outer side of each resonator as in Fig. B.2.a results in excitation of the first in-plane flexural mode. However, this simple modification in the filter architecture leads to drastic changes in filter frequency spectrum characteristics such as filter f_0 and BW . This might be expected actually by considering dramatic resonator and CB mode shape change for the in-phase and out-of-phase filter modes as shown in Fig. B.2.b.

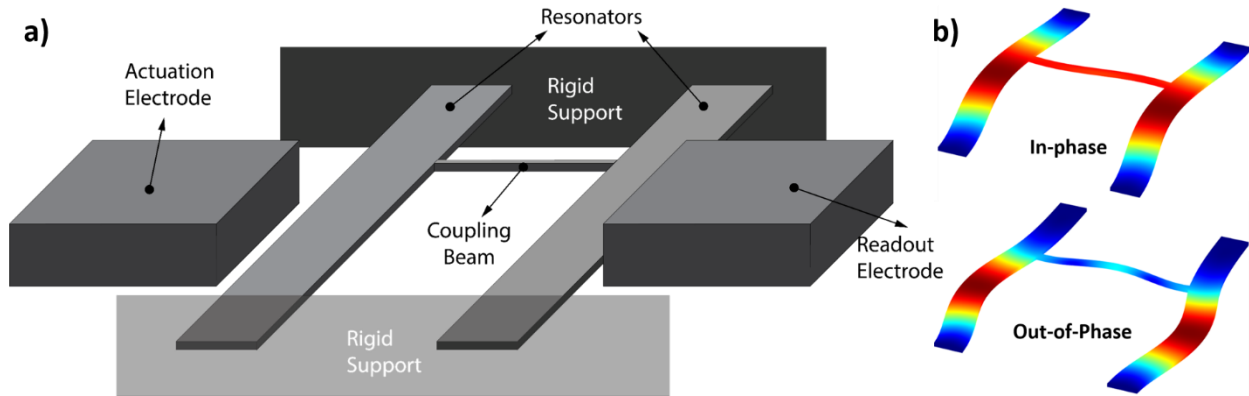


Figure B.10: a) Perspective view schematic of a second-order in-plane electromechanical filter together with actuation/readout electrodes b) resulting filter mode shapes are significantly different from the out-of-plane filter counterparts.

A clear distinction between electromechanical modeling of flexural beam based in-plane and out-of-plane electromechanical filters is the dependence of resonator mode shape on CB attachment location. Therefore, actual filter mode shape should be considered while determining resonator equivalent stiffness at a given coupling location for flexural beam based in-plane filters. Although flexural beam based in-plane series MEMS electromechanical filters are employed sporadically in the literature, development of a filter model has not been accomplished yet to the best of the authors' knowledge. Determining filter equivalent circuit using such a model leads to integration of an electromechanical filter with the rest of electrical components in a system to get the collective frequency spectrum.

In the remainder of the manuscript, contrast between electromechanical modeling of CBs of in-plane and out-of-plane filters is highlighted to prove that in-plane filter CB can be only modeled numerically using FEM modal analysis. To this end, varying mode shapes of the in-plane filter components with respect to filter design parameters are demonstrated. At the end, modeling of the in-plane electromechanical filter of Fig. B.2 is implemented by given BW and transformer turn ratio data.

2. Modeling of In-plane Series Filters

Although the idea of mechanical coupling and associated introduction of collective modes are interesting, the addition of a CB into the overall picture necessitates a proper CB design for a successful device implementation. When the CB mass is on the same order of the resonator mass unlike macroscale filters, this mass has to be taken into consideration, complicating CB design [12]. Electromechanical modeling of a single MEMS/NEMS resonator is well-established in the literature for various resonator boundary conditions [12-14]. However, these techniques cannot be borrowed to model coupling and support beams directly. In the literature, an analytical approach known as quarter-wavelength ($\lambda/4$) modeling is employed to design coupling and support beams [10, 11]. The CB of Fig. B.1 is modeled with the $\lambda/4$ modeling as in Fig. B.3.a. Fig. B.3.a illustrates a CB of the length, width and height of L_c , w_c and h , respectively, with guided boundary conditions. It is subject to mechanical forces of f_i resulting in velocity responses of $\dot{x}_i$. A general acoustic transmission line model consisting of a T-network of mechanical impedances shown in Fig. B.3.b was proposed to model equivalent mass (m_c) and stiffness (k_c) of the CB of Fig. B.2.a. [10]. CB dimensions and filter operation frequency (ω) are used to calculate CB mechanical impedances of Z_{ca} , Z_{cb} and Z_{cc} .

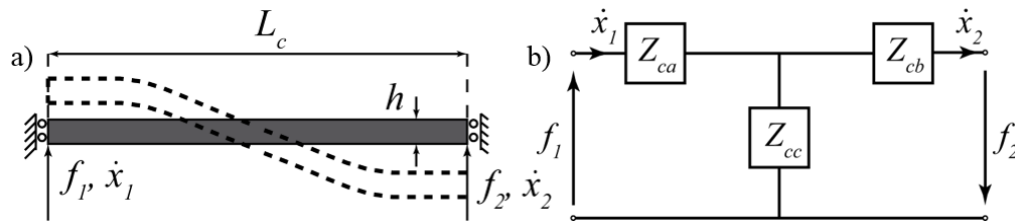


Figure B.11: a) CB of Fig. B.1 with guided boundary conditions b) a T-network of mechanical impedances is used to model the CB

Modeling of in-plane series electromechanical filters mainly consists of determining CB and resonator stiffness at a coupling location in accordance with Eq. 1. However, the $\lambda/4$ CB modeling methodology [12] cannot be applied to in-plane filters featuring the CB of Fig. B.2 which has a new set of boundary conditions shown in Fig. B.4.a. Nonetheless, this CB can still be modeled with the acoustic transmission line of Fig. B.3.b when a CB length is less than an eighth of the acoustic wavelength ($L_c \leq \lambda/8$) corresponding to a given filter operation frequency [12]. Moreover, the electromechanical filter of Fig. B.3.a can be modeled with the lumped-parameter equivalent mechanical circuit of Fig. B.4.b. In Fig. B.4.b, each resonator represented with equivalent mass (m_r), damping (c_r) and stiffness ($1/k_r$) elements undertakes half CB mass [12].

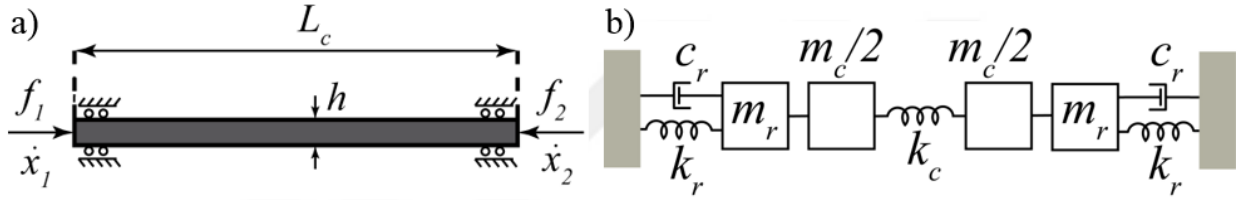


Figure B.12: a) A new set of boundary conditions for the CB of the in-plane filter of Fig. B.2.a necessitates a new CB model. b) The equivalent lumped-parameter mechanical model for the in-plane filter of Fig. B.2.a.

Complete equivalent mechanical circuit together with transformers with a turn ratio of η_c used to model mechanical impedance transformations between each resonator and CB is presented in Fig. B.5. For the sake of simplicity, equivalent damping parameter (c_r) is removed from the representation of resonators in the following filter analysis. This simplification can be justified as follows. Accurate determination of an equivalent damping parameter in lumped-parameter resonator modeling requires a Q measurement and very high Q s of MEMS/NEMS resonators are commonplace. As a result, equivalent mass and stiffness parameters for any resonator can be determined easily at any coupling location by assuming a resonator mode shape in addition to physical and material properties [12].

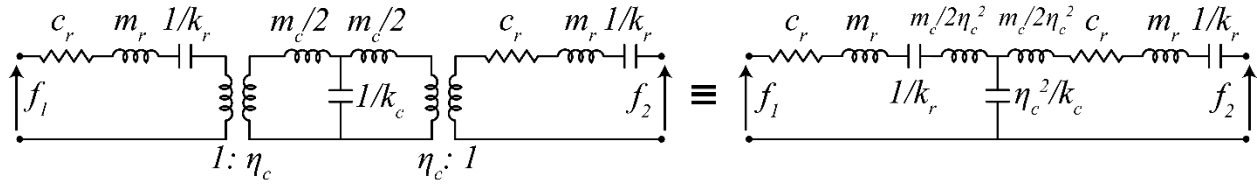


Figure B.13: Complete equivalent mechanical circuit consisting of mechanical impedance transformers in addition to resonator and CB lumped-parameters can be simulated conveniently with a circuit simulator

Modal analysis simulations are performed to evaluate the evolution of resonator and CB mode shapes with respect to filter design parameters. Modal analysis simulations are implemented using a commercial finite element modeling (FEM) software using 3D free-tetrahedral mesh elements. In FEM simulations, the effect of electrostatic spring softening by capacitive coupling to a side electrode and the effect of residual stress on resonance frequency are ignored while they can be incorporated easily for more rigorous analysis. Isotropic silicon with the mass density of 2329

kg/m³ and modulus of elasticity of 170 GPa is employed as the filter structural material. CB lengths are selected to match to those of CBs for out-of-plane series filters. $\lambda/4$ modeling calculations result in CB lengths of approximately half the resonator length. Resonators having aspect ratios (AR) i.e. resonator length over resonator width (L_r/w_r) in the range of 50-300 are examined. From the fabrication perspective, it is quite practical to set the thicknesses of a CB (h_c) and resonators (h_r) identical to such as the device layer thickness (h) of a silicon-on-insulator (SOI) wafer. Moreover, filter thickness is fixed to resonator width ($w_r/h_c=w_r/h_r=1$) for convenience. Hence, all in-plane filter dimensions can be scaled freely without any effect on filter characteristics.

Figs. B.6 and 7 demonstrate resonator and CB mode shapes respectively with respect to coupling location (L_a) along the resonator length. Mode shape dependence on coupling location is emphasized for both resonator and CB in case of the out-of-phase filter mode. Thus, Figs. B.6 and 7 underline the impossibility of assuming a specific mode shape for neither a resonator nor a CB to calculate equivalent mass and stiffness analytically.

Careful inspection of the resonator mode shapes shown in Fig. B.6.b-c for the out-of-phase filter mode reveals that the resonator mode shape can be approximated such that as if the CB acts as an anchor at the considered coupling locations. Thus, the resonator can be split at a coupling attachment point to two separate clamped-clamped beam segments. Moreover, the assumption for each resonator segment having the fundamental flexural mode shape might be good enough idea to overcome varying resonator mode shape issue. Interestingly, since equivalent stiffness of a flexural mode resonator is proportional to its length, it becomes essentially identical for both in-phase and out-of-phase filter modes at a coupling location. Treating a CB as a rigid anchor at a coupling location for the filter out-of-phase mode can be justified if one considers high stiffness of CBs having the axial force and boundary conditions of Fig. B.4.a. Hence, equivalent mass and stiffness parameters (m_r and k_r) of a resonator become fixed irrespective of coupling location (L_a) using this approach. However, since the assumption of a CB as an anchor leads to infinite resonator stiffness at a coupling point, resonator equivalent mass and stiffness parameters shown in the equivalent mechanical circuit of Fig. B.5 are calculated at a very small distance from coupling points such as $w_r/128$.

Thus, remaining unknown model parameters to complete the mechanical circuit of Fig. B.5 are equivalent mass (m_c) and stiffness (k_c) of CB and mechanical transformer turn ratio (η_c). Mechanical transformer turn ratio is calculated from resonator stiffness ratio at a coupling location (k_{rc}) and resonator midpoint (k_{rm}) by $\eta_c = \sqrt{k_{rc}/k_{rm}}$. Fortunately, analytical turn ratio calculation is quite accurate for out-of-plane filters. Since the dependence of resonator mode shape on CB is limited especially in case of very thin CBs. However, sensitivity of actual resonator mode shape on coupling location in Fig. B.6 implies very different case for in-plane filters.

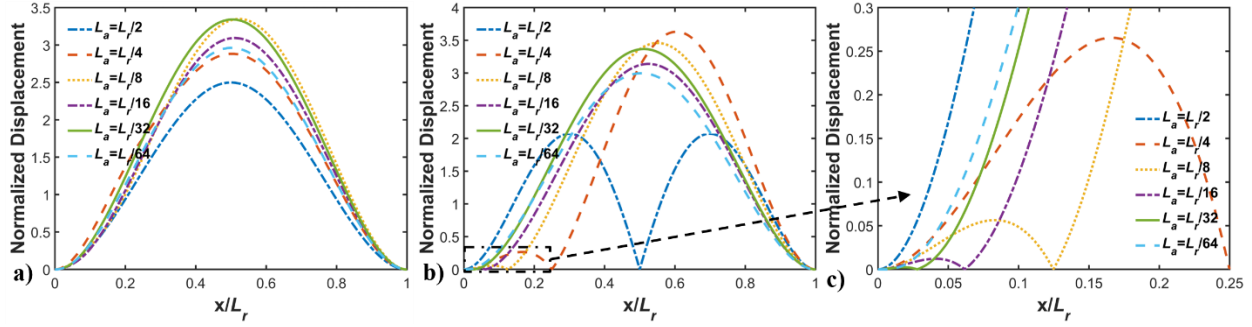


Figure B.14: In FEM modal analysis simulations, coupling location is swept from the middle of a resonator ($L_r/2$) towards its anchor ($L_r/64$). Resonator mode shapes are demonstrated for the filter a) in-phase and b) out-of-phase modes. c) Close-up results for the out-of-phase filter mode. Resonator: $1 \times 1 \times 200$ units ($w_r \times h_r \times L_r$), CB: $1 \times 1 \times 100$ units ($w_c \times h_c \times L_c$).

Unlike the CB in Fig. B.1 for out-of-plane filters, there is no analytical CB model in the literature for the CB of Fig. B.2 with the boundary conditions of Fig. B.4.a. Consideration of varying CB mode shape with respect to coupling location as shown in Fig. B.7 suggests employment of a numerical approach. A numerical modeling approach is used to determine CB lumped parameters and mechanical transformer turn ratio using FEM modal analysis simulations as follows.

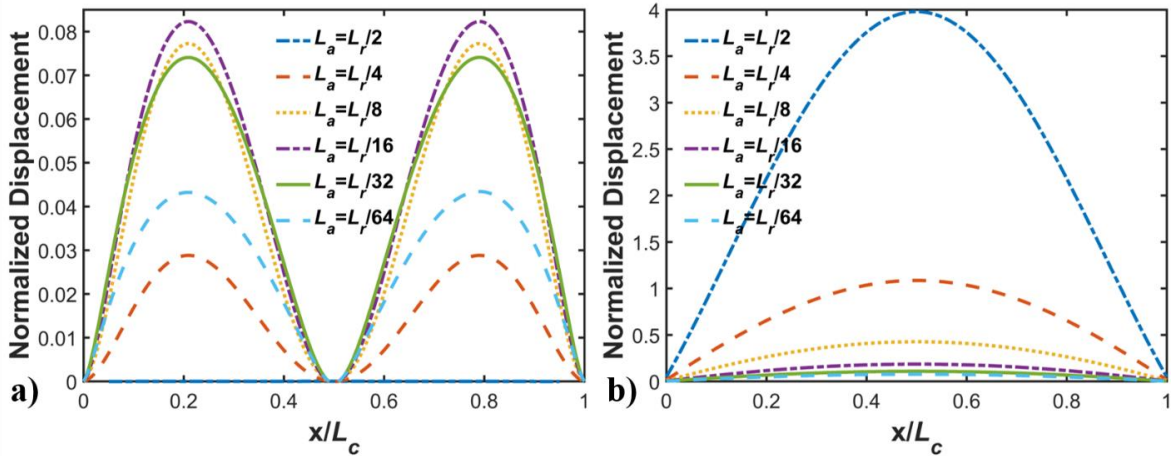


Figure B.15: CB mode shapes for the filter a) in-phase and b) out-of-phase modes for various coupling locations. Resonator: $1 \times 1 \times 200$ units ($w_r \times h_r \times L_r$), CB: $1 \times 1 \times 100$ units ($w_c \times h_c \times L_c$).

Some electromechanical filter frequency spectrum characteristics such as filter BW and f_0 can also be extracted from a simple FEM modal analysis simulation if filter Q is assumed very high. Then, simulation of the equivalent mechanical circuit of the second-order electromechanical filter of Fig. B.5 via a circuit simulator can be performed to match to a given filter BW and f_0 pair. In this way, unique CB equivalent mass and stiffness parameters corresponding to a specific resonator and CB layout of Fig. B.2 can be determined. Moreover, mechanical transformer turn ratio can be found with respect to coupling location by using specified CB and resonator mechanical lumped parameters for a given resonator and CB pair.

3. Results & Discussions

Mechanical transformer turn ratio (η_c) normalized to its value at $L_r/3$ is determined using the described numerical approach. Fig. B.8 summarizes the results with respect to coupling location normalized to resonator length *i.e.* L_a/L_r and resonator AR. Turn ratio is found independent from resonator AR as long as AR of the short segment of a resonator split at a coupling location is greater than 10. Moreover, less than 15% variation in transformer turn ratio and filter BW is obtained in case of short resonator segments having AR of 6. Transformer turn ratio and BW data from Fig. B.8 corresponding to a specific in-plane filter configuration can be utilized to obtain filter frequency spectrum using the equivalent mechanical circuit of Fig. B.5.

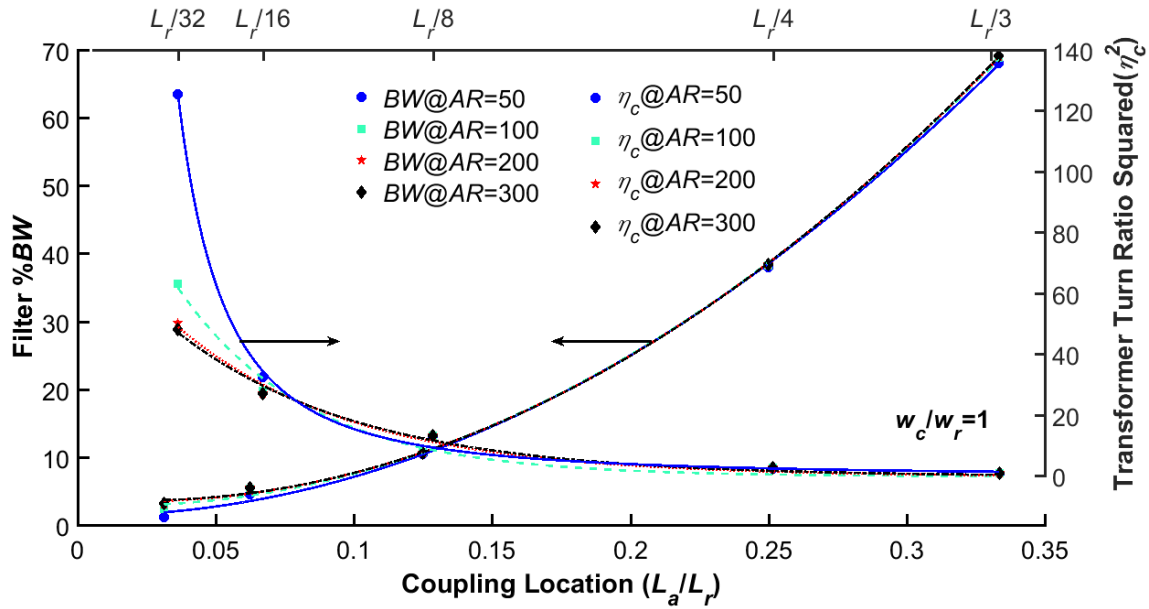


Figure B.16: Transformer turn ratio and filter BW data can be combined to extract CB lumped stiffness parameter to get filter frequency spectrum using the equivalent mechanical circuit of Fig B.5.

Lithographically-defined CB width is a convenient design parameter to realize filter banks with various filter BWs on a same die for out-of-plane electromechanical filters. On the other hand, the effect of CB width normalized to resonator width (w_c/w_r) can also be investigated in case of in-plane filters.

The complete mechanical circuit of Fig. B.5 shows that lumped-parameter CB stiffness (k_c/η^2) also depends on mechanical turn ratio. Hence, any possible mechanical turn ratio change with respect to normalized resonator width should also be taken into account. Since resonator mode shape is assumed above for each resonator segment, mechanical turn ratio will be determined indirectly in a different way from the case of out-of-plane filters. Numerically determined CB stiffness values for a given resonator and CB pair at different coupling locations is compared to extract mechanical turn ratio. Fig. B.9 presents transformer turn ratio with respect to coupling location for in-plane filters having various normalized CB widths.

Interestingly, normalized CB width within the range of 0.2-1.0 seems to affect mechanical turn ratio as shown in Fig. B.9. Sensitivity of mechanical turn ratio to normalized CB width increases as coupling location moves towards resonator anchors. This result might be associated with deficiencies of the employed numerical model from actual FEM. For instance, the existence of a rigid anchor at a coupling location is assumed above to derive resonator lumped parameters at that coupling location. A decrease in CB lumped stiffness by selecting smaller normalized CB widths or greater turn ratios may compromise this assumption. In addition, the flexural mode shape assumed for smaller resonator segments deviates increasingly from actual FEM counterparts as coupling location approaches a resonator anchor. Thus, the resulting complex relationships in Fig. B.9 between CB width, transformer turn ratio and filter BW parameters are obtained to compensate these approximations by matching to FEM simulations. The variation of transformer turn ratio with normalized CB width is ignored in the analytical filter modeling for out-of-plane filters by employing only very thin CBs.

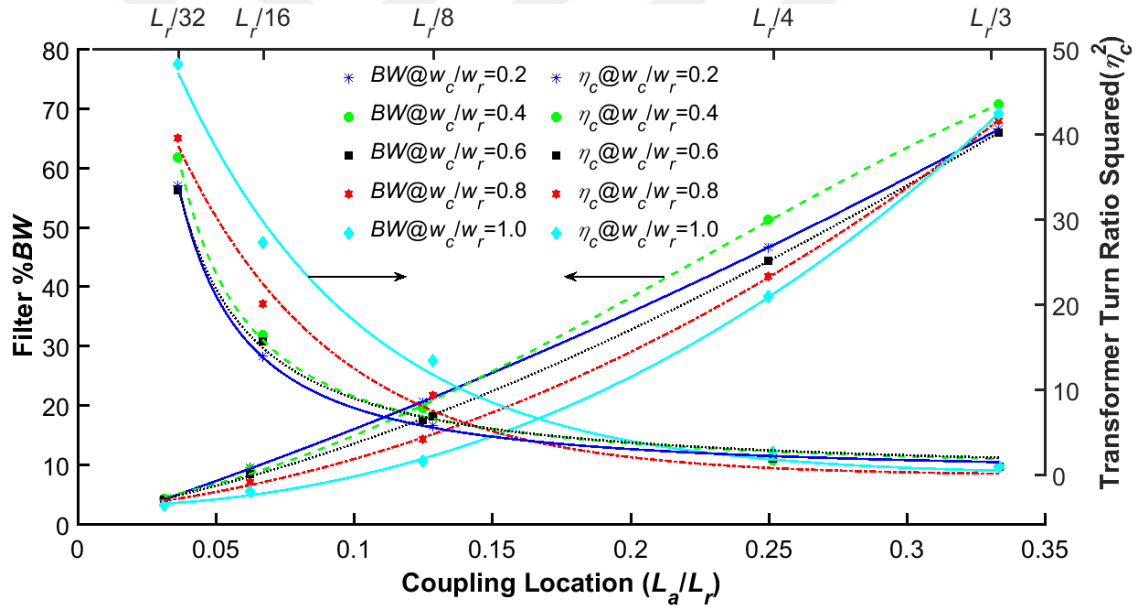


Figure B.17: Transformer turn ratio can be employed to calculate either in-plane filter BW or CB equivalent stiffness from the equivalent circuit of Fig. B.5.

Thus, it is possible to determine CB lumped stiffness in Fig. B.5 numerically from filter BW and transformer turn ratio data taken from Fig. B.9 for any in-plane filter geometry of Fig. B.2 since resonator lumped parameters are already calculated by assuming fundamental flexural mode shape for each resonator segment. As a result, Fig. B.9 is enough to design the in-plane filter of Fig. B.2 for the considered parameter space of interest.

According to Fig. B.9, this in-plane filter architecture seems to be best suited for realizing high filter BWs. Planar fabrication of filter components with actuation/readout electrodes using a common lithography mask presents an additional advantage for the in-plane filter of Fig. B.2. Modeling approach outlined in this work can be conveniently extended to higher order in-plane electromechanical filters. In addition to higher-order filters, Fig. B.10 demonstrates a composite

filter design where parallel and series resonator stacking coexist. In Fig. B.10, two vertical stacks of four clamped-clamped beams are coupled at their ends with common coupling elements. Then, these vertical stacks are bridged with a coupling beam from vertical coupling elements to realize a series in-plane electromechanical filter. Such filters can be fabricated from the device layer of a SOI wafer together with actuation/readout electrodes to accommodate electrostatic or piezoresistive readout. Advantages of such a design include providing readout signal improvement proportional to number of resonators in a vertical stack and more reliable filter operation by compensating any improperly fabricated resonator by other resonators.

When CB equivalent mass in Fig. B.5 becomes comparable to resonator equivalent mass, filter f_0 becomes no longer centered around common resonance frequency of resonators. Thus, as a CB gets wider and coupling location approaches resonator midpoint, filter f_0 extracted from FEM simulations diverges from fundamental flexural resonance frequency of a standalone fixed-fixed beam. However, these f_0 variations are less than 10% for the examined parameter space of interest.

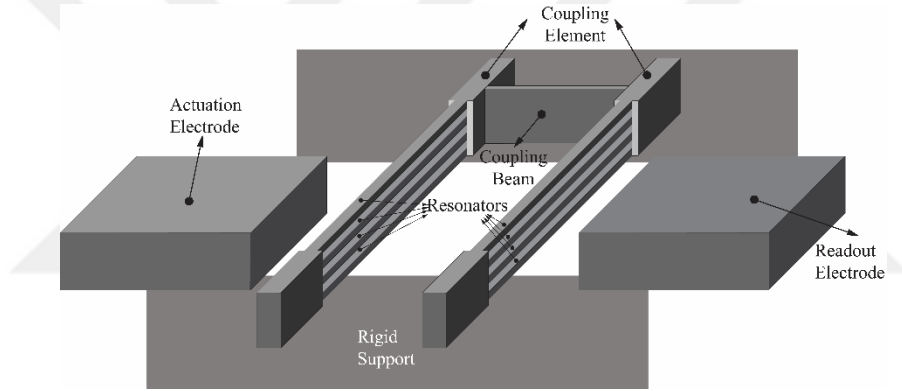


Figure B.18: In a stark contrast to commonplace horizontal resonator stacking in a parallel fashion, vertical stacking can be employed to reduce resonator motional resistance and phase noise, and increase device reliability for in-plane electromechanical filters.

4. Conclusions

Modeling of in-plane electromechanical filters differs from out-of-plane counterparts significantly. Since resonator and CB mode shapes are determined to vary considerably depending on coupling location and CB itself. Hence, the analytical $\lambda/4$ model used to design lumped-parameter CB stiffness for out-of-plane filters is not applicable for in-plane filters. However, CB is still modeled with a T network of mechanical impedances. Transformer turn ratio is found independent from resonator AR if AR of short segment of a resonator split at a coupling location is greater than 10. Due to substantial resonator mode shape dependence on coupling location, rigid anchor assumption at a coupling location is utilized to calculate resonator lumped parameters. Moreover, the effect of normalized CB width over the range of 0.2-1.0 on turn ratio and filter BW is investigated and related to utilized numerical model approximations.

As a result, electromechanical modeling of the in-plane electromechanical filter of Fig. B.2 is implemented with the knowledge of BW and transformer turn ratio data taken from Fig. B.9

without any need for further FEM simulations. Similar to out-of-plane filters, filter center frequencies are found to diverge less than 10% of standalone resonator natural frequencies.

Acknowledgements

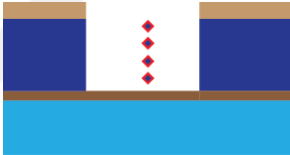
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APPENDIX C: FABRICATION FLOW

Step	Process description	Cross-section after process
0	✓ Wafer Cleaning • Full RCA (RCA1+RCA2) • HF ✓ n^{++} doping • 1 μm SOI device layer • $1\text{e}20\text{ cm}^{-3}\text{P}$ doping ✓ Wafer Annealing • $t=60\text{ min}$ at $T=1000\text{ }^{\circ}\text{C}$ ✓ Deglazing • Plade Reclaim Wetbench,	
1	✓ Metal Alignment Mark Formation • PMMA/PMMA coating & e-beam Lithography • E-beam Evaporation ○ 5 nm Ti adhesion ○ 50 nm Pt deposition • Lift-off ✓ PR Coating for Dicing • 2 μm thick PR	
2	✓ Wafer Dicing ✓ PR Removal ✓ Metal Deposition • PMMA/PMMA coating & e-beam Lithography • E-beam Evaporation ○ 5 nm Ti adhesion ○ 50 nm Pt deposition	
3	✓ Lift-off	

4	✓ <i>ZEP coating & E-beam Lithography</i>	n⁺⁺Si Si BOX Pt ZEP 
5	Dry Etch & E-beam Resist Removal Uniform NW Vertical Stack	n⁺⁺Si Si BOX Pt 
6	✓ <i>Dry Oxidation</i> 20 or 50 nm	n⁺⁺Si Si BOX Pt SiO2 
7	✓ <i>HF Vapour Etch</i>	n⁺⁺Si Si BOX Pt 