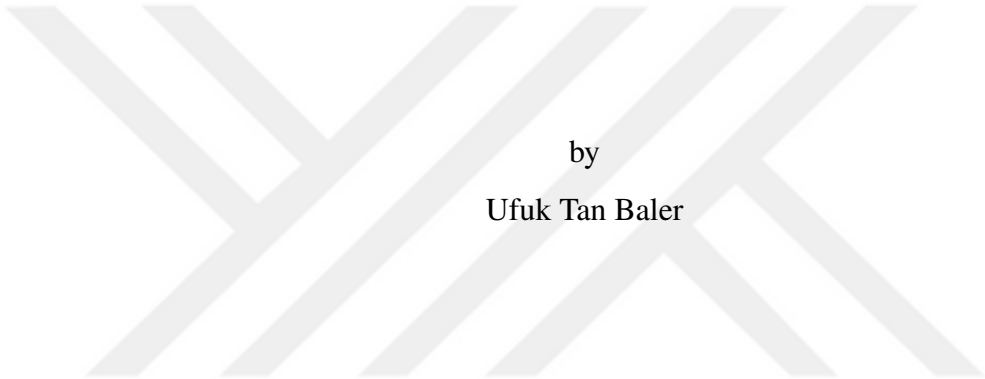


COMPUTATIONAL DYNAMIC ANALYSIS OF THE LAYERED PIEZOELECTRIC
SURFACE ACOUSTIC WAVE SENSORS FOR MASS SENSITIVITY IN LIQUIDS



by
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SURFACE ACOUSTIC WAVE SENSORS FOR MASS SENSITIVITY IN LIQUIDS

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ABSTRACT

COMPUTATIONAL DYNAMIC ANALYSIS OF THE LAYERED PIEZOELECTRIC SURFACE ACOUSTIC WAVE SENSORS FOR MASS SENSITIVITY IN LIQUIDS

Surface acoustic waves (SAWs) actuated by the inter-digital-transducers (IDT) on piezoelectric substrates are used in sensor technology. The configurations of IDT are resonator or delay-line, for which the responses show different dynamics. When a thin film is sputtered on the substrate/IDT combination, Love SAW mode is observed depending on the material selection. In this thesis we focus on Love SAW mode, which is mechanically feasible for detecting chemical agents in liquid environments. The manufacturing of these sensors should be done under very expensive equipment and meticulous operation. Setting the experimentation setup for testing also affects the microelectronic device reliability of the manufactured sensors due to pyroelectricity of the substrates. While testing, melting of the IDT material may occur due to high resistivity at some local regions. Not only that, but also the assessment of the dynamics of the waves requires specialized instruments, which might be inaccessible. Under these circumstances a robust computational workflow of the sensors might ease the overhead, and give invaluable data that can be achieved by just using a computer. Under this context, a computational analysis guideline is proposed using libre and open-source software. The goal of the guideline is to generate data to be analyzed towards making a reliable sensor device under given some design constraints. The responses of both IDT configurations shows different dynamics, yet the measure of success is set to an optimum layer thickness which gives an optimum mass sensitivity for both of them. Development of the guideline is started with modeling a simple thickness-shear mode problem. Developed FEniCS code is applied to reveal dispersive characteristics of a sensor through EVP results used in a postulated mass sensitivity calculation. Computed eigenfrequencies show close agreement with the experimental resonance frequencies. An optimum thickness is obtained to be used in transient solution for both the RVE and mock-up sensor geometry to analyse the displacements and electrical potential variables.

ÖZET

KATMANLI PİEZOELEKTRİK YÜZEY AKUSTİK DALGA SENSÖRLERİN HESAPLAMALI DİNAMİK ANALİZİ

Sensör teknolojisinde kullanılan yüzey akustik dalgalar (YAD) piezoelektrik alttaşları üzerinde bulunan ara-dijital-trandüserlerin (ADT) tahrik etmesi sonucu oluşur. ADT düzenleri farklı dinamikler gösterecek biçimde rezonatör veya gecikmeli-hat olabilir. Alttaş/ADT düzeninin üstüne püskürtme yöntemi ile üretilen ince katman sayesinde, kullanılan katmanın ve alttaşın malzemesine bağlı olarak Love dalga kipi gözlemlenir. Bu tezde sıvı ortamlarda kimyasal maddelerin tespit edilmesinde mekanik olarak elverişli olan Love YAD'ı incelenmektedir. Bu sensörlerin imalatı pahalı ekipmanlar ve titiz işçilik gerekmektedir. İmal edilmiş sensörlerin testleri için deneysel düzeneklerin kurulumları sırasında alttaşların piroelektrik özelliğinden kaynaklı olarak mikroelektronik cihaz güvenilirliğinin olumsuz etkilendiği görülmektedir. ADT malzemesi test sırasında olası yüksek direnç bölgelerinde eriyebilir. Ek olarak oluşan dalgaların dinamik davranışı erişimi zor olan özel aletler gerektirebilir. Bahsedilen şartlar altında sadece bir bilgisayarda çalışan hesaplamalı bir iş akış, oluşabilecek yükleri hafifletebilir ve değeri yüksek veri sağlayabilir. Özgür ve açık-kaynak yazılımlar kullanılarak bu bağlamda bir hesaplamalı analiz yönergesi önerilmiştir. Yönergenin amacı belirli tasarım kriterlerine uygun güvenilir bir sensör üretimine yönelik veri sağlamaktır. Bahsedilen iki ADT düzeni farklı dinamik yanıtlar göstermesine rağmen başarı ölçütü her ikisi için de optimum kılavuz katman kalınlığıdır. Yönergenin geliştirilmesi basit bir kalınlık-kesim titreşim kip problemiyle başlatılmıştır. Geliştirilen FEniCS kodu bir sensörün dağılım karakterinin ortaya çıkması için öne sürülen kütle duyarlılığı hesabını özdeğer probleminin çözümleriyle beraber kullanmıştır. Hesaplanan özfrekanslar deneysel rezonans frekanslarıyla uyumlu sonuçlar vermiştir. Temsili hacim elemanın (THE), kesit, ve model sensör geometrilerinin zamana bağlı deplasman ve elektrik potansiyel değişkenlerinin analiz edilebilmesi için bir optimum katman kalınlığı bulunmuştur.

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LIST OF SYMBOLS/ABBREVIATIONS

$\underline{e}_i$	Coordinate basis vector
$\underline{\Omega}$	Volume of the continuum model
$\underline{\partial\Omega}$	Boundary of the continuum model
$\underline{n}$	Surface normal of the continuum model
$\underline{X}$	Location of a point in the undeformed configuration
$\underline{x}$	Location of a point in the deformed configuration
t	Time
$\underline{\nabla}$	Gradient operator
$\underline{u}$	Displacement variable in the continuum model (m)
ϕ	Electric potential variable in the continuum model (V)
$\underline{\varepsilon}$	Infinitesimal strain tensor
$\underline{\sigma}$	Stress tensor (Pa)
$\underline{C}^{\text{mat}}$	Unrotated elasticity matrix (Pa)
$\underline{\tilde{T}}^{\text{mat}}$	Unrotated electro-mechanical coupling coefficient matrix (Pa V/m)
$\underline{\epsilon}^{\text{mat}}$	Permittivity matrix (C/V-m)
$\underline{C}$	Elasticity tensor (Pa)
$\underline{d}$	Piezoelectric strain matrix (V/m)
$\underline{\tilde{T}}$	Electro-mechanical coupling coefficient matrix (Pa V/m)
$\underline{\epsilon}_r$	Relative permittivity matrix
$\underline{\epsilon}_0$	Permittivity permittivity of the vacuum (C/V-m)
$\underline{\epsilon}$	Permittivity matrix (C/V-m)
ρ	Mass density (kg/m ³)
$\underline{f}$	Body acceleration (m/s ²)
$\underline{F}$	Electromagnetic force density (N/m ³)
$\underline{E}$	Electric field vector (V/m)
$\underline{D}$	Electrical displacement vector (C/m ²)
$\underline{\partial I}_{\text{gnd}}$	Ground potential surface boundary of the continuum model
$\underline{\partial I}_{\text{in}}$	Input potential surface boundary of the continuum model
$\underline{x}_{\text{src}}$	A point on the surface of periodic boundary source

$\underline{x}_{\text{trg}}$	A point on the surface of periodic boundary target
$\underline{d}_\alpha$	Relative placement vector between source and target surfaces of the applied periodic boundary condition
λ	Wavelength (m)
ω	Angular speed (rad/s)
L_e	Electrode length (m)
h	Thickness (m)
q	Electrical charge (C)
$\underline{p}$	Dipole moment (C-m)
$\underline{Q}$	Rotation matrix
$\underline{U}$	Known displacement (m)
Φ	Known electric potential (V)
$\underline{\delta}u$	Displacement test function
$\underline{\delta}\phi$	Electric potential test function
$\hat{V}_u$	Displacement test function space
$\hat{V}_\phi$	Electric potential test function space
$\hat{N}_i^{\text{ID}}$	Displacement test shape function
$\hat{N}^{\text{ID}}$	Electric potential test shape function
ID	Number of the DOF
N_i^{ID}	Displacement trial shape function
N^{ID}	Electric potential trial shape function
$\hat{\mathbf{u}}$	Vector of unknown displacements of the finite element model
$\hat{\boldsymbol{\phi}}$	Vector of unknown electric potentials of the finite element model
$\mathbf{K}$	Stiffness matrix
$\mathbf{M}$	Mass matrix
t_{max}	Maximum time (s)
n_{wave}	Number of solved waves
n_{pt}	Number of discrete solution points in a wave
Δt	Time increment (s)
ν_n	n_{th} resonance frequency (Hz)
Σ_{TSh}	Target eigenvalue (rad ² /s ²)

μ	Shear modulus (Pa)
v	Wave speed (m/s)
$\bar{h}$	Normalized thickness
S_m	Mass sensitivity (m ² /kg)



1. INTRODUCTION

Electrical phenomena can be coupled with mechanical response of a material. This coupling effect is seen in piezoelectric materials, and it can be utilized in lots of applications, ranging from submarine radar systems to vibration isolators. In this thesis surface acoustic wave (SAW) will be simulated.

SAWs are generated by inter-digital-transducers (IDTs) etched onto a piezoelectric substrate, which can be accompanied with a thin layer on top. Each IDT has two comb-shaped electrodes which are placed very close to each other like a zipper. Configurations of SAW sensors are divided into two port (input-output) or single port IDT. Two port (terminal) design is considered in this study for the sake of sensing bacteria or chemical agent in liquid or gas environment. In the two port configuration two IDTs are separated by a distance which is called delay length. On the delay area, the artifacts are stuck by means of chemical operations, and they act as a mass loading. Waves generated by the input IDTs are affected by the mass loading so that its frequency is shifted. The shift is read by an oscilloscope from the output IDTs.

Depending on the requirements, sensors are designed to have high sensitivity values. In product development, the experimentation and production of such devices might require high costs. In order to reduce the costs, a computational framework is proposed. An open source finite element code called FEniCS enable modeling piezoelectric materials in oprando mode. With this novel software advancement, we are able to find an optimized sensor design by just using a computer sitting in our residence.

We start the thesis by presenting literature survey in Chapter 2. The history of SAW research goes back to 1880's and still continues today. Kinematic relations, balance equations, and boundary conditions are given in Chapter 3 to construct variational formulation of the problem. A physical overview of the piezoelectricity, and regarding crystal cut conventions are explained in Chapter 4. Variational formulation prior to the finite element discretization is introduced in Chapter 5. Finite element method is employed on the variational formulation to be solved as a linear algebraic system in Chapter 6. Eigenvalue, and transient problems are defined in Chapter 7 using the discretized forms from Chapter 6. To test the FEniCS

implementation, the eigenvalue, and transient problems are verified for a vibrating infinite Quartz plate in Chapter 8. After the verification, a computational design guideline is proposed for a Love SAW sensor in Chapter 9 to obtain the optimum guide layer thickness in regards to achieve highest mass sensitivity. The optimum thickness is then utilized in Chapter 10 to analyse the transient waves observed in the sensors.



2. BACKGROUND

The surface waves might appear on a traction-free medium. For instance earthquakes can directly demonstrate the surface wave phenomenon as the thin layer of earth crust is displaced by some internal disturbance. Fluidic environments also show surface waves such as the water ripples caused by a hit of rock on a calm water pond. In this study we are interested in the dynamics of solids, which shows surface waves. Assuming the earth crust as a continuum, the particles on its free-surface can move vertically and longitudinally at the same time similar to an ocean wave. This typical mode is studied mathematically in [1] by Lord Rayleigh in 1885, and after named *Rayleigh*. Augustus Love shares some pitfalls of the general elastic theory, and the material property effect of the earth crust in [2] under the context of seismic vibrations. The type of SAW Augustus Love examined is after called *Love* waves, for which the particles move perpendicular to the wave motion. As an example the compact soil can have a layer of rocks, which move horizontally as opposed to vertically.

Rayleigh and Love waves are the fundamental outcomes of elasto-dynamics. As the time goes, they are slowly recognized in the realm of multiphysics. Gulyaev introduced the amplification of SAW layered piezoelectric and semiconductor materials in [3]. The electric and mechanical coupling of the piezoelectric materials becomes a fundamental basis to new emerging technologies in 1960s. [4] proposed an idea to generate SAW by the utilization of direct piezoelectric effect in 1965. The idea is to use photoetched 1000 Å-thick aluminum electrodes to apply electrical potential on a Quartz substrate. The gap between is set in terms of the application frequency, and directly affects the SAW frequency. The advantage of obtaining a specific operating frequency provides high frequency applications, which are suitable for sensing applications, which are reviewed in [5–11]. Chemical utilization of recognition layers are reviewed in [12–14]. First examples of tailor made bio-sensing layers are demonstrated in [15], which uses ST-cut Quartz as the substrate to immobilize the goat antihuman in a fluidic environment by capturing them on a sensing layer between two IDTs. One IDT generates the waves, and other one reads the signal. The capturing mechanism increases the mass on the surface, and therefore changes the SAW velocity. Inherent mode of the SAW for ST-cut Quartz is Rayleigh wave, which has some physical limitations. Modal disadvantage is the loss of SAW energy to the liquid above the surface.

Insertion loss, wave speed or frequency change, and mass sensitivity are related design parameters that are widely used in sensor characterization as stated in [16]. Mass sensitivity is a measure of the relative change of a quantity observed in the sensor with respect to the added mass. Frequency and/or insertion loss shift are the changes that can be evaluated. [17] gives a summary of derivation of the mass sensitivity measure. [18] calculates the mass sensitivity using perturbation theory, and takes the frequency change as the observed quantity.

[19] reports smaller insertion loss for shear-horizontal (SH) waves than Rayleigh waves under liquid environment. [20] theoretically compares SH-plate and Love wave modes in terms of the mass sensitivity. SH-plate and Love waves are obtained by only a Silicon Dioxide (SiO_2) plate and layering an amorph SiO_2 on a Silicon (Si) substrate, respectively. Kovacs et al. find that both configurations show different wave propagation speeds with respect to the plate and layer thicknesses, but Love wave mode provides superior mass sensitivity. Kovacs et al. also report experiments in [21] for the Love wave mode, which is obtained by ST-cut Quartz substrate and amorph SiO_2 layer. Gizeli et al. meanwhile study the mass sensitivity for a Love wave sensor in [22], yet they use Y-cut Quartz substrate with Polymethylmethacrylate (PMMA) layer. They find similar dispersive characteristics for the wave speeds with respect to the layer thickness, and it directly effects the mass sensitivity as given in [23]. [24] also finds the dispersion equation for a two-layer system, i.e. substrate/layer. [19] and [25] show the effect of the cut angle for the substrate and the layer material on the dispersion characteristics, respectively. Material and geometric parameters take crucial role in the design of a two-layer system as they directly effect the device performance.

In addition to the theoretical and experimental methods finite element method (FEM) fits well in the development process of Love wave sensors, due to the manufacturing and experiment challenges as stated in [5, 6, 26]. [27] uses a commercial software. In the simulations a 3D finite element of a layered substrate is solved in a transient manner. [28] resorts FEM to determine the thin film characterization. [29] solves a SAW sensor with microfluidic channel using frequency response analysis. [30] also simulates the frequency response of a single layer, i.e. substrate, SAW sensor modeled as a representative volume element (RVE) via a commercial software. Yet, a computational design and analysis framework is not come across. The lack of such framework is required, and can be accomplished by a open-source software.

3. GOVERNING EQUATIONS OF PIEZO-ELASTODYNAMICS

Unless the body rigid, it deforms under a mechanical loading. If we model the rigid body as a volume of infinitely many particals, the status of each particle can be defined under the material constitutive relations. This approximation is the basis of *continuum* approach, which is taught in [31]. It is a very powerful theory that can help formulating finite element weak forms which will be shown in the following text. We use indicial notation. Depending on the physical context mechanical displacement, $\underline{u}$, charge potential, ϕ , temperature, T , etc. of a particle might be defined.

3.1. KINEMATIC RELATIONS

In addition to the constitutive behaviour, there are mathematical representations how the physical quantites relate to each other. For instance, strain is a mechanical measure of how two points in a continuum move with respect to each other. They will be separated or got close by some amount, $d\underline{x}$, after the loading. If a point is selected in a three dimensional body, the

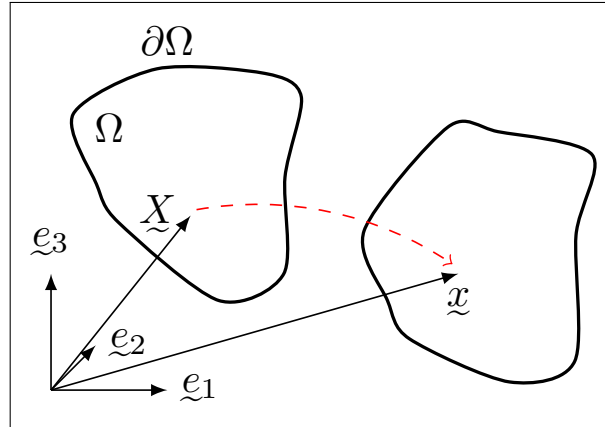


Figure 3.1. An arbitrary body in 3-dimensional space is shown. $\underline{X}$ and $\underline{x}$ are the location of any point in the undeformed and deformed body, respectively.

undeformed and the deformed locations at some time, t , are respectively represented by

$$\begin{aligned}\underline{X} &\equiv \underline{e}_j X_j, \\ \underline{x} &\equiv \underline{e}_j x_j,\end{aligned}\tag{3.1}$$

where i takes $\{1, 2, 3\}$. We use the *Einstein's Summation Convention* on the repeating indices. Then the displacement displacement of any point reads

$$u_i = x_i - X_i . \quad (3.2)$$

We assume the deformations are small enough to approximate displacements as the deformed state,

$$u_i \approx x_i . \quad (3.3)$$

The field of displacement change with respect to the undeformed configuration leads to use of gradient operator,

$$\underline{\nabla} \equiv \left(\frac{\partial}{\partial x_1} \quad \frac{\partial}{\partial x_2} \quad \frac{\partial}{\partial x_3} \right) \equiv \frac{\partial}{\partial x_i} , \quad (3.4)$$

such that

$$\underline{\nabla} u = \frac{\partial u_i}{\partial x_j} = \begin{pmatrix} \frac{\partial u_1}{\partial x_1} & \frac{\partial u_1}{\partial x_2} & \frac{\partial u_1}{\partial x_3} \\ \frac{\partial u_2}{\partial x_1} & \frac{\partial u_2}{\partial x_2} & \frac{\partial u_2}{\partial x_3} \\ \frac{\partial u_3}{\partial x_1} & \frac{\partial u_3}{\partial x_2} & \frac{\partial u_3}{\partial x_3} \end{pmatrix} . \quad (3.5)$$

Each element of $\frac{\partial u_i}{\partial x_j}$ means the normalized change of the distance in $\underline{e}_j$ direction between any points with respect $\underline{e}_j$ direction. Thus, we have nine states at a point in the material.

Since we are assuming infinitesimal changes of the particles and want to use linear approximation, higher order terms in the Lagrange strain tensor are dropped and *infinitesimal strain tensor* is defined as

$$\begin{aligned} \underline{\varepsilon} = \text{sym}(\underline{\nabla} u) &= \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \\ &\equiv \begin{pmatrix} \frac{1}{2} \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_1}{\partial x_1} \right) & \frac{1}{2} \left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right) & \frac{1}{2} \left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \right) \\ \frac{1}{2} \left(\frac{\partial u_2}{\partial x_1} + \frac{\partial u_1}{\partial x_2} \right) & \frac{1}{2} \left(\frac{\partial u_2}{\partial x_2} + \frac{\partial u_2}{\partial x_2} \right) & \frac{1}{2} \left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \right) \\ \frac{1}{2} \left(\frac{\partial u_3}{\partial x_1} + \frac{\partial u_1}{\partial x_3} \right) & \frac{1}{2} \left(\frac{\partial u_3}{\partial x_2} + \frac{\partial u_2}{\partial x_3} \right) & \frac{1}{2} \left(\frac{\partial u_3}{\partial x_3} + \frac{\partial u_3}{\partial x_3} \right) \end{pmatrix} \\ &= \begin{pmatrix} \frac{\partial u_1}{\partial x_1} & \frac{1}{2} \left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right) & \frac{1}{2} \left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \right) \\ \frac{1}{2} \left(\frac{\partial u_2}{\partial x_1} + \frac{\partial u_1}{\partial x_2} \right) & \frac{\partial u_2}{\partial x_2} & \frac{1}{2} \left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \right) \\ \frac{1}{2} \left(\frac{\partial u_3}{\partial x_1} + \frac{\partial u_1}{\partial x_3} \right) & \frac{1}{2} \left(\frac{\partial u_3}{\partial x_2} + \frac{\partial u_2}{\partial x_3} \right) & \frac{\partial u_3}{\partial x_3} \end{pmatrix} . \end{aligned} \quad (3.6)$$

FEniCS implementation of Equation (3.6) is given in Algorithm 3.1.

Algorithm 3.1. Strain definition

1	eps = sym(grad(u))
---	--------------------

3.2. BALANCE EQUATIONS

A continuum can be modeled as an elastic material. The integrity of the solid is provided by the internal forces between its atoms. At any point in the continuum, the internal forces are the result of displacement of atoms. When an arbitrary shaped body is pulled the internal force at an interested point is described by the *Hooke's Law*,

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl} , \quad (3.7)$$

where C_{ijkl} in N/m^2 is the *elasticity tensor* and valid for any solid material with various symmetries such as isotropy, anisotropy, etc.

As [32] shows some other the external disturbances might be present. All of these as well as σ_{ij} are written in the *balance of linear momentum* equation in N/m^3 ,

$$\rho \frac{\partial^2 u_i}{\partial t^2} - \sigma_{ij,j} - \rho f_i = F_i , \quad (3.8)$$

where $\rho \frac{\partial^2 u_i}{\partial t^2}$, ρf_i , F_i are the inertial, body, electromagnetic terms, respectively. The homogeneous counterpart of Eq. 3.8 is called *wave equation* in [33,34],

$$\rho \frac{\partial^2 u_i}{\partial t^2} - \sigma_{ij,j} = 0 . \quad (3.9)$$

Piezoelectric medium which is an anisotropic *dielectric* material, has a electro-mechanical coupling behaviour. In the next chapters this phenomenon will be explained. The stress in piezoelectric crystals and ceramics are modeled linearly such that Eq. 3.7 is rewritten,

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl} - \tilde{T}_{kij} E_k , \quad (3.10)$$

Algorithm 3.2. Stress definition

```

1 Sigma = {
2   'sub':as_tensor(C['sub'][j,i,k,l]*eps[k,l] \
3   - Ttilde['sub'][k,j,i]*E[k] , (j,i))

```

where $\tilde{T}_{kij}$ is the electro-mechanical coupling coefficient matrix in Pa V/m and E_k is the electric field vector in V/m. Equation (3.10) may also be applied to isotropic elastic materials. Piezoelectrics hold,

$$\begin{aligned} E_i &= -\phi_{,i} , \\ D_{i,i} &= 0 , \end{aligned} \tag{3.11}$$

Algorithm 3.3. Electric field definition

```

1 E = -grad(phi)

```

where D_i is the electrical displacement in C/m² and defined as

$$D_i = \tilde{T}_{ikl} \varepsilon_{kl} + \epsilon_{ik} E_k , \tag{3.12}$$

where ϵ_{ik} is the permittivity coefficient matrix.

Algorithm 3.4. Electric displacement definition

```

1 D = {
2   'sub':as_tensor(Ttilde['sub'][i,k,l]*eps[k,l] + \
3   eps_0 * eps_rel_el['sub'][i,k]*E[k] , (i,))
4 }

```

Eq. 3.10 and Eq. 3.12 are the constitutive equations to be substituted in Eq. 3.8, which will be used with Eq. 3.12 in the derivation of the weak form of the problem.

3.3. BOUNDARY CONDITIONS

A sensor can be modeled in a number of topologies. The model types suit some problems in terms of the computational resource usage and computing time. Yet, the approximation of a model may need new boundary condition implementations, for which the geometries are more complex. We first consider the most complex topology, which is a mock-up sensor including a substrate, IDT pairs and a layer in Figure 3.2. The model lacks of voltage probe

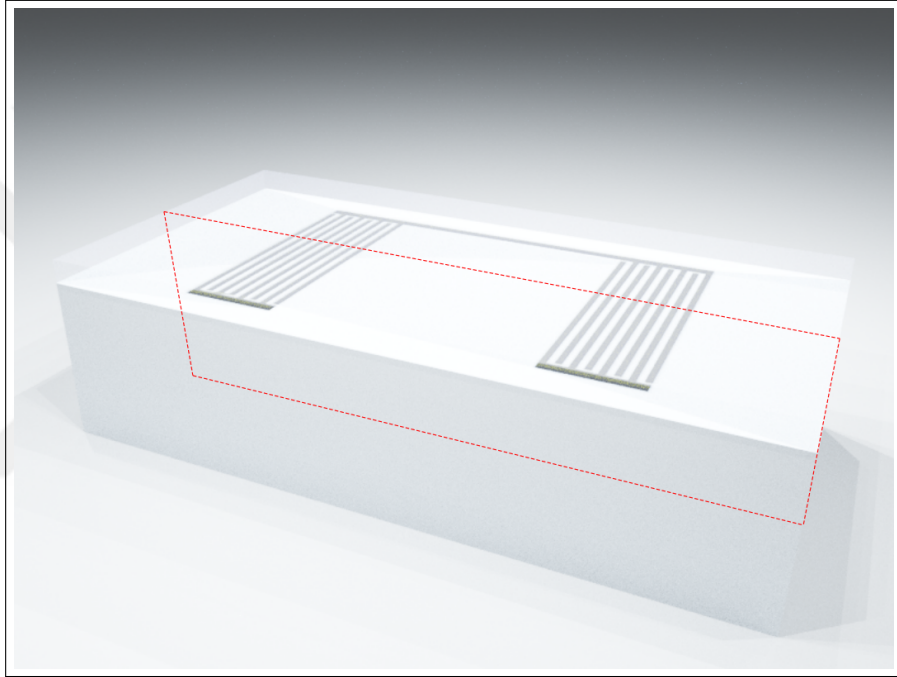


Figure 3.2. Full model of the Love SAW sensor

stations, but it is more than enough to analyze the dynamics of the Love SAW on the sensor. We call the model as the *full-sensor*. Bottom surface of the sensor is fixed,

$$u_i = 0 \text{ on } \partial\Omega_b . \quad (3.13)$$

In order to generate a surface wave on the piezoelectric substrate a time periodic electric field needs to be applied. We give charge potentials on the 2-dimensional region between the electrodes and substrate,

$$\begin{aligned} \phi_{\text{in}}(\underline{x}, t) &= \phi_0(\underline{x}) \sin \omega t \text{ on } \partial I_{\text{in}} , \\ \phi_{\text{gnd}}(\underline{x}, t) &= 0 \text{ on } \partial I_{\text{gnd}} , \end{aligned} \quad (3.14)$$

Algorithm 3.5. Boundary condition definitions

```

1 actuator = Expression("1.0*sin(2.0*pi*freq*t)",
2 freq=nu, t =0, degree=10, domain=mesh)
3 bc1 = DirichletBC(Space.sub(0), actuator, Patch1()) # input
4 bc2 = DirichletBC(Space.sub(0), 0., Patch2()) # ground
5 bc3 = DirichletBC(Space.sub(1), Constant((0., 0., 0.)),
6 facets, 4) # fixed

```

where ∂I_{in} and ∂I_{gnd} represent input and output electrodes, respectively. Thus using Equation (3.14) in Equation (4.6), we get the time dependent electric displacement field generated between two electrodes as shown in Figure 3.3,

$$D_i(\underline{x}, t) = -\epsilon_{ij} (\phi_{\text{in}} - \phi_{\text{gnd}})_{,j} \quad (3.15)$$

The 2-dimensional region between output electrodes and the substrate, ∂I_o , is left free.

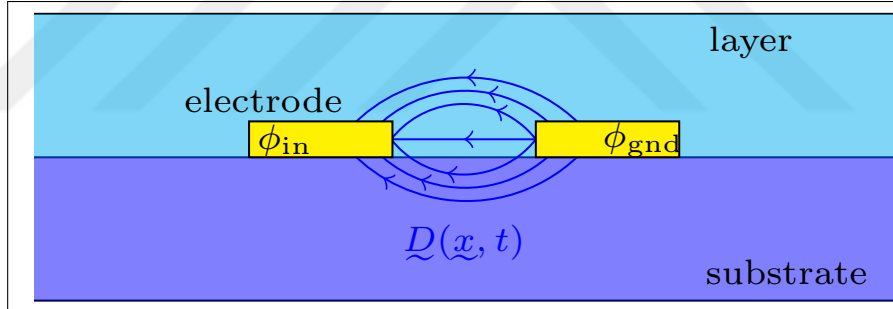


Figure 3.3. Generated D_i in a layered piezoelectric substrate

Equations (3.13) and (3.14) are well suited for the time dependent solution. We can further reduce the geometry by neglecting the effect of the connecting electrode, i.e. bus bar, between the IDTs. A hypothetical plane of symmetry is depicted in dashed red lines in Figure 3.2. If we cut a 3-dimensional section with a thickness in $\underline{e}_2$ direction, a cross-section perpendicular to 1-3 plane is obtained. To retain the motion of the waves in $\underline{e}_2$ direction, we apply periodic boundary condition (PBC) on the opposing surfaces perpendicular to the $\underline{e}_2$ direction as shown in Figure 3.5a. The degrees-of-freedom (DOF) on these surfaces are mapped utilizing a *source-target* relationship. Since we are trying to make a representative volume element (RVE), the configuration of such an element can be generalized using a rectangular prism in 3-dimensional infinite plate as shown in Figure 3.4. The infinite plate might be tessellated

into simple identical rectangular prisms. The RVE is the smallest assigned unit to span the finite element result in assigned directions. The RVE in Figure 3.4 has two source surfaces on where all the DOF are solved. The solution is then mapped to the target surface. The points which are inside the source surface is $\underline{x}_{\text{src}}$ and the target is $\underline{x}_{\text{trg}}$. The intersection line of two source surfaces needs to be defined as well, because it contains a common solution satisfying both surfaces,

$$\underline{x}_{\text{src}-0} \cap \underline{x}_{\text{src}-1} \in \underline{x}_{\text{src}-2} . \quad (3.16)$$

The mathematical representation of the mapping reads

$$\begin{aligned} u_i(\underline{x}_{\text{src}-\alpha}) &\mapsto u_i(\underline{x}_{\text{src}-\alpha} + \underline{d}_\alpha) , \\ \phi(\underline{x}_{\text{src}-\alpha}) &\mapsto \phi(\underline{x}_{\text{src}-\alpha} + \underline{d}_\alpha) , \end{aligned} \quad (3.17)$$

where $\alpha \in \{0, 1, 2\}$. The relative vector between source and target points are

$$\underline{d}_\alpha = \underline{x}_{\text{trg}-\alpha} - \underline{x}_{\text{src}-\alpha} . \quad (3.18)$$

Implementation of PBC can be extended or reduced to lower dimensions. For instance, 3.5a requires only a surface mapping across $\underline{e}_2$ direction such that Equation (3.16) is not valid and $\alpha = 0$ because only two opposing surfaces are to be mapped.

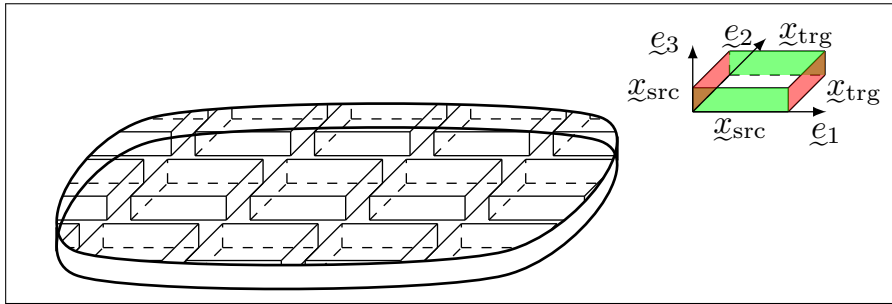


Figure 3.4. RVE representation of an infinite plate to depict the PBC concept.

Figure 3.5a might be further simplified by excluding the 3-dimensional electrodes as their inertial forces are considered to be negligible with respect to their occupied volumes. Yet, the ∂I_{in} and ∂I_{gnd} remains the same as depicted in Figure 3.5b for which Equations (3.13) and (3.14) are applied in addition to Equations (3.17) and (3.18). Slice model is also suitable for transient solutions with less DOF.

Algorithm 3.6. PBC template

```

1 class PeriodicBoundary(SubDomain):
2     def inside(self, x, on_boundary):
3         return <BOOLEAN>
4     def map(self, x, y):
5         <ALGORITHM>

```

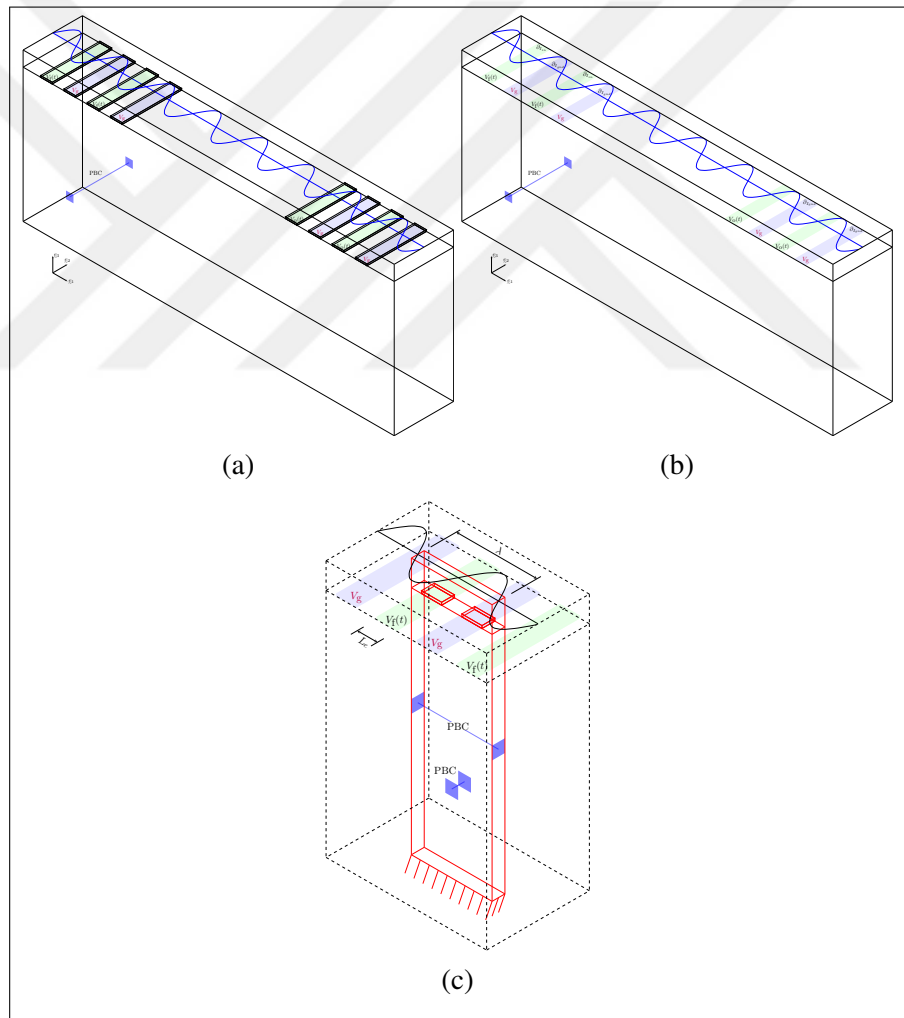


Figure 3.5. (a) 3-dimensional *slice* model, (b) Same topology of (a) excluding 3-dimensional electrodes which are substituted with 2-dimensional patches only, (c) Reduced topology of (b)

For an eigenvalue-problem (EVP) computer memory might be a limiting factor since the size of assembled mass and stiffness matrices are large depending on the number of DOF. To compensate the disadvantage, we can reduce the DOF by considering that the solution is λ -periodic, i.e. displacements on the surface is repeated on every four electrode length, L_e , in the wave propagation direction. Thus, we cut an RVE which fits $4L_e$ length in $\underline{e}_1$ direction from Figure 3.5b. As a result we obtain a new RVE depicted by Figure 3.5c. This model is used for the EVP and it obeys Equations (3.13) and (3.16) to (3.18).



4. PIEZOELECTRICITY MODELING

Piezoelectricity¹ is discovered by Pierre Curie and Jacques Curie in 1880. They observe charges on the outer surface of the piezoelectric material when it is in compression.

The working principle is a symmetry issue of the crystal configuration which constructs *unit cells*. Unit cells which have symmetry do not show polarization. For instance naturally found Quartz crystal is made of SiO₂ has a asymmetric crystal structure at specific lattice orientation as shown in Figure 4.1.

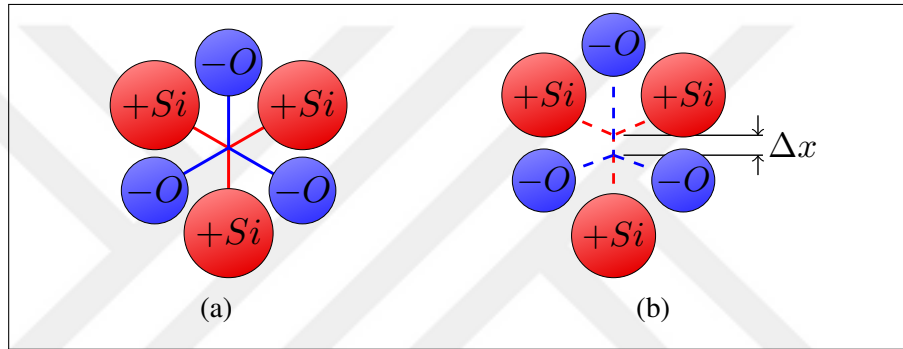


Figure 4.1. Undeformed and deformed configurations of the lattice. (a) Hexagonal SiO₂ crystal structure is at a specific lattice orientation (b) The charge centroids are displaced by a distance of Δx and an electric field, $\underline{D}$, is created.

Silicon (Si) and Oxygen (O) atoms have charge centroids inside the crystal. After the application of stress, atoms displaced some amount, thus the charge centroids. When a positive and a negative charge of the same magnitude, q , separated by a distance, Δx , a *dipole* is present and a *dipole moment* is defined as

$$\underline{p} = q\Delta\mathbf{x} . \quad (4.1)$$

Since a unit cell is the smallest crystalline structure of a solid, dipole moments are created in each cell when the material is pulled or compressed. Therefore, between the separated charges there is a small electric field appears, and the crystal structure is polarized in some direction. A piezoelectric material inside a vacuum environment exposed to an electrical

¹ *piezo* means "to press" in Greek [35]

field, $\underline{E}$, reads

$$\underline{E} = \underline{\epsilon}^{-1} \underline{D} \quad (4.2)$$

where $\underline{D}$ is the electric displacement vector also known as the electric flux density vector, and $\underline{\epsilon}$ is the electric permittivity which is equal to the multiplication of permittivity of the vacuum, ϵ_0 , and relative permittivity of the material, ϵ_r . The elements of ϵ is in $C/V - \mu m$

$$\epsilon_0 \epsilon_r \equiv \epsilon_{ij} = \begin{pmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{pmatrix}. \quad (4.3)$$

Algorithm 4.1. Definition of unrotated dielectric permittivity matrix parameters for Lithium Niobate from [36] in Voigt notation

```
1 eps_rel_el_p_11 = <VALUE>
2 ...
3 eps_rel_el_p_33 = <VALUE>
```

$\underline{D}$ is created by the charges inside the material as shown in Figure 4.1. The mechanical stress, $\underline{\sigma}$, which strains the object, and the electric displacement are related to each other for linear piezoelectric materials by a *piezoelectric strain* matrix, $\underline{d}$,

$$\underline{D} = \underline{d} \underline{\sigma}, \quad (4.4)$$

where the elements of $\underline{d}$ are in $V/\mu m$

$$d_{ijk} \equiv \begin{pmatrix} d_{111} & d_{122} & d_{133} & d_{123} & d_{131} & d_{112} \\ d_{211} & d_{222} & d_{233} & d_{223} & d_{231} & d_{212} \\ d_{311} & d_{322} & d_{333} & d_{323} & d_{331} & d_{312} \end{pmatrix}. \quad (4.5)$$

We can think of $\underline{D}$ as the small electric field. The small electric field creates a potential difference inside the unit cell, such that

$$\Delta V = - \int \underline{\epsilon}^{-1} \underline{D} \cdot d\underline{x}, \quad (4.6)$$

There are infinitely many unit cells in the material, and each voltage can be superposed to make a voltage source in a typical circuit. A measurable current flow from the object's surface is created. This phenomenon is called *direct* effect, which converts mechanical disturbance to electric current. In addition to $\underline{D}$, the material strains due to $\underline{\sigma}$

$$\underline{\varepsilon} = \underline{C}^{-1} \underline{\sigma} , \quad (4.7)$$

where stiffness tensor, $\underline{C}$, is a fourth rank tensor in TPa

$$C_{ijkl} = \begin{pmatrix} C_{1111} & C_{1122} & C_{1133} & C_{1123} & C_{1113} & C_{1112} \\ C_{2211} & C_{2222} & C_{2233} & C_{2223} & C_{2213} & C_{2212} \\ C_{3311} & C_{3322} & C_{3333} & C_{3323} & C_{3313} & C_{3312} \\ C_{2311} & C_{2322} & C_{2333} & C_{2323} & C_{2313} & C_{2312} \\ C_{1311} & C_{1322} & C_{1333} & C_{1323} & C_{1313} & C_{1312} \\ C_{1211} & C_{1222} & C_{1233} & C_{1223} & C_{1213} & C_{1212} \end{pmatrix} . \quad (4.8)$$

Algorithm 4.2. Definition of unrotated elastic stiffness tensor parameters for Lithium Niobate from [36] in Voigt notation

1	C11_p = <VALUE> # in TPa
2	...
3	C66_p = <VALUE> # in TPa

Direct effect is reversible, and it is called *converse* effect which is obtained when $\underline{E}$ is applied. The linear relationship between $\underline{\varepsilon}$ and $\underline{E}$ is

$$\underline{\varepsilon} = d\underline{E} . \quad (4.9)$$

Combining Equations (4.2), (4.4), (4.7) and (4.9) leads to

$$\begin{aligned} \underline{\varepsilon} &= \underline{C}^{-1} \underline{\sigma} + d\underline{E} , \\ \underline{D} &= d\underline{\sigma} + \underline{\epsilon} \underline{E} . \end{aligned} \quad (4.10)$$

If $\underline{\sigma}$ and $\underline{D}$ are selected as the dependent variables,

$$\begin{aligned}\underline{\sigma} &= \underline{C}\underline{\varepsilon} - \underline{\tilde{T}}\underline{E} , \\ \underline{D} &= \underline{\tilde{T}}\underline{\varepsilon} + \underline{\epsilon}\underline{E} ,\end{aligned}\tag{4.11}$$

where $\underline{\tilde{T}}$ is the *piezoelectric coupling* coefficient matrix

$$\underline{\tilde{T}} = \underline{C}\underline{d} .\tag{4.12}$$

Algorithm 4.3. Definition of unrotated piezoelectric coupling coefficient matrix parameters for Lithium Niobate from [36] in Voigt notation

```
1 Ttilde_p_11 = <VALUE> # in muC/mum2
2 ...
3 Ttilde_p_36 = <VALUE> # in muC/mum2
```

4.1. LITHIUM NIOBATE

The plane on which the crystal atoms are placed is the deciding factor in which direction the piezoelectric material deforms as shown in Figure 4.1. There are infinitely many choices of plane orientations, but the intended wave mode exhibits a certain orientation. Lithium Niobate (Linobate, LiNbO_3) is a tailor-made material which contains Lithium (Li^+), Niobium (Nb^{+5}) and Oxygen (O^{-2}) atoms. A detailed explanation of its microstructure is explained in [37]. We are interested in the macro-scale properties such as the crystal principle axes: $\{X, Y, Z\}$. Yet, the principle axes are configured by the orientation of the mirror planes, m , which are dependent on the crystal structure. On the macro-scale they are depicted in Figure 4.2a, and therefore LiNbO_3 belongs to $3m$ *point group* or *crystal class*.

4.1.1. 64YX Cut

In practice the interested plane is bottom surface of the substrate, and perpendicular to the thickness. A conventional naming for designating the cut angles is as follows

###AB-cut ,
 <angle of rotation in degrees><thickness direction><rotation axis>-cut .

For example, there are common cuts such as Y-cut, for which the ZXZ-Euler angles of rotation is $(0, 0, 0)^\circ$ as shown in Figure 4.2a. 64YX-cut LiNbO₃ showing leaky SAW² is found to have high electromechanical coupling coefficient in [38]. As depicted in Figure 4.2b normal of the free-surface of the substrate is towards +Y axis, then the crystal is cut at an angle of $(0, 64, 0)^\circ$ from the +Z axis. The initial direction of the free-surface normal might be +Z

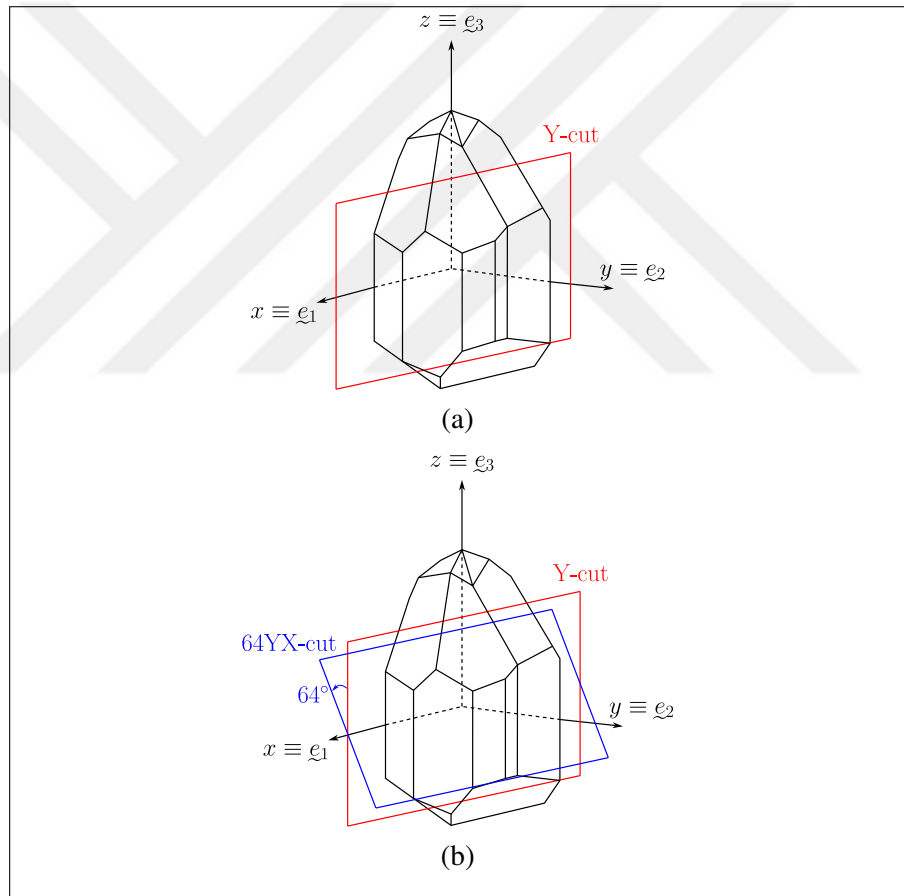


Figure 4.2. Common LiNbO₃ cuts on the crystal medium. (a) Y-cut perpendicular to the crystal's +Y axis.

axis, which is generally the case in CAD models. Same orientation of the substrate as in the 64YX-cut case is achieved by rotating the substrate $(0, -26, 0)^\circ$ from the +Y axis as shown in Figure 4.3b. Although Figure 4.3b is theoretically 154ZX-cut, it is not common in the

² A SAW showing similar characteristics as Love type SAW, but there is no layer on the substrate.

literature.

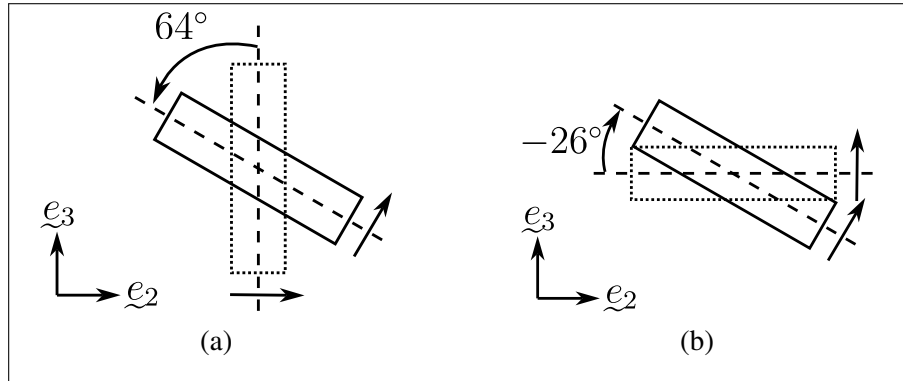


Figure 4.3. Equivalent rotations for 64YX-cut. Arrows show the thickness directions or the free-surface normals. Initial configuration is the dotted rectangle. (a) 64YX-cut (b) 154ZX-cut.

4.1.2. 128-YX Cut

Finding the optimum angle for Rayleigh SAW is also considered in [39], where large electromechanical coupling coefficient is obtained at 127.86° rotated from +Y axis about +X axis. In the literature, 128-YX is widely used for the Rayleigh mode. We can similarly show the equivalent rotations for the free-surface normal oriented at +Y and +Z directions in 4.4. Although Figure 4.4b is theoretically 38ZX-cut, it is not common in the literature as well.

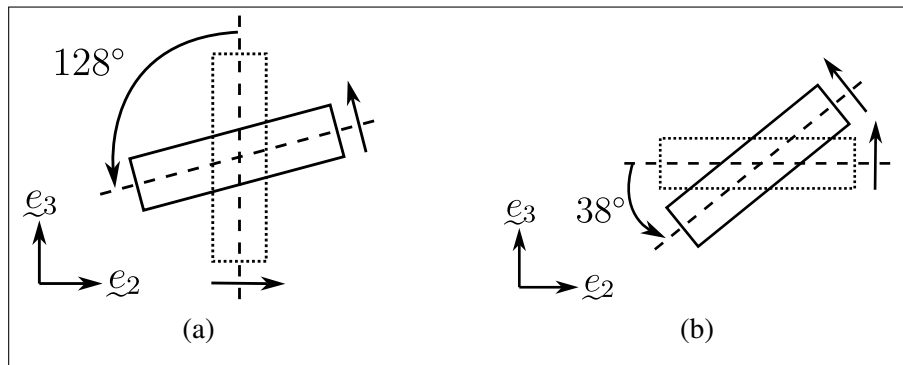


Figure 4.4. Equivalent rotations for 128YX-cut. Arrows show the thickness directions or the free-surface normals. Initial configuration is the dotted rectangle. (a) 128YX-cut (b) 38ZX-cut.

4.2. AT-CUT QUARTZ

Silicon Dioxide (Silica, SiO_2) in crystal form is named Quartz, which is made of Silicon (Si^{+4}) and Oxygen atoms. It is widely used in resonator applications as a piezoelectric material. It shows thickness-shear (TSh) mode, at AT-cut, which corresponds to -35.42° YX-cut or $(0, -35.42, 0)^\circ$ rotation about +X axis.

4.3. ROTATION OF MATERIAL MATRICES

We have the material matrices $\underline{C}$, $\underline{d}$, $\underline{\tilde{T}}$ and ϵ . They are defined with respect to the crystal axes. Different orientation of the substrate results different material matrices. Therefore, we need to define a mapping that converts the parameters from the crystal axes to the rotated frame. In indicial notation, the mapping reads

$$\begin{aligned}\epsilon'_{ij} &= Q_{ai} Q_{bj} \epsilon_{ab} , \\ \tilde{T}'_{ijk} &= Q_{ai} Q_{bj} Q_{ck} e_{abc} , \\ C'_{ijkl} &= Q_{ai} Q_{bj} Q_{ck} Q_{dl} C_{abcd} .\end{aligned}\tag{4.13}$$

According to the previous rotations ZXZ Euler angles is sufficient. Rotation matrix, Q_{ij} , is equal to

$$\begin{aligned}Q_{ij} &= \underline{e}'_i \cdot \underline{e}_j \\ Q_{ij}|_{(0,\theta,0)^\circ} &\equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta^\circ & \sin \theta^\circ \\ 0 & -\sin \theta^\circ & \cos \theta^\circ \end{pmatrix} .\end{aligned}\tag{4.14}$$

Algorithm 4.4. Rotation of material parameter matrices for 64YX convention

```

1  # Rotate the piezoelectric material tensors
2  Q = R.from_euler('ZXZ', [<VALUE>,<VALUE>,<VALUE>], degrees=True)
3  Q_rot = Q.as_matrix()
4
5  C_tensor_pR = np.einsum('ai,bj,ck,dl,abcd->ijkl',
6  Q_rot, Q_rot, Q_rot, Q_rot, C_tensor_p)
7  Ttilde_tensor_pR = np.einsum('ck,ai,bj,cab->kij',
8  Q_rot, Q_rot, Q_rot, Ttilde_tensor_p)
9  eps_rel_el_tensor_pR = np.einsum('ai,bj,ab->ij',
10 Q_rot, Q_rot, eps_rel_el_tensor_p)

```

5. VARIATIONAL FORMULATION

Finite element method is a mathematical tool that solves the continuous differential equations by discretizing them via *finite elements*. The result of discretization process is a linear system of equations to be solved. [40, 41] show the derivation of the matrices. In our case the differential equations are Eq. 3.8 and Eq. 3.12. From these equations u_i and ϕ needs to be solved. First procedure is to write the *strong form* of the problem,

$$\begin{aligned}\rho \ddot{u}_i - \sigma_{ji,j} &= 0 \text{ in } \Omega , \\ D_{i,i} &= 0 \text{ in } \Omega , \\ u_i &= U_i \text{ and } \phi = \Phi \text{ on } \partial\Omega ,\end{aligned}\tag{5.1}$$

which is multiplied by a test function δu_i , and integrated over the volume,

$$\int_{\Omega} (\rho \ddot{u}_i - \sigma_{ji,j}) \delta u_i \, dV = 0 .\tag{5.2}$$

More explicitly we get

$$\rho \int_{\Omega} \ddot{u}_i \delta u_i \, dV - \int_{\Omega} \sigma_{ji,j} \delta u_i \, dV = 0 ,\tag{5.3}$$

where $\sigma_{ji,j} \delta u_i$ might be rewritten by integration by parts,

$$(\sigma_{ji} \delta u_i)_{,j} = \sigma_{ji} \delta u_{i,j} + \sigma_{ji,j} \delta u_i\tag{5.4}$$

Then, Equation (5.3) reads

$$\rho \int_{\Omega} \ddot{u}_i \delta u_i \, dV - \int_{\Omega} (\sigma_{ji} \delta u_i)_{,j} \, dV + \int_{\Omega} \sigma_{ji} \delta u_{i,j} \, dV = 0\tag{5.5}$$

After applying *Gauss' Divergence Theorem* to the second expression in Equation (5.5), the weak form constituting mechanical displacements reads

$$\int_V \rho \ddot{u}_i \delta u_i \, dV + \int_V \sigma_{ji} \delta u_{i,j} \, dV - \int_{\partial\Omega} n_j \sigma_{ji} \delta u_i \, dA = 0\tag{5.6}$$

A similar procedure might be applied to Equation (5.1). However, test function for this case is now a scalar function $\delta\phi$, which represents the voltage. Therefore, Equation (5.1) becomes

$$-\int_{\Omega} D_{i,i} \delta\phi \, dV = 0 \quad (5.7)$$

Integrand might be rewritten by integration by parts,

$$(D_i \delta\phi)_{,i} = D_i \delta\phi_{,i} + D_{i,i} \delta\phi \quad (5.8)$$

Then, Equation (5.7) is rewritten as

$$\int_{\Omega} D_i \delta\phi_{,i} \, dV - \int_{\Omega} (D_i \delta\phi)_{,i} \, dV = 0 \quad (5.9)$$

After applying Gauss' Divergence Theorem to the first expression of Equation (5.9), the weak form constituting mechanical displacements reads

$$\int_{\Omega} D_i \delta\phi_{,i} \, dV - \int_{\partial\Omega} n_i D_i \delta\phi \, dA = 0 . \quad (5.10)$$

6. FINITE ELEMENT DISCRETIZATION

We are after solving u_j and ϕ as trial functions in Equation (5.6). Yet, the test function spaces $\hat{V}_u$ and $\hat{V}_\phi$ which respectively contains δu_j and $\delta \phi$ shall be defined first,

$$\begin{aligned}\hat{V}_u &= \{\delta u_i \in H^1(\Omega) : \delta u_i = 0 \text{ on } \partial\Omega\}, \\ \hat{V}_\phi &= \{\delta \phi \in H^1(\Omega) : \delta \phi = 0 \text{ on } \partial\Omega\}.\end{aligned}\tag{6.1}$$

H^1 is a vector space of functions having discontinuous derivatives in addition to the ones with continuous derivatives. The trial counterpart satisfies the Dirichlet³ boundary condition at the known DOF,

$$\begin{aligned}V_u &= \{u_i \in H^1(\Omega) : u_i = u_d \text{ on } \partial\Omega\}, \\ V_\phi &= \{\phi \in H^1(\Omega) : \phi = \phi_d \text{ on } \partial\Omega\}.\end{aligned}\tag{6.2}$$

Thus Equations (5.6) and (5.10) is discretized as follows

Find $u_i \in V_u$ and $\phi \in V_\phi$ such that

$$\begin{aligned}\int_V \rho \ddot{u}_i \delta u_i \, dV + \int_V \sigma_{ji} \delta u_{i,j} \, dV - \int_{\partial\Omega} n_j \sigma_{ji} \delta u_i \, dA &= 0 \quad \forall \delta u_i \in \hat{V}_u, \\ \int_\Omega D_i \delta \phi_{,i} \, dV - \int_{\partial\Omega} n_i D_i \delta \phi \, dA &= 0 \quad \forall \delta \phi \in \hat{V}_\phi.\end{aligned}\tag{6.3}$$

Equation (6.7) is in continuous form. In fact we can approximate them using the shape, also named as interpolation or basis, functions from the sets defined in Equation (6.2)

$$\begin{aligned}u_i &= \sum_{\text{ID}} N_i^{\text{ID}} \hat{u}^{\text{ID}}, \quad \delta u_i = \sum_{\text{ID}} \hat{N}_i^{\text{ID}} \mathbf{1}^{\text{ID}} \\ \phi &= \sum_{\text{ID}} N^{\text{ID}} \hat{\phi}^{\text{ID}}, \quad \delta \phi = \sum_{\text{ID}} \hat{N}^{\text{ID}} \mathbf{1}^{\text{ID}}\end{aligned}\tag{6.4}$$

where ID is the number of the DOF within the computational domain. Also N_i^{ID} and N^{ID} are the trial shape functions, $\hat{N}_i^{\text{ID}}$ and $\hat{N}^{\text{ID}}$ are the test shape functions.

The Equation (6.3) has boundary integrals containing Dirichlet, ∂_{Ω_D} , Neumann,⁴ $\partial_{\Omega_N} =$

³ A boundary condition type for which the nodal values are prescribed.

⁴ A boundary condition type on where partial differentiation of a function, f , with respect to a boundary

$\partial\Omega - \partial\Omega_D$, boundary conditions. Since on $\partial\Omega_D$ Equation (6.1) holds, the integrals on $\partial\Omega_D$ are eliminated from Equation (6.3). Furthermore, the problems in this thesis do not contain any Neumann boundary condition, i.e. $n_j\sigma_j = 0$ and $n_iD_i = 0$ due to the fact that traction-free surfaces and no electric displacement flux present at the boundaries, respectively. Thus, the integrals on $\partial\Omega_N$ domains are also eliminated, and we are left with

$$\begin{aligned} \int_{\Omega} \left(\rho \ddot{u}_i \delta u_i + \sigma_{ji} \delta u_{i,j} \right) dV &= 0, \\ \int_{\Omega} \left(D_i \delta \phi_{,i} \right) dV &= 0, \end{aligned} \quad (6.5)$$

We can substitute σ_{ji} and D_i in Equation (6.5) using the constitutive relations in Equations (3.10) and (3.12), and sum them to get

$$\int_{\Omega} \left(\rho \ddot{u}_i \delta u_i + \delta u_{i,j} C_{jikl} \varepsilon_{kl} - \delta u_{i,j} T_{kji} E_k + \delta \phi_{,i} T_{ikl} \varepsilon_{kl} + \delta \phi_{,i} \epsilon_{ik} E_k \right) dV = 0. \quad (6.6)$$

Prior to Chapter 7, Equation (6.6) is treated to get mass, M , and stiffness matrices, K —, according to the procedure shown in [40, 42, 43]. By using linear material modeling, we obtain a linear system such that a perturbation as a sinus or cosinus form leads to a vibration in a sinus or cosinus form. This linear property allows us to rewrite the equations by decomposing space and time dependencies that is called a Bernoulli separation ansatz, as follows:

$$\begin{aligned} u_j(x, t) &= u_j(x) \exp(-i\omega t), \\ \phi(x, t) &= \phi(x) \exp(-i\omega t), \end{aligned} \quad (6.7)$$

where exponential function collects sinus and cosinus responds with the Euler equation. In this manner, inertial term in Equation (6.6) is rewritten, $\ddot{u}_j = -\omega^2 u_j$. Therefore, we obtain

normal, $\underline{n}$, is prescribed, i.e. $\frac{\partial f}{\partial \underline{n}} = g$.

mass and stiffness matrices

$$\begin{aligned}
\mathbf{K}_{uu} \cdot \hat{\mathbf{u}} &= \sum_e \int_{\Omega} \delta u_{j,i} C_{ijkl} \varepsilon_{kl} dV, \\
\mathbf{K}_{u\phi} \cdot \hat{\phi} &= - \sum_e \int_{\Omega} \delta u_{j,i} \tilde{T}_{kij} E_k dV, \\
\mathbf{K}_{\phi u} \cdot \hat{\mathbf{u}} &= \sum_e \int_{\Omega} \delta \phi_{,i} \tilde{T}_{ikl} \varepsilon_{kl} dV, \\
\mathbf{K}_{\phi\phi} \cdot \hat{\phi} &= \sum_e \int_{\Omega} \delta \phi_{,i} \epsilon_{ik} E_k dV, \\
-\omega^2 \mathbf{M} \cdot \hat{\mathbf{u}} &= \sum_e \int_{\Omega} \rho \delta u_j \ddot{u}_j dV = - \sum_e \omega^2 \int_{\Omega} \rho \delta u_j u_j dV,
\end{aligned} \tag{6.8}$$

which will be used in eigenvalue-problem in Chapter 7. The computational implementation is given in Algorithm 6.1.

Algorithm 6.1. Assembly

```

1 M, K_uu, K_up, K_pu, K_pp = EigenMatrix(), EigenMatrix(), \
2 EigenMatrix(), EigenMatrix(), EigenMatrix()
3 epsilon = sym(grad(u))
4 delta_epsilon = sym(grad(delta_u))
5
6 assemble(C[p,q,r,s]*epsilon[r,s]*delta_epsilon[p,q]*dx ,
7 tensor = K_uu)
8 K_uu_s = K_uu.sparray().tocsc()
9 del K_uu
10
11 assemble(-e[r,p,q]*(-phi.dx(r))*delta_epsilon[p,q]*dx ,
12 tensor = K_up)
13 K_up_s = K_up.sparray().tocsc()
14 del K_up
15
16 assemble(-eps[p,q]*(-phi.dx(q))*(-delta_phi.dx(p))*dx ,
17 tensor = K_pp)
18 K_pp_s = K_pp.sparray().tocsc()
19 del K_pp
20
21 assemble(rho*delta_u[j]*u[j]*dx , tensor = M)
22 M_s = M.sparray().tocsr()
23 del M

```

Finite elements are topological objects that have DOF and basis functions, as shown in Equation (6.5). For this problem we use Lagrange elements, which is H^1 -conforming as given in Equations (6.1) and (6.2). To construct a finite element we first need to define a local

coordinate system, $\xi_i e_j$, as depicted in Figure 6.1.

Since FEniCS v2019 allows us to use tetrahedron elements shown in Figure 6.1, there are four DOF in the simplest case. [44] shows the four basis functions on the tetrahedron element

$$\begin{aligned}
 N_0(\underline{\xi}) &= -\xi_1 - \xi_2 - \xi_3 + 1 , \\
 N_1(\underline{\xi}) &= \xi_1 , \\
 N_2(\underline{\xi}) &= \xi_2 , \\
 N_3(\underline{\xi}) &= \xi_3 .
 \end{aligned}
 \tag{6.9}$$

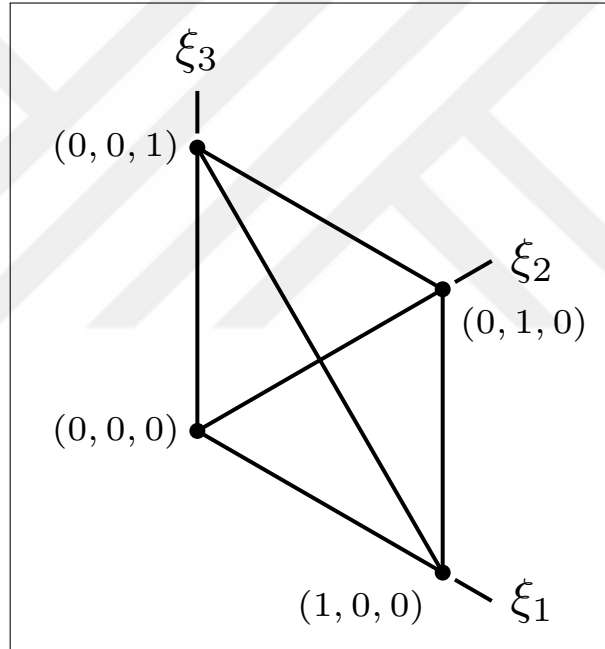


Figure 6.1. Tetrahedron element

7. ANALYSIS TYPES

The interested concept is the *dynamics* of the objects which accelerate or decelerate, because we want to study more specialized concepts used in *micro-scale* sensors. To do that we shall construct two analyses frameworks for eigenvalue and transient problems. Eigenvalue problem is used when the resonance of a system is concerned. Elastic and reversible dynamic systems show infinite displacements at resonance frequencies. Resonance phenomenon may or may not be desired depending on the application. For the SAW sensors and bulk resonators it is desired to work at a resonance frequency because it would be accurate to observe any change in the operating frequency. In Chapters 8 and 9 we will utilize the eigenvalue solution of AT-cut infinite Quartz plates to be a pre-analysis for an extension to the SAW sensors. Transient problems on the other hand reveal the solution variables in a time dependent manner. Eigenvalue solution can be verified by transient to see the resonance or not. Thus, at the resonance wave patterns on might be examined, and using the displacement information any stress at a point and time might be calculated via the transient solution.

7.1. EIGENVALUE PROBLEM

For the eigenvalue problem, discretization of Equation (6.8) is achieved by two different Sobolev spaces for displacements, vectorial, and electric potential, scalar, quantities as given in Equations (6.1) and (6.2). We code two Sobolev spaces in Algorithm 7.1#6 and #7, respectively. Then trial u , ϕ and test functions δu , $\delta \phi$ are generated from those spaces.

By observing Eq. 6.8_{2,3}, we realize that $\mathbf{K}_{\phi u}$ is the transpose of $\mathbf{K}_{u\phi}$. Now, we rewrite in the matrix form

$$\left(\begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{u\phi} \\ \mathbf{K}_{u\phi}^T & \mathbf{K}_{\phi\phi} \end{bmatrix} - \omega^2 \begin{bmatrix} \mathbf{M} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \right) \begin{Bmatrix} \hat{u} \\ \hat{\phi} \end{Bmatrix} = \mathbf{0} . \quad (7.1)$$

The second line is observed only and it reads

$$\begin{aligned} \mathbf{K}_{u\phi}^T \cdot \hat{u} + \mathbf{K}_{\phi\phi} \cdot \hat{\phi} &= 0 \\ -\mathbf{K}_{\phi\phi}^{-1} \cdot \mathbf{K}_{u\phi}^T \cdot \hat{u} &= \hat{\phi} . \end{aligned} \quad (7.2)$$

Algorithm 7.1. Function space definitions

```

1 deg = 1
2 Ve = VectorElement("CG", mesh.ufl_cell(), deg)
3 Ue = FiniteElement("CG", mesh.ufl_cell(), deg)
4
5 VectorSpace = FunctionSpace(mesh, Ve,
6 constrained_domain=PeriodicBoundary())
7 ScalarSpace = FunctionSpace(mesh, Ue,
8 constrained_domain=PeriodicBoundary())
9
10 delta_u = TestFunction(VectorSpace)
11 delta_phi = TestFunction(ScalarSpace)
12 u = TrialFunction(VectorSpace)
13 phi = TrialFunction(ScalarSpace)

```

By inserting the latter into the first line in Equation (7.1), we acquire

$$\mathbf{K}_{uu} \cdot \hat{\mathbf{u}} - \mathbf{K}_{u\phi} \cdot \mathbf{K}_{\phi\phi}^{-1} \cdot \mathbf{K}_{u\phi}^T \cdot \hat{\mathbf{u}} - \omega^2 \mathbf{M} \cdot \hat{\mathbf{u}} = 0 . \quad (7.3)$$

The *condensed* stiffness matrix,

$$\mathbf{K}^* = \mathbf{K}_{uu} - \mathbf{K}_{u\phi} \cdot \mathbf{K}_{\phi\phi}^{-1} \cdot \mathbf{K}_{u\phi}^T , \quad (7.4)$$

which is implemented in Algorithm 7.2

Algorithm 7.2. Static condensation

```

1 K_star_s = K_uu_s - K_up_s*sparse_inv(K_pp_s)*K_up_s.transpose()

```

Eq. Equation (7.4) enables to rewrite Equation (7.1) as

$$(\mathbf{K}^* - \omega^2 \mathbf{M}) \hat{\mathbf{u}} = 0 . \quad (7.5)$$

This form is a special case called the generalized eigenvalue problem having two Hermitian⁵ (equivalent to symmetric since all entries are real numbers) non-identity matrices, while $\mathbf{M}$ shall be a positive definite matrix [45]. Corresponding eigenvectors, or the modeshapes, to

⁵ A matrix whose conjugate transpose is equal to itself.

the calculated eigenvalues, ω^2 , are the displacements, $\mathbf{u}$. SLEPc provides iterative methods such as arpack to solve the eigenvalues of large matrices more efficiently. We utilize spectral transform in order to specify a target eigenvalue, Σ , around which a number of eigenvalues, n_{eig} , are solved. Σ selection is dependent on the problem type, and the computed eigenvector might be within $\Sigma \pm \Sigma_0$.

The computational implementation of the eigenvalue problem requires PETSc matrices which are converted from the assembled EigenMatrix types. The procedure in Algorithm 7.3 is employed for conversion of matrix data types. Solution of Equation (7.5) is obtained by Algorithm 7.4, where freq is Σ and lmbda is ω^2 .

Algorithm 7.3. Scipy to PETSc conversion

```

1 K_star_s_d = K_star_s.tocsr() # dummy
2 del K_star_s
3 K_star_pet = pet.Mat().createAIJ(size=K_star_s_d.shape,
4 csr=(K_star_s_d.indptr, K_star_s_d.indices, K_star_s_d.data))
5 del K_star_s_d
6 K_star_PETSc = PETScMatrix(K_star_pet)
7 del K_star_pet
8 M_pet = pet.Mat().createAIJ(size=M_s.shape,
9 csr=(M_s.indptr, M_s.indices, M_s.data))
10 del M_s
11 M_PETSc = PETScMatrix(M_pet)
12 del M_pet

```

Algorithm 7.4 is used to solve EVPs.

Algorithm 7.4. Eigensolver setup

```

1 freq = <VALUE>
2 lmbda = (2*np.pi*freq)**2
3
4 eigensolver = SLEPcEigenSolver(K_star_PETSc, M_PETSc)
5 eigensolver.parameters["problem_type"] = "gen_hermitian"
6 eigensolver.parameters["spectral_transform"] = "shift-and-invert"
7 eigensolver.parameters["spectral_shift"] = lmbda
8 eigensolver.parameters["spectrum"] = "target real"
9 eigensolver.parameters["solver"] = "arpack"
10
11 del K_star_PETSc; del M_PETSc
12
13 N_eig = <VALUE>
14 eigensolver.solve(N_eig)

```

7.2. TRANSIENT BY DIRECT INTEGRATION

Equation (6.6) is the starting point to construct the transient weak form. Since the form has spatial discretization, the time derivative shall be treated. There are different techniques to discretize the partial derivatives of the temporal quantities. We prefer the simple algorithms, therefore we choose *Euler backward difference* algorithm. The derivative of an arbitrary function, $f(x)$, is approximated as

$$\begin{aligned}\frac{\partial f}{\partial t} &= \frac{f(t_2) - f(t_1)}{t_2 - t_1}, \\ \frac{\partial^2 f}{\partial t^2} &= \frac{f(t_3) - 2f(t_2) - f(t_1)}{(t_2 - t_1)^2},\end{aligned}\tag{7.6}$$

where $t_2 - t_1 = t_3 - t_2$. We can implement this method to the first expression of Equation (6.6),

$$\begin{aligned}\text{Form} = \int_{\Omega} \left(\rho \delta u_i \frac{u_i - 2u_i^0 + u_i^{00}}{\Delta t^2} + \delta u_{i,j} C_{jikl} \varepsilon_{kl} - \delta u_{i,j} \tilde{T}_{kji} E_k \right. \\ \left. + \delta \phi_{,i} \tilde{T}_{ikl} \varepsilon_{kl} + \delta \phi_{,i} \epsilon_{ik} E_k \right) dV,\end{aligned}\tag{7.7}$$

where 0 and 00 show the time sequence in the decreasing order. Δt is the time difference depending on maximum solution time, $t_{\max}$, number of waves to be solved, n_{wave} , operating frequency of the SAW sensor, ν , and number of time increments fit in a wave, n_{pt} ,

$$\begin{aligned}t_{\max} &= \frac{n_{\text{wave}}}{\nu}, \\ \Delta t &= \frac{t_{\max}}{n_{\text{wave}} n_{\text{pt}}}.\end{aligned}\tag{7.8}$$

Algorithm 7.5 is used to solve the transient problems.

Algorithm 7.5. Transient solver setup

```

1  c_step = 1
2  file_phi << (unkn.split())[0], t)
3  file_u   << (unkn.split())[1], t)
4  start_time = time.time()
5  while t < t_max:
6      if processID == 0:
7          elapsed = int(time.time() - start_time)
8          e_h, e_m, e_s = int(elapsed/3600), \
9              int(elapsed % 3600 / 60), \
10             int( ( elapsed % 3600 ) % 60 )
11         print('step %.0f, %.3f MHz' %(c_step, nu))
12         print('----- time %e s in %.0f h %.0f min %.0f s ' \
13             % (t, e_h, e_m, e_s) )
14         t += Dt
15
16     actuator.t = t
17
18     solve(Form == 0, unkn, bc, J=Gain,
19         solver_parameters={ \
20             "newton_solver":{"linear_solver":"mumps",
21                 "preconditioner":"none",
22                 "relative_tolerance": 1e-5}},
23         form_compiler_parameters={"cpp_optimize": True,
24             "representation":"uflacs"})
25
26     file_phi << (unkn.split())[0], t)
27     file_u   << (unkn.split())[1], t)
28
29     assign(unkn00, unkn0)
30     assign(unkn0, unkn)
31
32     c_step += 1

```

8. THICKNESS-SHEAR VIBRATIONS IN PIEZOELECTRIC PLATES

The thickness-shear (TSh) mode is a bulk mode in contrast to SAW. The waves are in the thickness of a bulk material. The bulk material is sandwiched between two thin electrode plates and the one of them is grounded while the other exposed to alternating electric potential. The system is similar to a capacitor element. Applied electric potentials create a uniform electric field to excite the piezoelectric material. Excitation returns in a characteristic deformation mode depending on the used material. TSh is amongst them, and commonly used in bulk acoustic wave (BAW) sensors to sense chemical agents inside some fluidic environment. The oscillating application of electric potential causes to material vibrate at its resonance frequency to amplify the response. AT-cut Quartz is one of the materials used in BAW sensors as it is less sensitive to the temperature changes. We are examining the AT-cut Quartz because it is a benchmark problem for us to evaluate our code in terms of the resonance frequency spectrum and the transient response at a frequency in the spectrum.

The TSh problem is well defined in [46,47], and illustrated in Figure 8.1. $x_2 = 0$ and $x_2 = h$ surfaces are traction free such that

$$n_j \sigma_{ji} = 0 . \quad (8.1)$$

Although electrodes have some thickness as well, it is negligible as they are very thin compared to the plate. Therefore, geometry of the electrodes are not included in Figure 8.1. The infinite plate is modeled with an RVE shown in Figure 8.2, and coded in Algorithm 8.1.

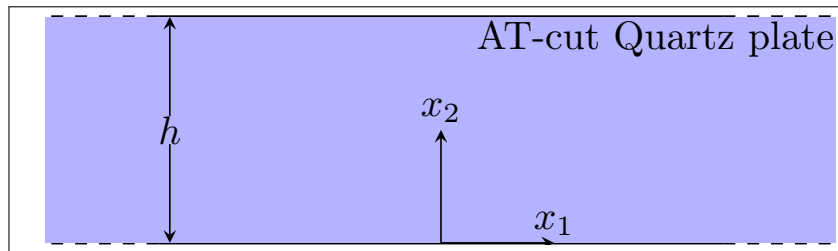


Figure 8.1. Cross-section of an infinite piezoelectric plate with thickness, h .

In order to satisfy the unidirectional PBC, i.e. in x_1 and x_2 directions, <BOOLEAN> and <ALGORITHM> in Algorithm 3.6 are replaced by Algorithms 8.2 and 8.3, respectively.

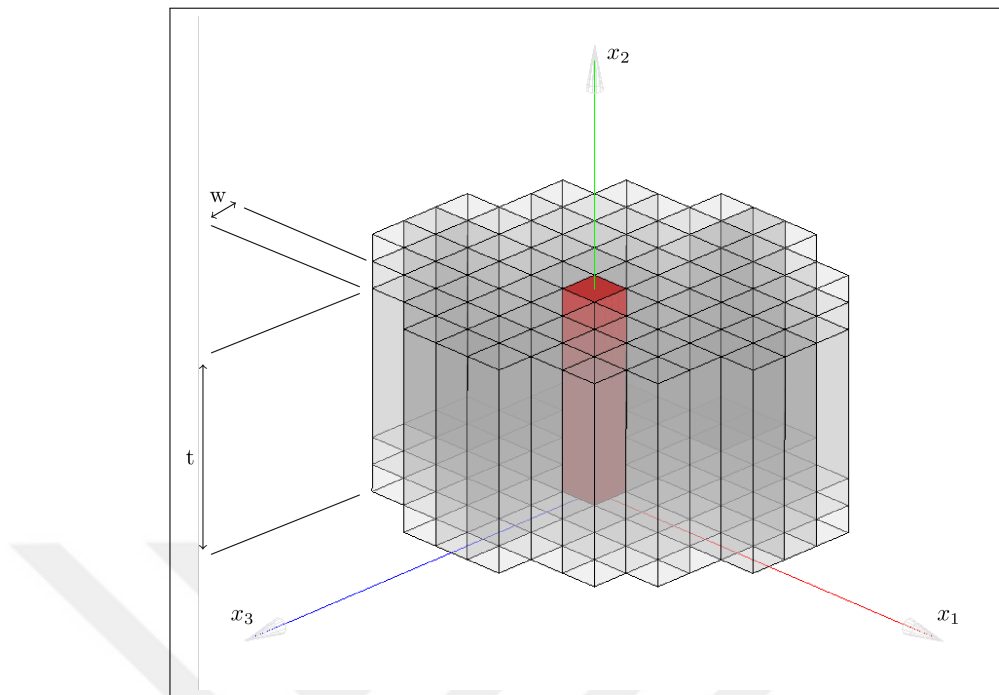


Figure 8.2. RVE of the infinite plate colored in magenta.

Algorithm 8.1. TSh RVE geometry and mesh declarations

```

1 xmin, xmax = 0, 0.000125
2 ymin, ymax = 0, 0.002
3 zmin, zmax = 0, 0.000125
4
5 l1 = xmax; l2 = ymax; l3 = l1
6 N1 = 1; N2 = 16; N3 = N1
7 mesh = BoxMesh(Point(0,0,0), Point(l1, l2, l3), N1, N2, N3)

```

Algorithm 8.2. <BOOLEAN> in Algorithm 3.6

```

1 bool ( on_boundary and (
2   ( near ( x [0] , xmin , TOL ) and not \
3   ( near ( x [2] , zmax , TOL ) \
4   and near ( x [0] , xmin, TOL ) ) ) or \
5   ( near ( x [2] , zmin , TOL ) \
6   and not ( near ( x [2] , zmin , TOL ) and near \
7   ( x [0] , xmax , TOL ) ) )
8 ))

```

Algorithm 8.3. <ALGORITHM> in Algorithm 3.6

```

1  if near ( x [2] , xmax , TOL ) and near ( x [0] , xmax , TOL ) :
2      y [0] = x [0] - ( xmax - xmin )
3      y [1] = x [1]
4      y [2] = x [2] - ( xmax - xmin )
5  elif near ( x [0] , xmax , TOL ) :
6      y [0] = x [0] - ( xmax - xmin )
7      y [1] = x [1]
8      y [2] = x [2]
9  else :
10     y [0] = x [0]
11     y [1] = x [1]
12     y [2] = x [2] - ( xmax - xmin )

```

Mesh and functions are declared as in Algorithm 7.1, and the matrices in Equation (6.8) are assembled in Algorithm 6.1. Static condensation given in Equation (7.4) is implemented in Algorithm 7.2. Material parameters in Algorithms 4.1 to 4.3 are given by AT-cut Quartz,

$$\begin{aligned}
 \mathbf{C}^{\text{mat}} &= \begin{bmatrix} 8.6736 & 2.550 & -6.611 & 8.299 & 0 & 0 \\ 2.550 & 2.473 & -3.11 & -17.91 & 0 & 0 \\ -6.611 & -3.11 & 107.19 & 0 & 0 & 0 \\ 8.299 & -17.91 & 0 & 0.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.5 & -17.91 \\ 0 & 0 & 0 & 0 & -17.91 & 39.88 \end{bmatrix} \times 10^{-12} \text{ TPa} \\
 \tilde{\mathbf{T}}^{\text{mat}} &= \begin{bmatrix} -20.9 & -0.171 & 0 & 0.0436 & 0 & 0 \\ 0 & -53.3 & 0 & 0 & 0.0 & 0.813 \\ 0 & 0 & 0 & 0 & 0 & 8.41 \end{bmatrix} \text{ C/m}^2 \\
 \boldsymbol{\epsilon}^{\text{mat}} &= \begin{bmatrix} 39.84 & 0 & 0 \\ 0 & 39.84 & 0 \\ 0 & 0 & 40.73 \end{bmatrix} \times 10^{-12} \text{ C/V - m}
 \end{aligned} \tag{8.2}$$

n_{th} resonance frequency of the TSh mode is calculated with respect to C_{1212} and the thickness of the plate,

$$\nu_n = \frac{n}{2h} \sqrt{\frac{C_{1212}}{\rho}}, \tag{8.3}$$

where $\rho = 2651 \text{ kg/m}^3$. Therefore, we select first resonance frequency as the target frequency

for the SLEPc solver,

$$\nu_1 = \frac{1}{2h} \sqrt{\frac{C_{1212}}{\rho}} = 827.045 \text{ kHz} , \quad (8.4)$$

$$\Sigma_{\text{TSh}} = (2\pi\nu_1)^2$$

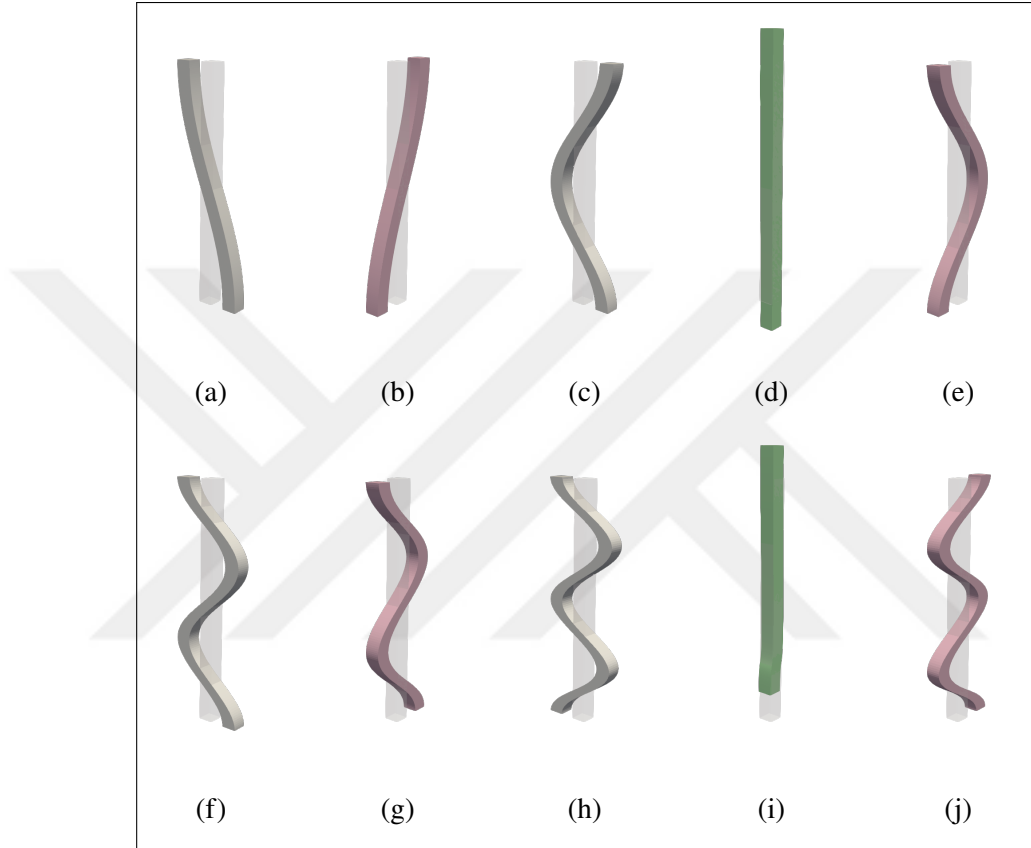


Figure 8.3. SLEPc solver results (in kHz) of the $8 \times 128 \times 8$ mesh for ten eigenvectors around 830 kHz (same scale factor is used), colors denote differing directions, gray and red deformations are bending along x and z -axes, green is stretching along y -axis. (a) 830 (b) 950 (c) 1660 (d) 1752 (e) 1900 (f) 2491 (g) 2850 (h) 3322 (i) 3503 (j) 3800

For the transient solutions, the effect of n_{pt} in Equation (7.8) is also examined. n_{pt} takes the values in $\{40, 80, 160, 320\}$. Corresponding time intervals are represented by $\{\Delta t, \Delta t/2, \Delta t/4, \Delta t/8\}$. Then three frequencies are selected: smaller than, equal to, and larger than ν_1 ,

$$\nu \in \{100.000, 827.045, 3000.000\} \text{ kHz} . \quad (8.5)$$

ν , is given as the excitation frequency in the form of Equation (3.14) from the top surface, and the bottom surface is grounded. 20 waves are solved, and the displacements in x_1 direction, u_1 , from the middle point of the top surface is plotted in Figures 8.4a to 8.4c.

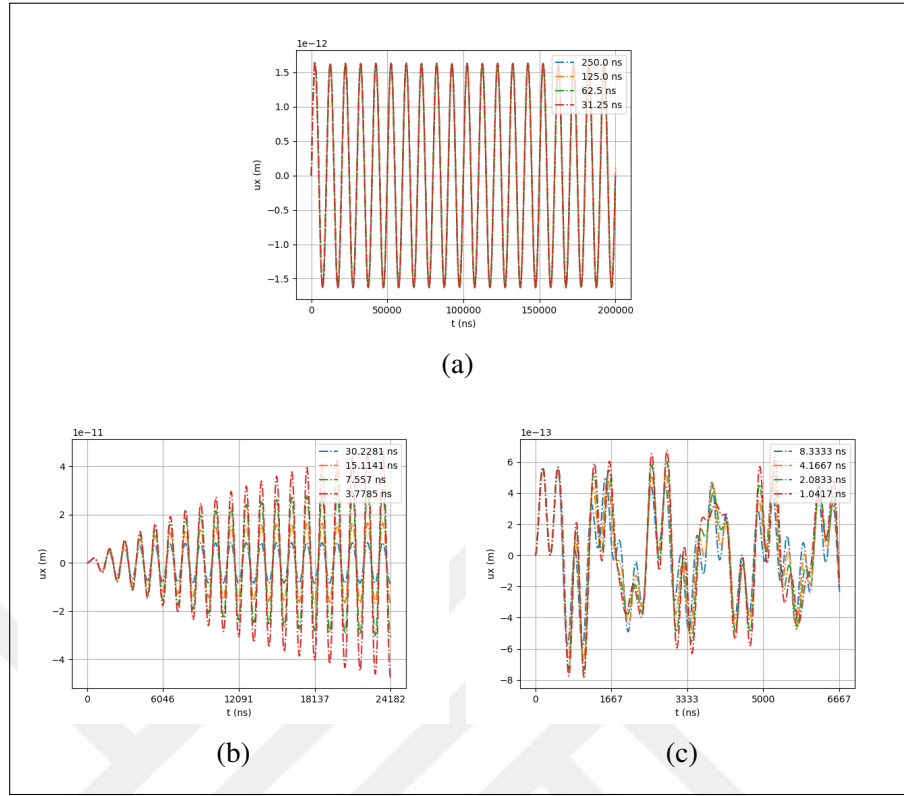


Figure 8.4. TSh transient benchmark for u_1 for different n_{pt} and v . (a) Comparison of u_x at 100.000 kHz; Δt (250.0 ns), $\Delta t/2$ (125.0 ns), $\Delta t/4$ (62.5 ns), and $\Delta t/8$ (31.25 ns) (b) Comparison of u_x at 827.045 kHz; Δt (30.2281 ns), $\Delta t/2$ (15.1141 ns), $\Delta t/4$ (7.557 ns), and $\Delta t/8$ (3.7785 ns) (c) Comparison of u_x at 3000.000 kHz; Δt (8.3333 ns), $\Delta t/2$ (4.1667 ns), $\Delta t/4$ (2.0833 ns), and $\Delta t/8$ (1.0417 ns)

All the results are expected in Figure 8.4; since displacements are not amplified below the resonance frequency, resonance occurs at the resonance frequency, and no resonance occurs but the mode of the vibration is not the fundamental mode anymore above the resonance frequency for all time discretizations.



9. DESIGN GUIDELINE FOR LOVE TYPE SAW SENSORS

A design guideline is needed for getting data to characterize the layered sensors. Finite element is also viable in addition to analytical solutions, and finite element method can be extended to novel concepts such as wave guiding application under SAW concept. Scope of the design guideline is a piezoelectric substrate with a dielectric layer showing Love mode under liquidic environment. Although the sensor works under fluid, we do not consider the fluid in the simulations because Love type sensors do not radiate acoustic wave energy as much as Rayleigh mode. Therefore, kinematics of the particles on the surface is assumed to be not affected by the fluid environment. An λ -periodic RVE is constructed for the sensor, and the resonance frequencies are calculated by the method developed in Chapter 8. Calculated frequencies are then used as fitted variables for an analytical mass sensitivity solution. Some material properties are let free in the fitting operation.

A typical operational environment is given in Figure 9.1. As the number of particles increase on the sensitive layer, the accumulated mass changes the wave speed, Δv , and therefore the frequency of the waves, Δf , through

$$f = \frac{v}{\lambda}. \quad (9.1)$$

The change in the Love wave speed and frequency for substrate/layer system are shown to be dependent on the layer thickness in [21] for a delay line or standing wave oscillator. This phenomenon is called *dispersion*, and can be modeled by the *dispersion equation* in [23,48]. We need to know the wave speed, also known as *phase speed*, v , shear horizontal wave speed of the substrate and layer, v_s and v_g respectively, shear moduli of the substrate and layer, μ_s and μ_g respectively. These parameters are related to thickness of the h material through the dispersion equation

$$\tan \left(2\pi v \frac{h}{\lambda} \sqrt{\frac{1}{v_g^2} - \frac{1}{v^2}} \right) = \frac{\mu_s}{\mu_g} \sqrt{\frac{1 - (v^2/v_s^2)}{(v^2/v_g^2) - 1}}. \quad (9.2)$$

As a standard procedure v in Equation (9.2) is the dependent variable due to the fact that h is changing as the design parameter such that $v = v(\hat{h})$. Yet, v cannot be solved directly.

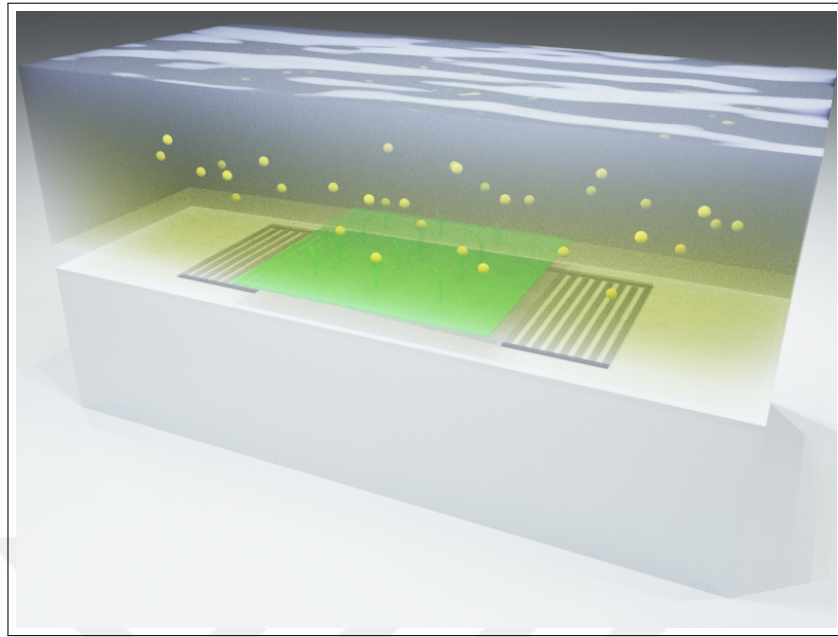


Figure 9.1. Love mode SAW sensor working under liquid environment. Particles are captured by the sensitive layer (green).

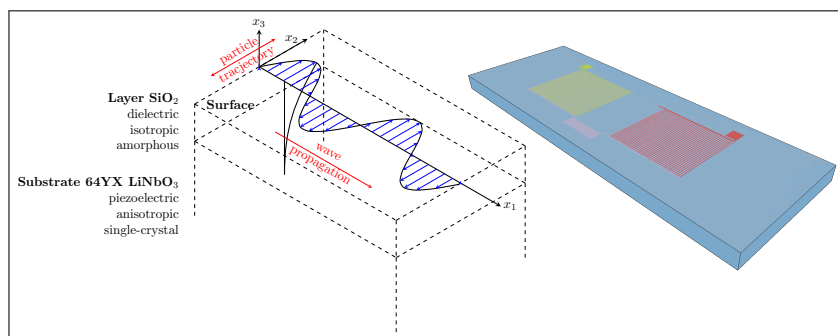


Figure 9.2. Love wave configuration

Instead, we can solve for the normalized thickness, $\hat{h} = \frac{h}{\lambda}$, shown in Figure 3.5c

$$\hat{h}(v) = \frac{1}{2\pi\sqrt{v^2/v_g^2 - 1}} \arctan \left[\frac{\mu_s}{\mu_g} \sqrt{\frac{1 - v^2/v_s^2}{v^2/v_g^2 - 1}} \right], \quad (9.3)$$

where

$$v_s = \sqrt{\frac{\mu_s}{\rho_s}}, \quad v_g = \sqrt{\frac{\mu_g}{\rho_g}}. \quad (9.4)$$

We can introduce some free parameters to validate the EVP results, which are depicted in Figure 9.3. The $\hat{h}$ is changed within $[0, 1]$, yet some eigenvectors do not show the Love mode. Wave speeds for the correct eigenvectors are written in Table 9.1. The set of free parameters is $\beta = \left\{ \alpha = \frac{\mu_s}{\mu_g}, v_s, v_g \right\}$. We fit Equation (9.3) curve on the data in Table 9.1, $D = \{(v_i, \hat{h}_i)\}$, by the Levenberg–Marquardt algorithm (LMA) [49]

$$\hat{\beta} \in \arg \min_{\beta} \sum_{i=1}^{\#D} \left[\hat{h}_i - \hat{h}(v_i, \beta) \right]^2. \quad (9.5)$$

Table 9.1. EVP data obtained by FEniCS for the geometry in Figure 3.5c.

$\hat{h}_i$	g_h (μ m)	v_i (m/s)
0.0	0.0	4696
0.000625	0.65	n/a
0.00125	1.3	n/a
0.025	2.6	4606
0.05	5.2	4629
0.1	10.4	4555
0.2	20.8	4280
0.4	41.6	3983
0.6	62.4	3807
0.8	83.2	3756
1.0	104.0	3690

Initial values for β is equal to $\beta_0 = \{2.32, 4606 \text{ m/s}, 3583.83 \text{ m/s}\}$. LMA stops after 3 iterations, and the final sum of squares of residuals and relative change during last iteration are 0.00860711 and $-8.17992(10^{-6})$, respectively.

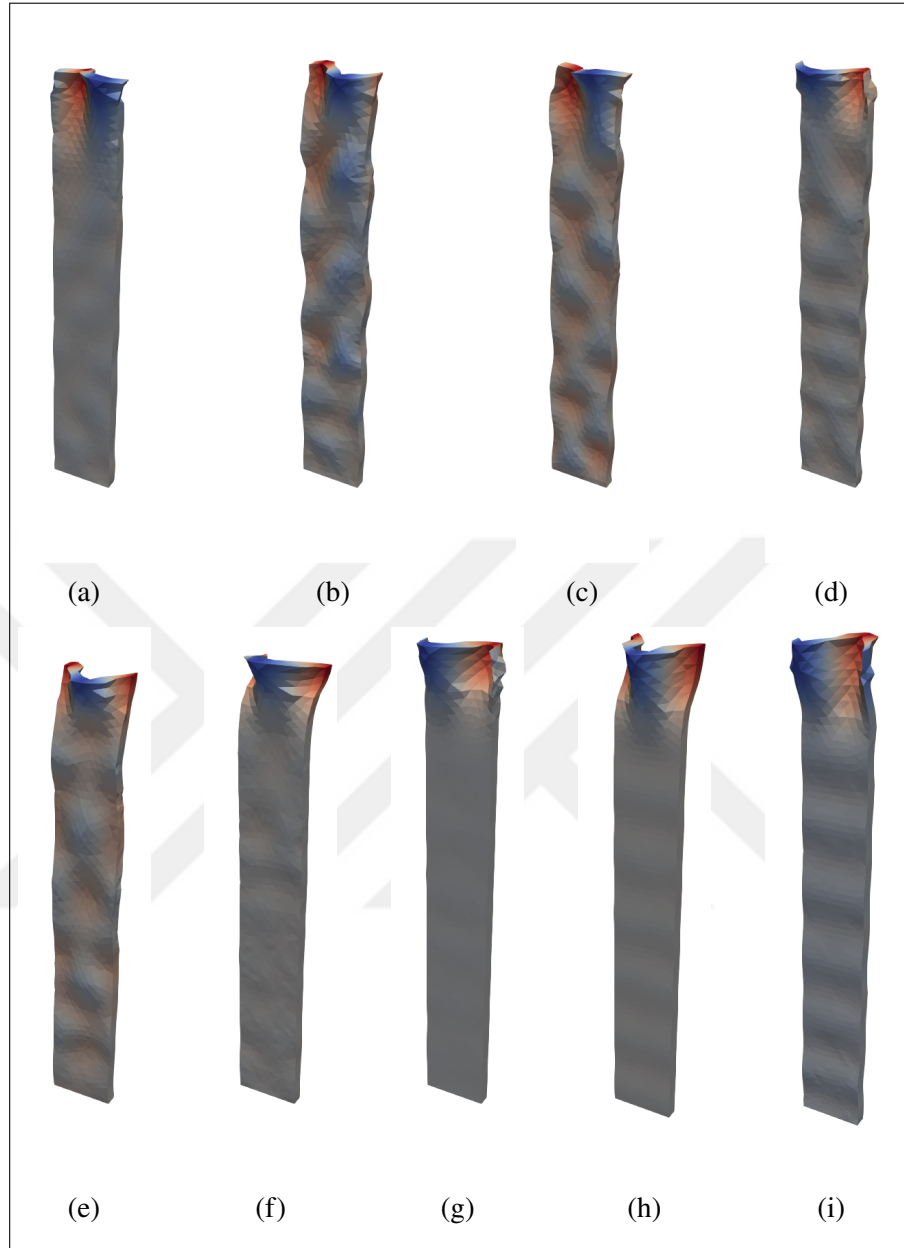


Figure 9.3. SLEPc solver results for 64YX LN/SiO₂. u_2 is colored. Their wave speeds are written in Table 9.1. Layer thicknesses in μm : (a) 0.0 (b) 2.6 (c) 5.2 (d) 10.4 (e) 20.8 (f) 41.6 (g) 62.4 (h) 83.2 (i) 104.0

Final set of parameters, and their asymptotic standard error (ASE) are given in Table 9.2

Table 9.2. LMA results obtained by Gnuplot

Parameter	Value	ASE ($\pm$)	ASE (%)
α	2.32061	0.5207	22.44
v_s (m/s)	4610.78	18.48	0.4008
v_g (m/s)	3603.72	7.396	0.2052

To plot the obtained fit, we rewrite Equation (9.3) as a parametric function

$$\begin{aligned} v &= f_y(t) = a + (b - a)t, \\ \hat{h} &= f_x(t) = \hat{h}(f_y(t)), \end{aligned} \quad (9.6)$$

such that as we change the parameter, t , within $[0, 1]$ the solution points on the dispersion curve, η , is obtained

$$\eta(f_x(t), f_y(t)) = 0. \quad (9.7)$$

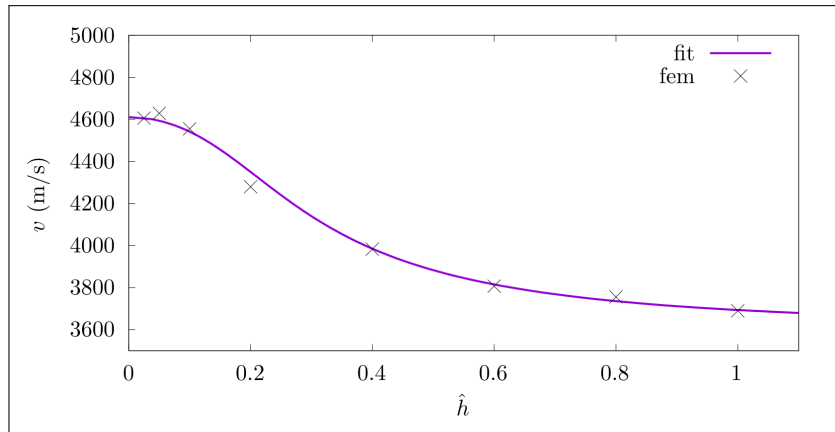


Figure 9.4. Dispersion curve using the parametric functions with fitted parameters.

Mass sensitivity concept is a measure of success for an optimal Love type SAW sensor design. There are various types of mass sensitivity definitions. We propose a mass sensitivity calculation. In order to derive such a definition, an initial equation is given

$$S = \lim_{\Delta M \rightarrow 0} \frac{\Delta R}{\Delta M} = \frac{\partial R}{\partial M}, \quad (9.8)$$

where R is the response, and M is the measured quantity from the sensor. From Equation (9.8), we can observe that there is a proportional change between the response, and the measurement. Consider a substrate/layer system. If the layer thickness increases, v decreases from the experimental results. This behaviour is interpreted as a gradual encapsulation of the acoustic wave energy into the layer due to the fact that increase in volume of the layer material.

R can be taken as v , and we also know that addition of a layer brings a mass due to ρ_g . The added mass is defined as mass added per area of the substrate

$$\Delta M = \frac{\rho_g h A}{A} = \rho_g h . \quad (9.9)$$

Therefore, Equation (9.8) is rewritten in terms of the phase velocity, and the added mass due to the guide layer

$$S = \lim_{\Delta \rho_g h \rightarrow 0} \frac{\Delta v}{\Delta \rho_g h} = \frac{\partial v}{\partial \rho_g h} . \quad (9.10)$$

Equation (9.10) is in $\text{m}^3/\text{kg}\cdot\text{s}$. We can further multiply and divide the denominator by λ , and normalize Equation (9.10) by the fitted v_s ,

$$S_m = \frac{S}{v_s} = \frac{1}{v_s} \frac{1}{\lambda \rho_g} \frac{\partial v}{\partial \hat{h}} . \quad (9.11)$$

Equation (9.11) is in m^2/kg , and the velocity change with respect to normalized thickness is achieved.

Thus if we solve for $\frac{\partial v}{\partial \hat{h}}$ from Equation (9.2) with parametric functions in Equation (9.6), we get Equation (B.1). v and $\frac{\partial v}{\partial \hat{h}}$ in Equation (9.11) are substituted with Equations (9.7) and (B.1), respectively. Therefore, S_m calculated using parameter t .

Thus we propose a design guideline to obtain the mass sensitivity for a substrate/layer type sensor, which is illustrated in an algorithmic fashion in Figure 9.6. The algorithm works for Love mode SAW sensors having standard bidirectional IDT configuration, because they are dispersive. We first decide on the materials, the cut angle for the substrate, and one of the operational frequency/electrode length needed for the intended wave mode.

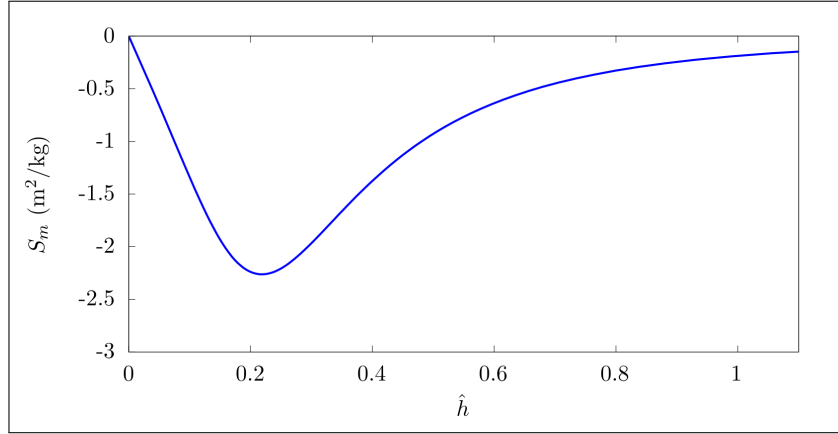


Figure 9.5. Mass sensitivity curve using the proposed derivation with fitted parameters.

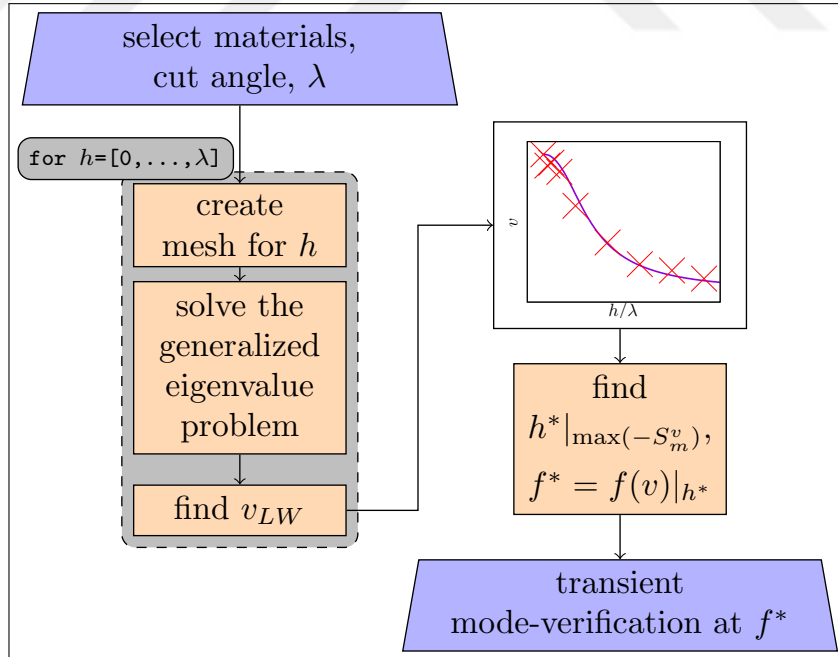


Figure 9.6. Design guideline to obtain maximum sensitivity of a dispersive Love type SAW sensor

10. TRANSIENT SOLUTIONS

Transient solutions are used to obtain the displacements and voltages while time goes from 0 μs to $t_{\max}$. The main idea here is to compare the variables of different models: RVE, slice, and full-sensor. These three models are in the order of increasing DOF. In addition, we can compare the variables from EVP and transient for the same configuration and mesh. We specifically look at the differences between EVP, and transient solutions of the RVE shown in Figure 3.5c. The effect of the voltage Dirichlet conditions in transient, and patchless model of the EVP will be emphasized. For the slice, and full-sensor models the variables are further compared.

Patchless, and patched configurations are first evaluated. The same geometry, and mesh as shown in Figure 10.1 is used. The elements on the interface is configured such that there are 8 elements in x_1 -direction, and 2 elements in x_2 -direction; because we will apply boundary patch boundary conditions as given in Algorithm 10.1. The dimensions of the unit-cell sensor RVE is composed of the guiding layer thickness in x_3 -direction, $g_h = 41.6 \mu m$, substrate thickness in x_3 -direction, $s_h = 700 \mu m$, width in x_2 -direction, $y_{\max} = 20 \mu m$, and length in x_1 -direction, $\lambda = 104 \mu m$.

In order to see the effect of Dirichlet boundary conditions in transient solution, we first need to reveal the potential difference on the path of $(0, y_{\max}/2, s_h) - (\lambda, y_{\max}/2, s_h)$. The eigenvalue results are shown in Figures 10.2a and 10.2b for warped u_i but colored with respect to u_2 , and ϕ , respectively. Figure 10.2b is also clipped from the substrate/layer interface, and resulting images are shown in Figures 10.2c and 10.3. The path plot for Figure 10.3 is shown in Figure 10.3. As it can be seen ϕ makes a λ -periodic fluctuation over the nodes of the path.

Same mesh is used in the transient solution. In this case, Algorithm 10.1 is applied to the elements on the interface. We solved for 20 waves, which has 1000 time steps. Therefore, 988 step is taken to get the peak of ϕ for a considerable stable solution. Similar presentation of the results are given in Figure 10.4. As it can be seen from Figure 10.4a, the vibration mode is different from the EVP counterpart in Figure 10.2a. Difference is also valid for Figures 10.4b, 10.4c and 10.5. The path plot in Figure 10.5 shows the difference in the application of the Dirichlet boundary condition. Although different modes of vibration are observed due to the

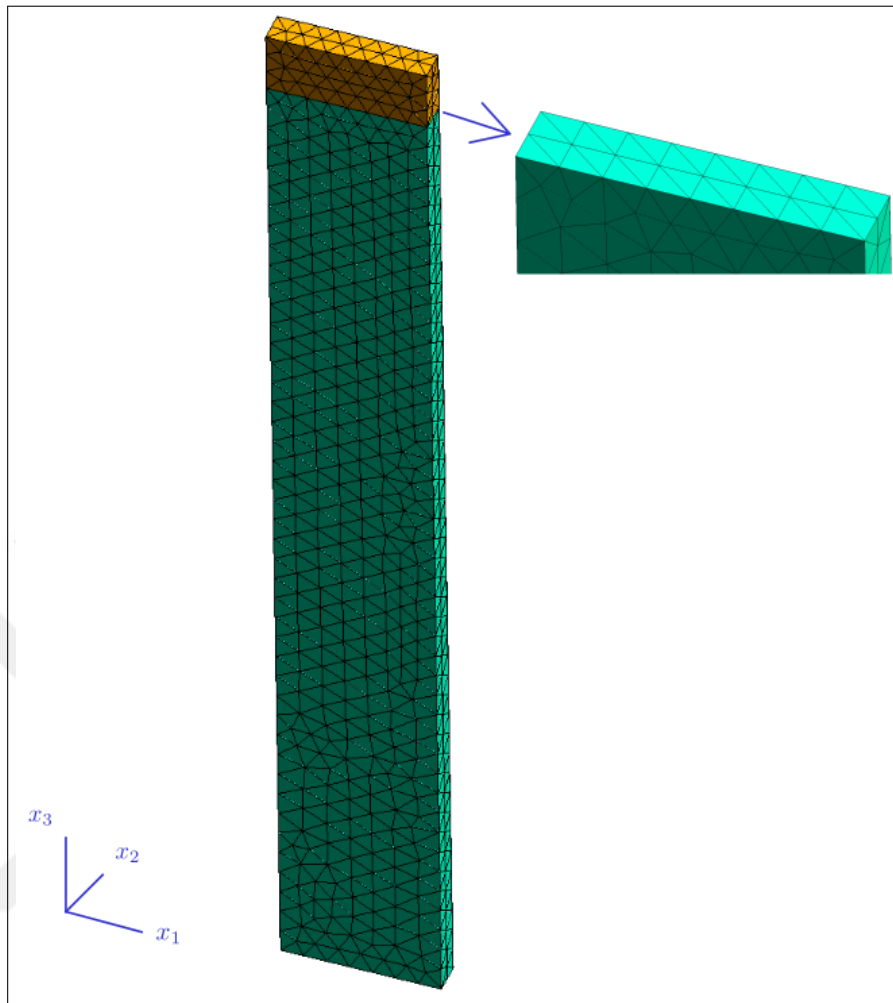


Figure 10.1. Mesh of the 41.6 μm layer thickness of SiO_2 on top of 64YX LN

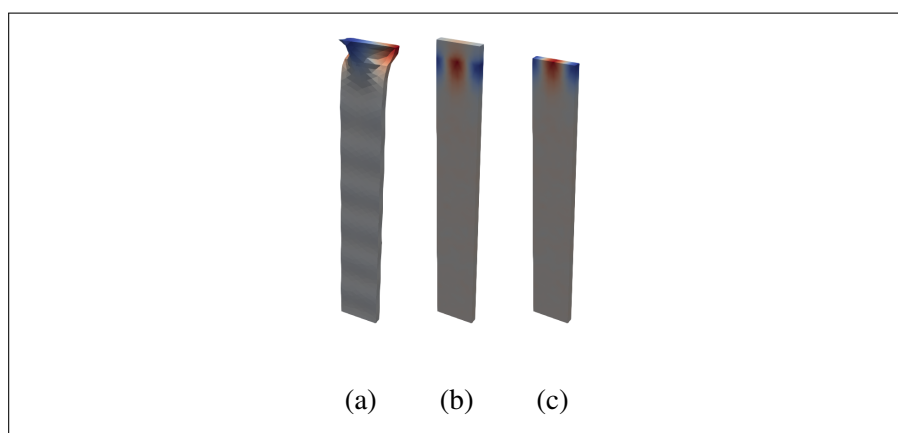


Figure 10.2. Eigenvectors, and voltage plot for 64YX LN/ SiO_2 with layer thickness of 41.6 μm . The eigenvectors are obtained at 3981 m/s. (a) Displacement eigenvector (b) Electric potential eigenvector (c) Voltage at the substrate/layer interface, i.e. the layer is clipped

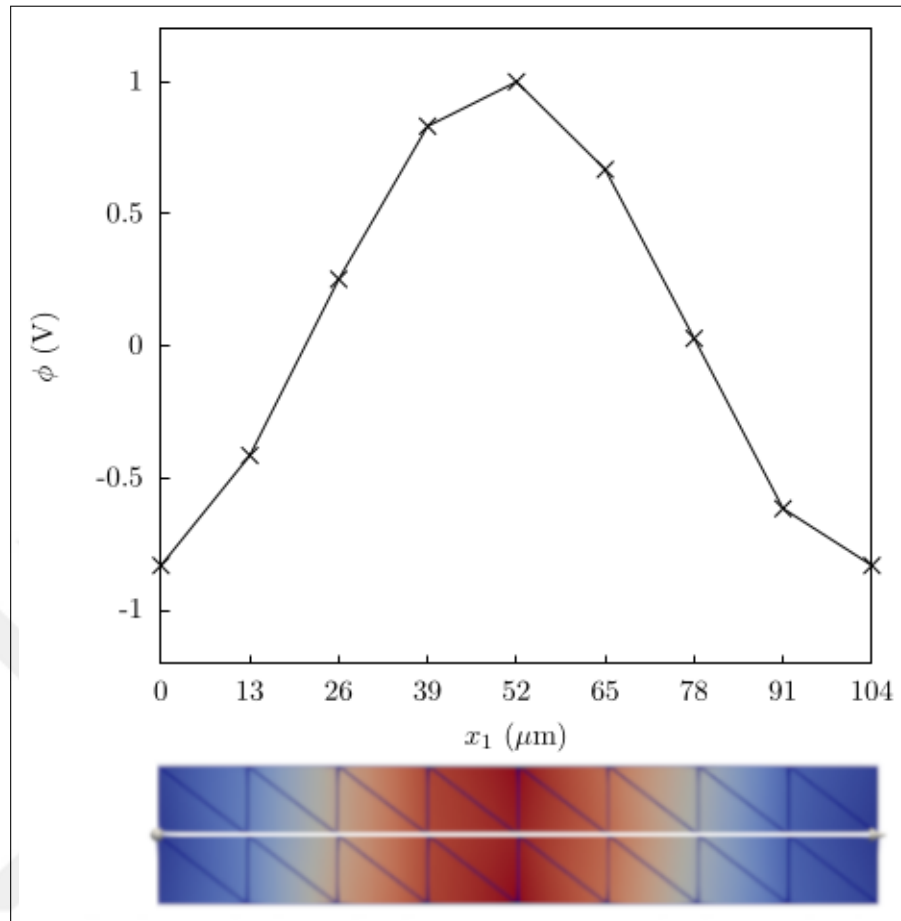


Figure 10.3. Interface voltage plot over the line $(0, y_{\max}/2, s_h) - (\lambda, y_{\max}/2, s_h)$ of Figure 10.2c

different ϕ applications, we can say that the transient application is successfully achieved.

Algorithm 10.1. Patch configurations for the application of Dirichlet boundary conditions

```

1  class Patch1(SubDomain):
2      def inside(self, x, on_boundary):
3          tol = 1E-8
4          p_h = near(x[2], s_h, tol)
5          p_A = x[0] > (lmbda/8) - tol and x[0] < \
6              (lmbda/8 + lmbda/4) + tol
7          return p_h and p_A
8
9  class Patch2(SubDomain):
10     def inside(self, x, on_boundary):
11         tol = 1E-8
12         p_h = near(x[2], s_h, tol)
13         p_A = x[0] > (lmbda/8 + lmbda/4 + lmbda/4) - tol and \
14             x[0] < (lmbda/8 + lmbda/4 + lmbda/4 + lmbda/4) + tol
15         return p_h and p_A

```

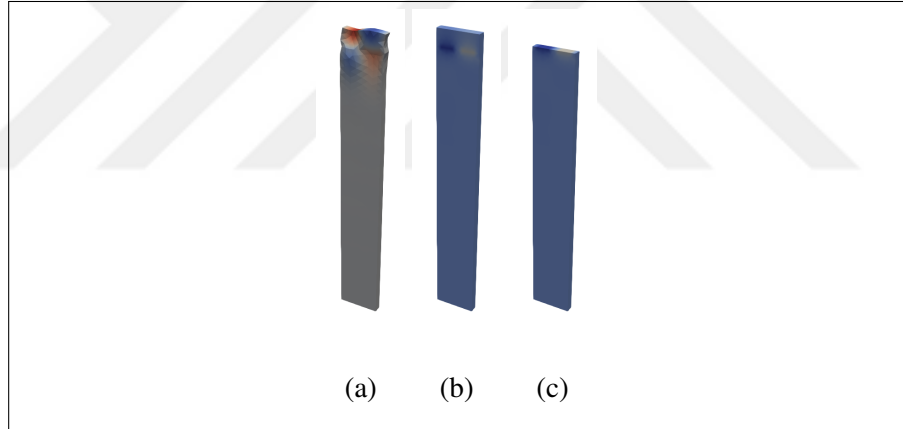


Figure 10.4. Transient solutions, and voltage plot for 64YX LN/SiO₂ with layer thickness of 41.6 μm . The solutions are obtained at 0.5162 μs , and 3981 m/s. (a) Displacement solution (b) Electric potential solution (c) Voltage at the substrate/layer interface, i.e. the layer is clipped

Equation (7.7) is now can be applied to further applications. In this case, a finite element (FE) model for the SAW sensor is created to verify wave modes depending on the material parameters via transient solution. The model is reduced from the full-sensor geometry, since only the wave modes are concerned. Due to the symmetry on the $x_1 - x_3$ plane of the middle section of the large delay length area, a 3D cross-sectional cut is taken from the full-sensor geometry as shown in Figure 3.2.

Geometry consists of 64YX LN/Silica, 2D IDT patches. The model is indicated in

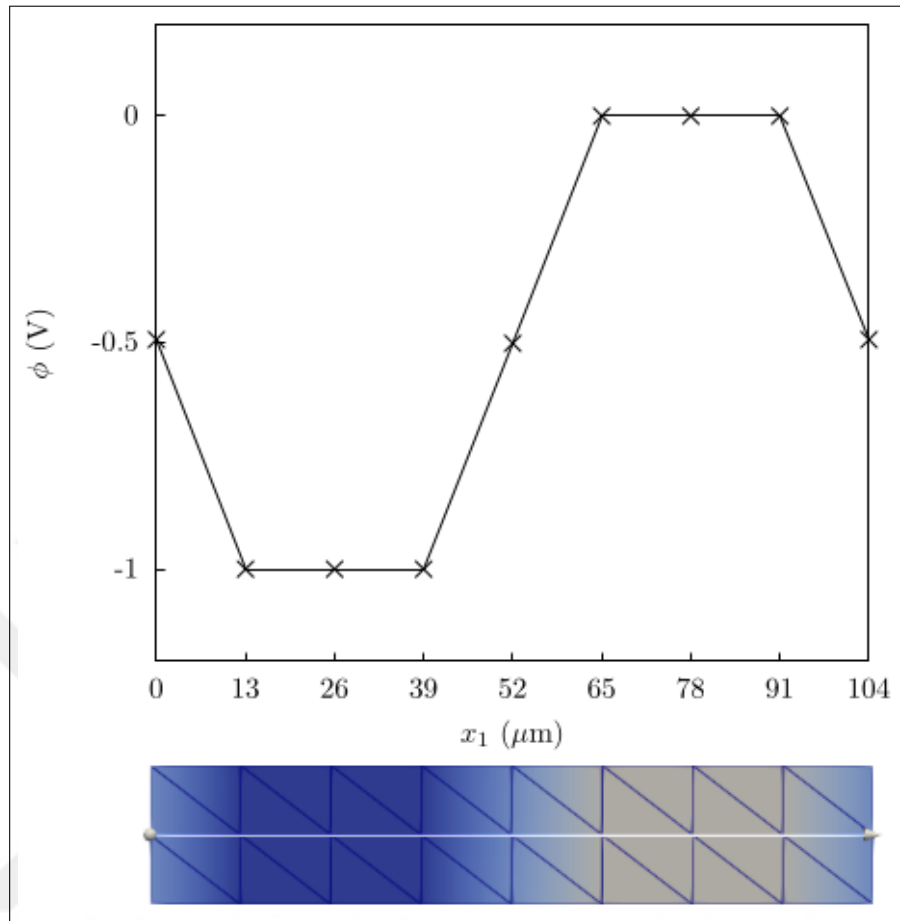


Figure 10.5. Interface voltage plot over the line $(0, y_{\max}/2, s_h) - (\lambda, y_{\max}/2, s_h)$ of Figure 10.4c

Figure 10.6. IDT is placed in the middle of the slice geometry in $\underline{e}_1$ direction, and consists of four pairs of voltage-ground electrodes as 2D patches. From the IDT to either ends is 20λ , such that no reflections from each end is not present for a 20 wave solution.

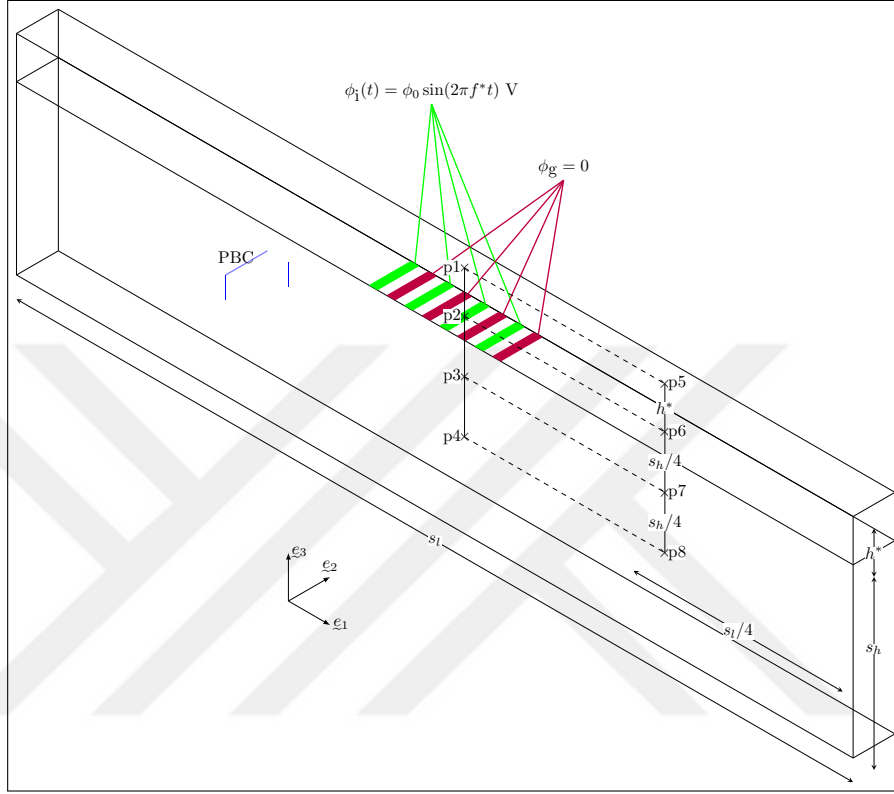


Figure 10.6. Transient slice geometry and boundary condition definitions for the optimized thickness

ω of Equation (3.14) is calculated by Equation (9.1) where ν is obtained from Figure 9.5, and λ is determined from the placement electrodes. Thus, applied frequency is $f^* = 41.107725$ MHz. A sinusoidal ϕ is applied from input voltage 2D patches as Dirichlet BC to excite the system as shown in Figure 10.6. ϕ for the ground patches are given as $\phi = 0$ V. PBC is applied on the planes perpendicular to $\underline{e}_2$ directions.

80 waves are solved, and a wave is generated within four electrode distance, and propagated to two ends of the geometry as seen in Figures 10.7 to 10.11.

The results are evaluated more precisely by looking at the time-history plots for u_i . A probe is located at p1 location shown in Figure 10.12 to get the solved variables. Group velocity effect is observed. If fast fourier transform is applied on the transient data, present frequencies including phase and group velocities can be extracted from the magnitude spectrum.

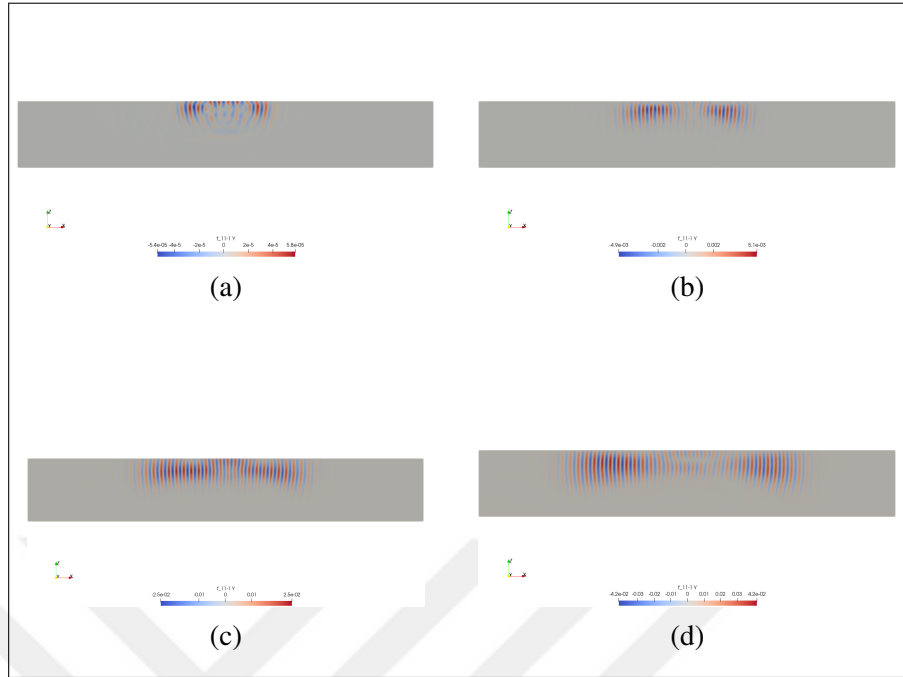


Figure 10.7. Contour plots of 64YX LN/Silica with the optimized thickness after (a) 4λ , (b) 8λ , (c) 12λ , (d) 16λ is solved.

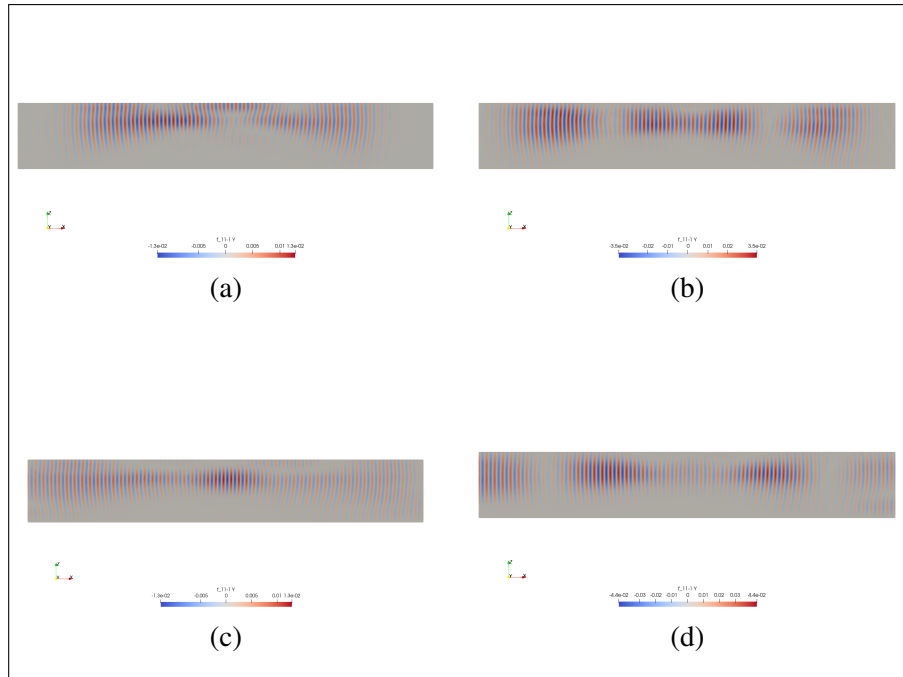


Figure 10.8. Contour plots of 64YX LN/Silica with the optimized thickness after (a) 20λ , (b) 24λ , (c) 28λ , (d) 32λ is solved.

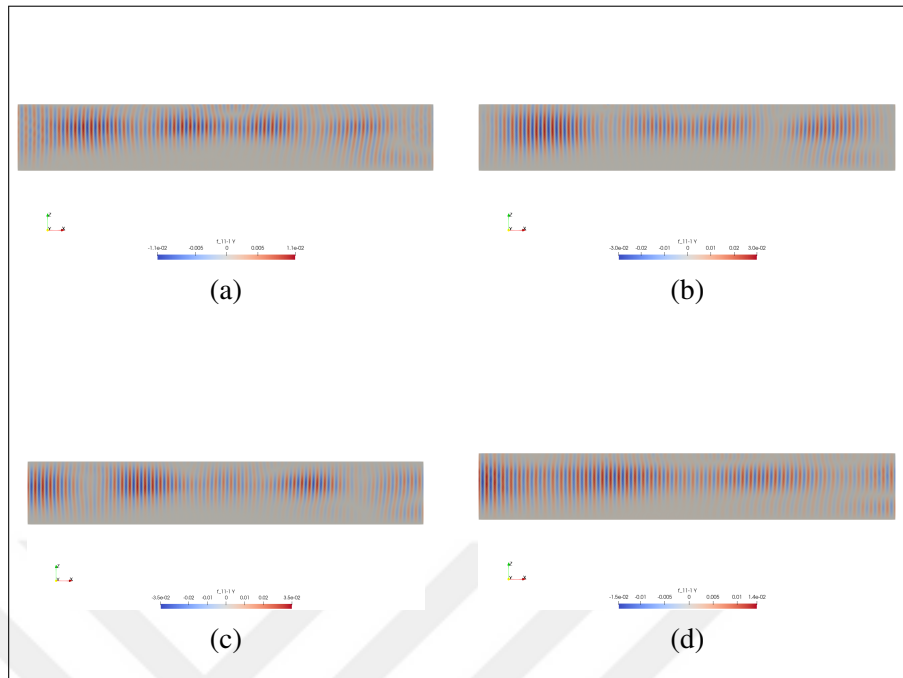


Figure 10.9. Contour plots of 64YX LN/Silica with the optimized thickness after (a) 36λ , (b) 40λ , (c) 44λ , (d) 48λ is solved.

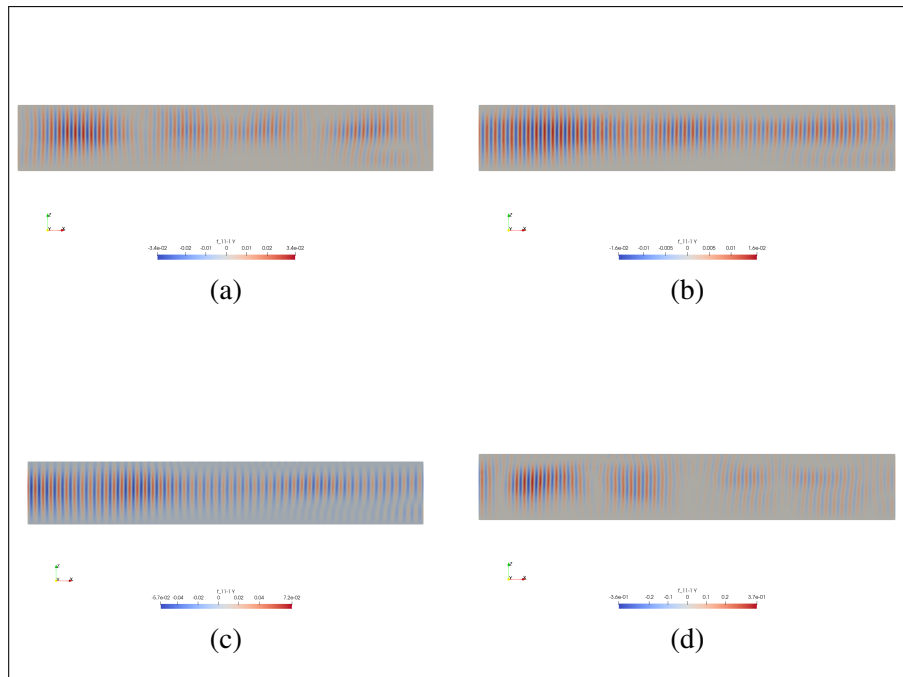


Figure 10.10. Contour plots of 64YX LN/Silica with the optimized thickness after (a) 52λ , (b) 56λ , (c) 60λ , (d) 64λ is solved.

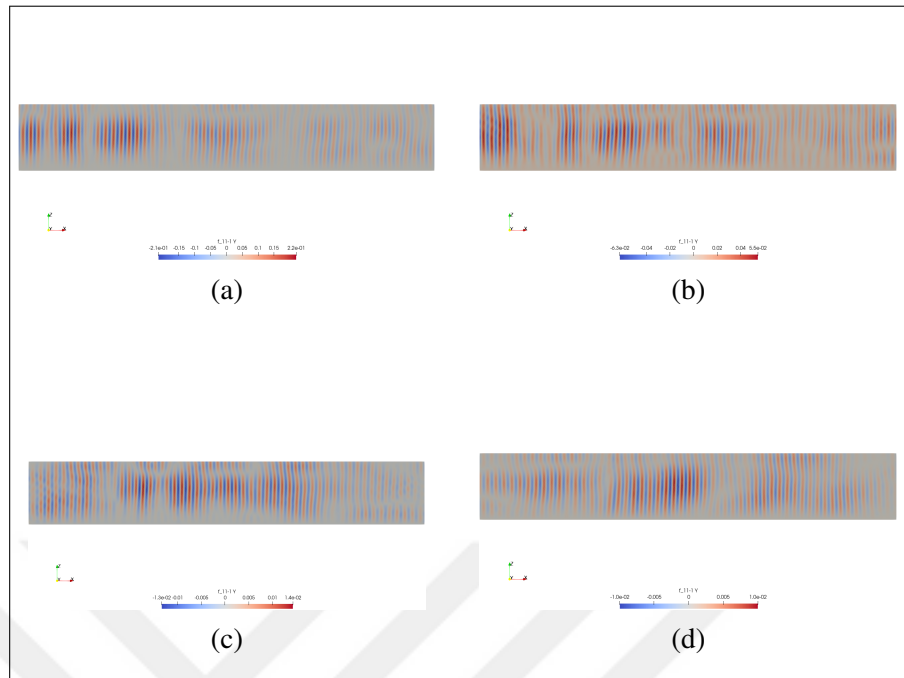


Figure 10.11. Contour plots of 64YX LN/Silica with the optimized thickness after (a) 68λ , (b) 72λ , (c) 76λ , (d) 80λ is solved.

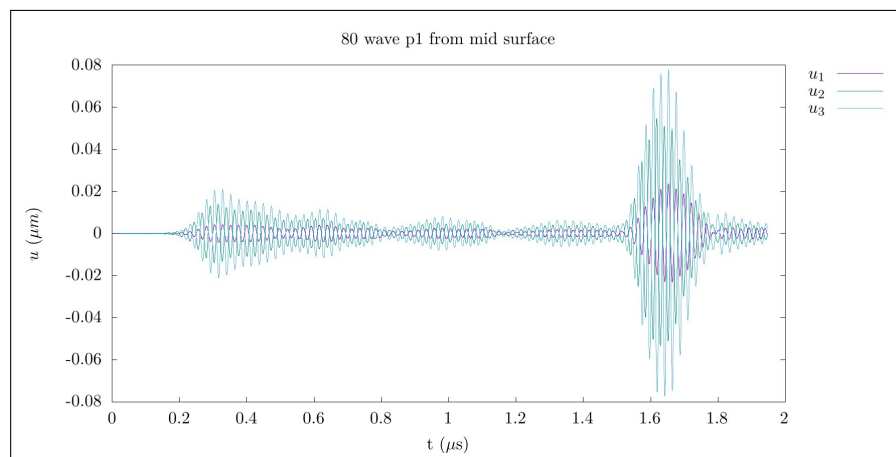


Figure 10.12. Time history plots of displacements of 64YX LN/Silica at the optimized thickness

Phase plotting is utilized to observe the displacement profile of the generated waves. For the Figure 3.5c, Figure 10.13 contains different thicknesses to analyse the thickness effect on the change of displacement magnitudes. From 41.6 μm , u_3 is increased.

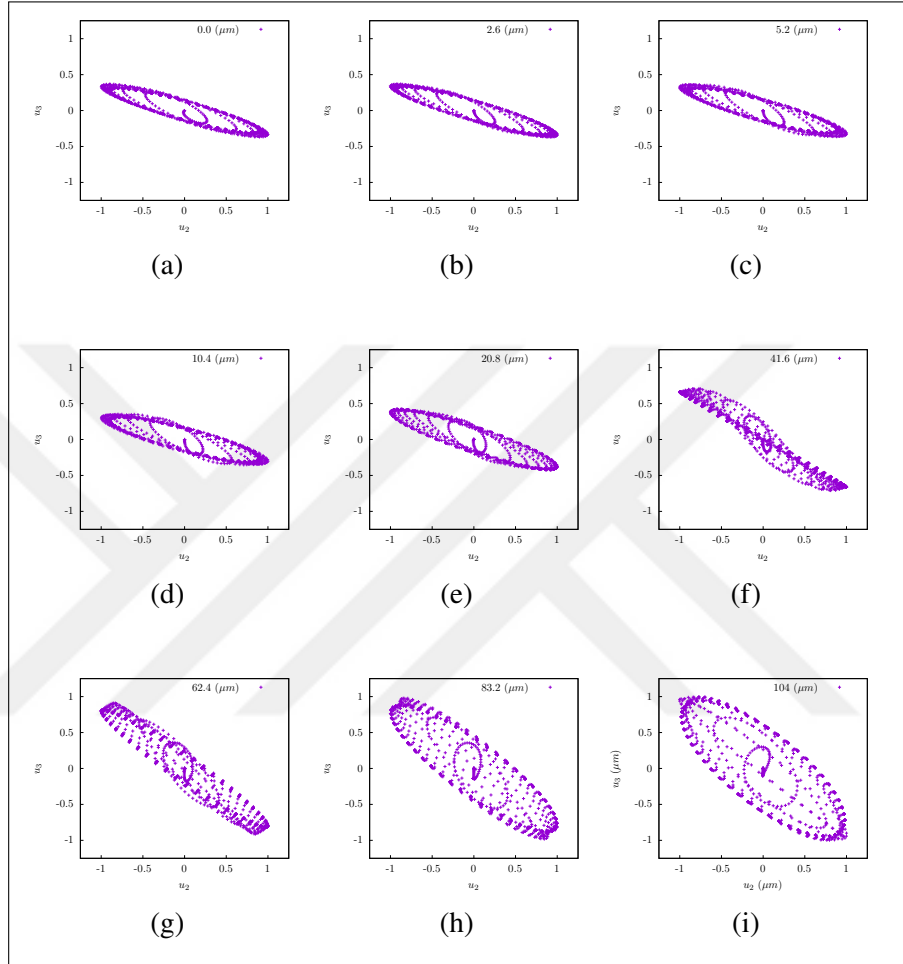


Figure 10.13. Phase plots for 64YX LN/Silica for the RVE (a) $g_h = 0 \mu\text{m}$ (b) $g_h = 2.6 \mu\text{m}$ (c) $g_h = 5.2 \mu\text{m}$ (d) $g_h = 10.4 \mu\text{m}$ (e) $g_h = 20.8 \mu\text{m}$ (f) $g_h = 41.6 \mu\text{m}$ (g) $g_h = 62.4 \mu\text{m}$ (h) $g_h = 83.2 \mu\text{m}$ (i) $g_h = 104 \mu\text{m}$

Further investigation of displacement profiles are conducted from the probes depicted in Figure 10.6. Results are given in Figure 10.14. Significant silence in displacements observed at p4 location which is under the middle input patch.

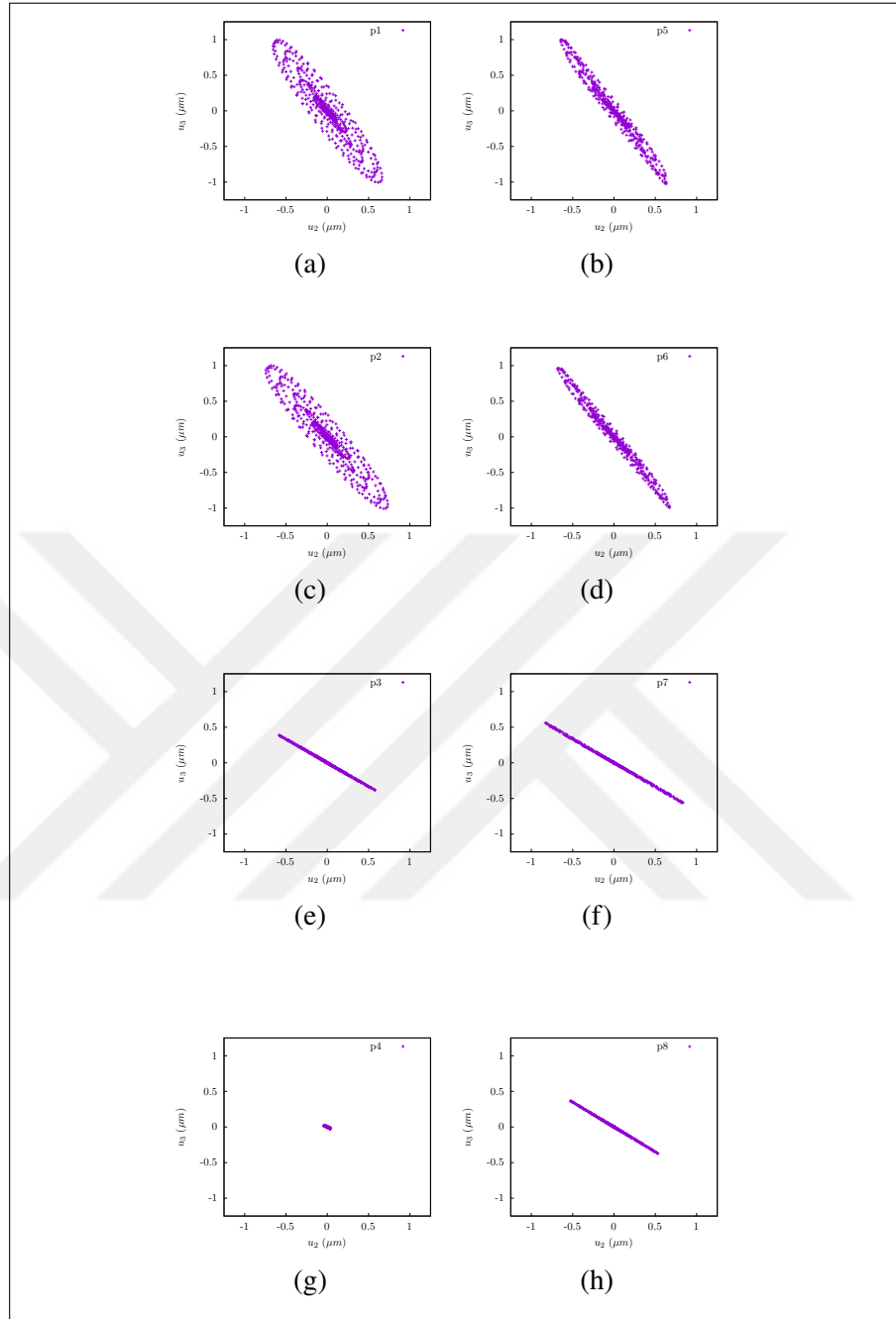


Figure 10.14. Phase plots for 64YX LN/Silica for the single IDT slice model (a) p1 (c) p2 (e) p3 (g) p4 (b) p5 (d) p6 (f) p7 (h) p8

11. CONCLUSIONS

In this thesis, computational modeling of the Love mode SAW sensors are discussed. The governing equations include balance, and constitutive equations that lead to variational formulation of a piezoelectric substrate with a layer on top. Discretization of the variational formulation is done in FEniCS. Equations are easily ported, and shown by code snippets through the thesis. The codes are presented in a modular fashion. Developed codes are applied to two analysis types: eigenvalue, and transient problems. These analyses are utilized in more specialized applications. First application is thickness-shear mode of a infinite AT-cut Quartz plate, which is a fundamental problem used in oscillator technology. Developed eigenvalue problem code is tested on an RVE of the geometry due to its simplicity. The results of the eigenvalue problem is verified by comparing them with the transient counterpart of the identical configuration. Second application is to construct a computational guideline aided with analytical solution to obtain the mass sensitivity of a Love type SAW sensor made with 64YX LN/SiO₂. In this application, verified code from the first application is applied to the eigenvalue problem of an RVE of a standard bidirectional IDT configuration. While changing the thickness of the guiding layer, the wave speeds of the eigenvectors showing Love mode are fitted onto an analytical dispersion equation to verify the computational algorithm. A proposed mass sensitivity measure is utilized to find an optimum guiding layer thickness for the maximum sensitivity for a given dispersive substrate/layer Love mode SAW sensor. Third application is the examination of the effect of Dirichlet boundary condition on the electric potential distribution, and the modes of vibration of the same RVE models of a Love mode SAW sensor. There are considerable differences in the modes, but the transient method is found to be applied properly on both models. Fourth application is the transient solution of a representative slice geometry taken from a prototype Love mode SAW sensor. In this application time-history plots of the displacements, and electric potentials are compared to observe the differences of grounded, and non-grounded output IDT electrodes. At the end, we concluded that a computational analysis framework is achieved to analyse Love mode SAW sensors to aid the development, and manufacturing.

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APPENDIX A: TOOLS

FEniCS has been around for 20 years. It incorporates different software components that are used to solve differential equations with finite elements. FEniCS library is open-sourced and easy to implement a problem using some functions. A successful solution may be achieved after changing the solution parameters depending on the problem type. In this thesis FEniCS v2019.2.0.dev0 is used.

Meshing an object is required to convert a continuum into an approximate solution domain. Gmsh and Salome are employed, but they are used in different cases. Gmsh is rather used when simpler geometries and full mesh control are required. Salome on the other hand is utilized for complex geometries and mesh control is not concerned. Gmsh has its own scripting language, which is easy to code. Main challenge is to make the computational aided design (CAD) model while controlling the resulting object in the graphical user interface (GUI). The script can be then executed to reproduce the same topology while changing the dimensions of the geometry. Salome works in a similar way but it is a more complex CAD program. It has a modular architecture as it uses Python. A macro Python script can be traced in the GUI while modeling, and the model parameters can be edited on the same script. Aside from the CAD modeling, submeshing in Salome generates somewhat unexpected meshes.

FEM results are postprocessed using Paraview. It has many utilities to interpret the numerical results. To give an example, transient solution can be rendered as an animation with very small amount of storage compared to the solution files. In addition, solved variables can be extracted with respect to time as comma separated value (.csv) files. To plot them Gnuplot is used. It is a program that is capable of data analysis, e.g. curve fits, as well. Both of programs can be driven by macro scripts.

APPENDIX B: DERIVATIVE OF THE DISPERSION CURVE

$$\frac{\partial v}{\partial \hat{h}}(t) = - \frac{\left(f_y^6 - 3v_g^2 f_y^4 + 3v_g^4 f_y^2 - v_g^6\right)}{\left(f_x f_y^5 - 2v_g^2 f_x f_y^3 + v_g^4 f_x f_y\right) + \frac{\alpha v_g^4 \left(v_s^2 - v_g^2\right) \sqrt{\frac{1}{v_g^2} - f_y^2}}{2\pi v_s^2 \sqrt{\frac{1}{\frac{f_y^2}{v_g^2} - 1} - \frac{f_y^2}{\frac{v_s^2 f_y^2}{v_g^2} - v_s^2}} \sec^2\left(2\pi f_x f_y \sqrt{\frac{1}{v_g^2} - \frac{1}{f_y^2}}\right)}} \quad (\text{B.1})$$