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Design, Modeling and Fabrication of Shear Mode Bulk Acoustic Wave Sensor as a Potential Biosensor

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DESIGN, MODELING AND FABRICATION OF SHEAR MODE BULK ACOUSTIC WAVE SENSOR AS A POTENTIAL BIOSENSOR

by

Chi-Jung Cheng

A Dissertation
Submitted to the
Faculty of The Graduate College
in partial fulfillment of the
requirements for the
Degree of Doctor of Philosophy
Department of Electrical and Computer Engineering
Advisor: Massood Atashbar, Ph.D.

Western Michigan University
Kalamazoo, Michigan
June 2012
WE HEREBY APPROVE THE DISSERTATION SUBMITTED BY

Chi-Jung Cheng

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DEGREE OF Doctor of Philosophy

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Chi-Jung Cheng, Ph.D.

Western Michigan University, 2012

There has been an increasing interest in development of thin film bulk acoustic wave resonator (FBAR) devices for chemical and biological sensing applications in the environmental and biomedical industries. The zinc oxide (ZnO) thin film based FBAR devices provides attractive advantages, such as high resonant frequency, small size, and rapid response. Typically, the ZnO-based FBAR devices are operated in the longitudinal wave mode where the ZnO crystallites are perpendicular to the substrate. In gaseous environments, the longitudinal mode FBAR device provides high sensitivity for mass sensing. However, the longitudinal wave mode is adversely affected when used in liquid environments because the longitudinal wave is easily dissipated in a liquid media such as water, blood or serum. This phenomenon causes the decrease of quality factor (Q) and thus reduces the mass sensing resolution.

To overcome this limitation, the shear mode solidly mounted film bulk acoustic wave resonator (SMFBAR) device is presented in this dissertation. The shear acoustic wave propagation is an ideal acoustic wave mode for liquid sensing applications because it allows minor damping effects and thus reduces the energy dissipation in liquid media. Two proposed structures, the lateral field excitation structure and the c-axis inclined structure, for generating a shear acoustic wave are
discussed in this study. The resonant frequency, electromechanical properties, and frequency response of the device are analyzed through the one-dimensional Mason’s equivalent circuit method. The two- and three-dimensional finite element structures were also built to study the wave propagation direction and the particle displacement. In addition, the effect of the thickness of the ZnO thin film and Bragg reflector layers on the resonance frequency was also discussed.

The shear mode SMFBAR device, with overall dimension of 12260 µm × 11900 µm was fabricated on a 4” silicon (Si) wafer. The devices were tested for parameters of interest such as resonant frequency quality factor, and electromechanical coupling as well as their ability to operate in liquids. The results show that the shear mode SMFBAR offers great potential as a biosensor. Lastly, the accomplishments of this study are summarized and future perspectives are provided.
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CHAPTER 1

INTRODUCTION

1.1 Background

Over the last few decades, the research interest in the field of healthcare diagnostics had focused on developing new and innovative methods to detect the biomolecular species. Various biomolecular species, such as bacteria and viruses, are found widely in our living environment and the human body. Many of these molecules have an essential function in nature, but some potentially harmful molecules can have deep negative effects on humans [1]. With the recent advances in medicine, many substances associated with various diseases have been identified, and thus presence and progress of these diseases can be determined by detecting its associated substances. The possibility of curing a disease increases dramatically by early detection. Early detection is particularly important in the case of cancer. It is highly treatable when the disease is detected in early stage [2]. To find diseases in its early stage, it is necessary to detect these molecules even at low concentration. This means that there is a great demand for developing a new sensing technology with high sensitivity.

1.2 Conventional Detection Methods

Currently, a number of sensing techniques have been reported and used for the detection of pathogenic bacteria in a variety of applications, including the colony count, polymerase chain reaction (PCR), enzyme-linked immunosorbent assay (ELISA) and biosensors.
The colony counting method is one of the oldest standard microbiological techniques used to estimate the concentration of a micro-organism species such as bacteria and cells in a liquid [3]. The method is to count colonies of micro-organism species or bacteria growing in a wide area of agar plate. The bacterial cell in the original sample should reproduce and form a single colony if the bacteria are spread out enough. Generally, the colony counting is the most time-consuming method. For example, in the case of Campylobacter, it takes at least 4 days to obtain a negative result and at least 14 days for confirmation of a positive result [4].

The polymerase chain reaction provides an extremely sensitive measurement by amplifying small quantities of DNA, which was developed by Kary Mullis in 1987 [5]. The basic concept of the polymerase chain reaction is based on isolation, amplification and quantification of a short DNA sequence. Although the PCR technique has ability to detect a single molecule of DNA, the extreme sensitivity feature causes its main limitation such as the false-positive results from background DNA contamination, limited detection space of the assay or platform for simultaneous identification of multiple species, virulence factors, or drug resistance [6].

Enzyme-linked immunosorbent assay, ELISA, is a method of measuring the degree of concentration of a particular biomolecular such as antibody or antigen. The basic concept of immunoassay was first described by Landsteiner in 1945, when he discovered that antibodies could bind with associated small molecules when they were conjugated to a carrier molecule [7]. ELISA testing starts with the immobilization of the antigen and antibody onto a solid support such as a test tube, followed by adding enzyme conjugated secondary antibody. Adding the substrate and treating enzyme cause a catalytic reaction that produces a color-change
of the substrate. Finally, the sample is washed to remove unbound molecules and the amount of colored product is measured using a spectrophotometer [8].

Although colony count, PCR and ELISA have been widely used in clinical diagnosis and life science, these methods are relatively expensive, time consuming and labor intensive, which required at least some training and a significant amount of practical experience to perform successfully. Desired improvements on ELISA capability would include label-free detection, near real-time response, greater sensitivity, and capacity for multiplexing.

1.3 Biosensors

A biosensor is similar to a chemical sensor that converts physical or chemical response to a measureable signal [9]. A biosensor is defined by the Union of Pure and Applied Chemistry (IUPAC) Commission [10] as a detecting device that combines a transducer with a biological component, called a biosensor. As shown in Figure 1.1, when a specific target molecule interacts with the bioreceptor such as immobilized enzymes, antibody and microorganism, a measurable signal is produced proportional to the concentration of the substance [11]. Currently, the biosensors are used for detecting even the smallest amount biomolecular such as a protein, nucleic, acid and enzyme [12]. According to the transducer type, the biosensor can be classified into five categories: electrochemical sensor [13], electrical sensor [14], optical sensor [15], acoustic wave sensor [16] and thermal sensor [17].
Acoustic wave based devices are an appealing sensing scheme compared to the other methods because they are small, relatively inexpensive to fabricate, and offer a potentially superior sensitivity to surface perturbations [18] [19]. Recently, there have been bodies of research efforts to use acoustic wave devices as bioanalytical tools [20] [21] [22]. Acoustic wave devices are considered as a type of gravimetric sensors which utilize a mechanical wave (acoustic wave) as the sensing mechanism. As the acoustic waves generate and propagate through the piezoelectric material, any physical quantities change in the wave propagation path affects the velocity of the acoustic wave and thus changes the resonant frequency of the device. Several types of acoustic wave devices have been developed, which includes the surface acoustic wave (SAW) device and the quartz crystal microbalance (QCM). Recently, thin film bulk acoustic resonators (FBARs) on silicon substrates have developed as a substitute for QCM and SAW devices in the filter and sensor applications. It is due to its ease of miniaturization and superior resonant frequency and high sensitivity. Since fabrication of thin films is a routine practice in the microelectronics industry, it makes FBAR technology compatible with silicon wafer processing [23]. However, the typical

![Figure 1.1: The principle of component of biosensor includes bioreceptor and transducer.](image)
FBAR with compression wave, operating in longitudinal mode, is not suitable for detecting biomolecular substance in liquid environment because the energy of acoustic waves easily dissipate into a contacting liquid. This result in the decrease of quality factor and thus reduce the mass sensing resolution.

1.4 Author’s Contributions

The present work led to several publications including two journal papers and five conference presentations as given in the list of publications in Appendix B. In addition, another three manuscripts have been accepted for presentation at the IMCS 2012 and APCOT 2012.

1.5 Organization of the Dissertation

The rest of the dissertation is divided into 5 chapters. Chapter 2 provides an introduction of piezoelectricity, piezoelectric effect and acoustic wave sensor technologies. Chapter 3 presents a detailed description of the design, modeling and simulation of thin film bulk acoustic wave device using MATLAB and CoventorWare. Chapter 4 discusses the theoretical analysis of c-axis inclined structure and lateral field excitation structure. Chapter 5 discusses the design, fabrication and measurement of lateral field excitation solidly mounted film bulk acoustic wave resonator (LFE SMFBAR) devices. It also discusses the fabrication issues. Chapter 6 concludes this project and also gives suggestions for the future work.
CHAPTER 2

ACOUSTIC WAVE SENSOR

In this chapter, a brief historical background to understand the theoretical basis of this dissertation will be provided. First, the concept of the piezoelectricity and the role of the piezoelectric material will be explained, and the basic theory of the piezoelectricity will also be described. Second, in section 2.2, I will provide an overview of acoustic wave devices and evaluate current acoustic wave technologies in the fields of chemistry and biology.

2.1 Introduction of Piezoelectricity

The underlying physical phenomenon operating in acoustic wave devices is a piezoelectricity. The word piezoelectricity comes from Greek and means “electricity by pressure.” It was proposed by Hankel [24] in 1881, to name the phenomenon discovered by the brothers Pierre Curie and Jacques Curie in 1880 [25]. The Curie brothers discovered that positive and negative charges appear on certain crystal surfaces when the crystal is compressed in different directions.

This phenomenon can be explained by using a simplified molecular model as illustrated in Figure 2.1. Before the piezoelectric material was applied to any external stress, the positive (+) and negative (-) charges share a common center of gravity, and the positive and negative charges coincide. In this moment, the molecular is neutral and the polarization is zero [26] (Figure 2.1(b)). When the external compressive force is applied on the piezoelectric material (Figure 2.1(a)), the internal structure is deformed, in such a way as to bring two of the negative charges close together at the top of the surface and the positive charges at the bottom of the surface. This form a
dipole where one end of structure is positive and the other is negative therefore, the whole structure becomes electrically polarized. If the direction of the forces reverses (Figure 2.1(c)), the structure will be pulled upwards, which results in an opposite polarization [27].

![Piezoelectricity in an ionic crystal](image)

Figure 2.1: Piezoelectricity in an ionic crystal.

For an entire piezoelectric crystal, one can easily imagine that a crystal structure make up of these arrangements of molecular, all lined up in an orderly matrix throughout the bulk of the crystal volume [28] as shown in Figure 2.2. When the piezoelectric crystal is deformed, each molecular would contribute to a net polarization across the entire crystal.
In addition, one of the unique characteristics of the piezoelectric material is that the piezoelectric effect is reversible. As shown in Figure 2.3, the mechanical stress converts to electric voltage is called the *direct piezoelectric effect*. Conversely, the application of an electric voltage to an unrestrained piezoelectric body results in deformation and this phenomenon is called *inverse piezoelectric effect*. The amount of movement is a function of the polarity of the voltage applied. When an AC (alternating current) voltage applied to the piezoelectric material, the material will deform mechanically such as shrinking or stretching and begin vibrating. The vibration is occurred at the frequency of the applied voltage. For example, if the frequency of the voltage is 30 hertz or 30 cycles per second, this is also the frequency at which the piezoelectric material will vibrate.

**Figure 2.2: Cross section of modeled hexagonal structure.**
2.1.1 Elastic Constitutive Equations

The above two-dimensional models illustrated the piezoelectric effect; however, they are too simple to provide a comprehensive understanding for the complexity of piezoelectricity in real-world applications. Therefore, a more complex model with mechanical properties is desired to describe the piezoelectric phenomenon.

In general, when the external stress is applied to a piezoelectric or non-piezoelectric object, the object will generate strains in the direction opposed to applied stress and the direction perpendicular to the stress. For example, when the stress is applied in the x-direction, the material would generate strains in x-, y- and z-directions. To better understand these facts, the three-dimensional Hooke’s Law [29] is employed to explain the relationship between the stress and the strain. Hooke’s Law
states that the strain is linearly proportional to the stress, or conversely, that the stress is linearly proportional to the strain, which can be written as follows [30]:

\[ T_{ij} = c_{ijkl}s_{kl} \quad (2.1) \]

\[ S_{ij} = s_{ijkl}T_{kl} \quad (2.2) \]

where \( T \) and \( S \) are stress (N/m²) and strain (m/m), respectively, \( c_{ijkl} \) and \( s_{ijkl} \) are a fourth-order tensor of elastic stiffness constants (N/m²) and a fourth order compliance constant (m²/N), respectively. The indices \( i, j, k \) and \( l \) represent the three-dimensional Cartesian coordinate system of \( x, y \) and \( z \). Based on each of the indices, we expect a total of 81 \((3^3=81)\) independent components in elastic stiffness and compliance constants; thus, the full expression of Equation (2.1) and (2.2) can be written as the following:

\[
\begin{bmatrix}
T_{xx} \\
T_{xy} \\
T_{xz} \\
T_{yy} \\
T_{yz} \\
T_{zz}
\end{bmatrix} =
\begin{bmatrix}
c_{xxxx} & c_{xxyy} & c_{xyxx} & c_{xyxy} & c_{xyzy} & c_{xyzz} & c_{xxzz} & c_{xyzz} & c_{xyzz} \\
c_{yxxx} & c_{yxyy} & c_{xyxy} & c_{xyxy} & c_{xyzy} & c_{xyzz} & c_{xxzz} & c_{xyzz} & c_{xyzz} \\
c_{yxzx} & c_{xyzx} & c_{xyxy} & c_{xyxy} & c_{xyzy} & c_{xyzz} & c_{xxzz} & c_{xyzz} & c_{xyzz} \\
c_{yyyx} & c_{yyxy} & c_{xyxy} & c_{xyxy} & c_{xyzy} & c_{xyzz} & c_{xxzz} & c_{xyzz} & c_{xyzz} \\
c_{yyzy} & c_{yzyx} & c_{xyxy} & c_{xyxy} & c_{xyzy} & c_{xyzz} & c_{xxzz} & c_{xyzz} & c_{xyzz} \\
c_{yyzz} & c_{yzzx} & c_{xyxy} & c_{xyxy} & c_{xyzy} & c_{xyzz} & c_{xxzz} & c_{xyzz} & c_{xyzz}
\end{bmatrix}
\begin{bmatrix}
S_{xx} \\
S_{xy} \\
S_{xz} \\
S_{yy} \\
S_{yz} \\
S_{zz}
\end{bmatrix}
\]

\[
\begin{bmatrix}
S_{xx} \\
S_{xy} \\
S_{xz} \\
S_{yy} \\
S_{yz} \\
S_{zz}
\end{bmatrix} =
\begin{bmatrix}
s_{xxxx} & s_{xxyy} & s_{xyxx} & s_{xyxy} & s_{xyzy} & s_{xyzz} & s_{xxzz} & s_{xyzz} & s_{xyzz} \\
s_{yxxx} & s_{yxyy} & s_{xyxy} & s_{xyxy} & s_{xyzy} & s_{xyzz} & s_{xxzz} & s_{xyzz} & s_{xyzz} \\
s_{yxzx} & s_{xyzx} & s_{xyxy} & s_{xyxy} & s_{xyzy} & s_{xyzz} & s_{xxzz} & s_{xyzz} & s_{xyzz} \\
s_{yyyx} & s_{yyxy} & s_{xyxy} & s_{xyxy} & s_{xyzy} & s_{xyzz} & s_{xxzz} & s_{xyzz} & s_{xyzz} \\
s_{yyzy} & s_{yzyx} & s_{xyxy} & s_{xyxy} & s_{xyzy} & s_{xyzz} & s_{xxzz} & s_{xyzz} & s_{xyzz} \\
s_{yyzz} & s_{yzzx} & s_{xyxy} & s_{xyxy} & s_{xyzy} & s_{xyzz} & s_{xxzz} & s_{xyzz} & s_{xyzz}
\end{bmatrix}
\begin{bmatrix}
T_{xx} \\
T_{xy} \\
T_{xz} \\
T_{yy} \\
T_{yz} \\
T_{zz}
\end{bmatrix}
\]
Equations (2.3) and (2.4) clearly illustrate the inconvenience of using full subscript notation for writing and transforming Hooke’s Law. However, this difficulty can be avoided by using the symmetry characteristics of stiffness and compliance which are defined as the following:

\[
\begin{align*}
  c_{ijkl} &= c_{jikl} = c_{jilk} = c_{jkl}\quad (2.5) \\
  s_{ijkl} &= s_{jikl} = s_{jilk} = s_{jkl}
\end{align*}
\]

The symmetric characteristics of stiffness and compliance reduce the expression from nine-dimensional vector into a six-dimensional vector with the matrices being simplified as follows [31]:

\[
\begin{align*}
  c &= \begin{bmatrix}
  c_{xxx} & c_{xyy} & c_{xzz} & c_{xyz} & c_{xyz} & c_{xxz} \\
  c_{xyy} & c_{yyy} & c_{yyz} & c_{yzy} & c_{yzy} & c_{yzz} \\
  c_{xzz} & c_{yyz} & c_{zzz} & c_{zyz} & c_{zyz} & c_{zzz} \\
  c_{xyz} & c_{yzy} & c_{zyz} & c_{zzz} & c_{zzz} & c_{zzz} \\
  c_{xyz} & c_{zyz} & c_{zyz} & c_{zzz} & c_{zzz} & c_{zzz} \\
  c_{xxz} & c_{yzy} & c_{zyz} & c_{zzz} & c_{zzz} & c_{zzz} 
\end{bmatrix} \\
  s &= \begin{bmatrix}
  s_{xxx} & s_{xyy} & s_{xzz} & s_{xyz} & s_{xyz} & s_{xxz} \\
  s_{xyy} & s_{yyy} & s_{yyz} & s_{yzy} & s_{yzy} & s_{yzz} \\
  s_{xzz} & s_{yyz} & s_{zzz} & s_{zyz} & s_{zyz} & s_{zzz} \\
  s_{xyz} & s_{yzy} & s_{zyz} & s_{zzz} & s_{zzz} & s_{zzz} \\
  s_{xyz} & s_{zyz} & s_{zyz} & s_{zzz} & s_{zzz} & s_{zzz} \\
  s_{xxz} & s_{yzy} & s_{zyz} & s_{zzz} & s_{zzz} & s_{zzz} 
\end{bmatrix} \quad (2.6, 2.7)
\]

With those constraints on the stiffness and compliance constants, the subscripts can be further reduced by using abbreviated subscript notation, where \(1 = xx\), \(2 = yy\), \(3 = zz\), \(4 = yz\) or \(zy\), \(5 = xz\) or \(zx\) and \(6 = xy\) or \(yx\). Thus, the final expressions for the stress and strain show the following: (elastic constitutive equations)
2.1.2 Constitutive Equations

For the piezoelectric material, both coupled and uncoupled polarization must be considered in order to properly characterize the piezoelectricity. As described above, when an electrical potential is applied across a piezoelectric material, molecular dipoles accumulate throughout the volume of the crystal and cause polarization. The electrical quantities are related in the following manner [32]:

\[
\vec{D} = \varepsilon_0 \vec{E} + \vec{P}
\]  

(2.10)

where \(\vec{D}\) is electric displacement (m), \(\vec{E}\) is the electric field (V/m) and \(\vec{P}\) (C/m\(^2\)) is the electric polarization. The term \(\varepsilon_0 = 8.85 \times 10^{-12}\) F/m is the permittivity of free space, which is a measure of the ability of a material to be polarized by an electric field. The polarization depends on the applied electric field. In a piezoelectric material, an electric polarization can also result from a strain and applied stress. Therefore relationship among the polarization, strain and stress can be expressed as follows [33]:
\[ P_k = d_{kl} T_{ij} \quad k = 1 \text{ to } 3, \quad ij = 1 \text{ to } 6 \quad (2.11) \]
\[ P_k = e_{kl} S_{ij} \quad k = 1 \text{ to } 3, \quad ij = 1 \text{ to } 6 \quad (2.12) \]

In the converse piezoelectric effect, the stress or strain forces are formed by an electric field applied to the material and can be expressed as the following:

\[ S_{ij} = d_{ijk} E_k \quad k = 1 \text{ to } 3, \quad ij = 1 \text{ to } 6 \quad (2.13) \]
\[ T_{ij} = e_{ijk} E_k \quad k = 1 \text{ to } 3, \quad ij = 1 \text{ to } 6 \quad (2.14) \]

where \( d \, (\text{C/N}) \) and \( e \, (\text{C/m}^2) \) is the piezoelectric coupling coefficient for the strain-charge and stress-charge forms, respectively.

Finally, for the linear piezoelectric material, the relations between the mechanical and electrical variables can be described by combining Equation (2.1) to (2.14). Depending on the variable choice, two sets of constitutive equations are defined as below [34]:

\[
\begin{cases}
T_{ij} = c_{ijkl} S_{kl} - e_{ijk} E_k \\
D_i = e_{ik} S_{ki} + e_j E_j
\end{cases}
\quad \text{Stress-Charge Form} \quad (2.15)
\]
\[
\begin{cases}
S_{ij} = s_{ijkl} T_{kl} + d_{ijk} E_k \\
D_i = d_{ik} T_{ki} + e_j E_j
\end{cases}
\quad \text{Strain-Charge Form} \quad (2.16)
\]

In this section, we confirm the reduction process of constitutive equations. Those equations will be used to estimate the propagation properties of acoustic wave devices in Chapter 3 and Chapter 4.

### 2.2 Overview Acoustic Wave Devices

Since Dr. Cady demonstrated a first oscillator using quartz crystal in 1920 [35], many companies such as Bell, GE, IBM and Motorola explored quartz crystal’s
piezoelectric character and used in the technologies of radio and electronic devices [36]. Recently, acoustic wave devices have been widely used as a sensor for detecting and measuring the change of physical properties such as mass, density, viscosity and conductivity [37] [38]. It is because acoustic wave devices have great advantages in terms of versatility, sensitivity and reliability [39].

Acoustic wave devices are defined by the mode of wave propagation through or on a piezoelectric substrate. Generally, acoustic wave devices can be classified into two groups depending on the device structure and acoustic wave propagation behavior: Surface Acoustic Wave (SAW) devices and Bulk Acoustic Wave (BAW) devices. In SAW devices, the acoustic wave travel along a surface of the piezoelectric substrate; in BAW devices, the acoustic wave propagates through the volume of the substrate.

2.2.1 Surface Acoustic Wave (SAW) Devices

The surface acoustic wave was first discovered and demonstrated by Lord Rayleigh in 1885 [40]. The wave, also called a Rayleigh wave, propagates near the surface of piezoelectric substrate. In the Raleigh wave, surface particles move in elliptical path with two types of wave motions: bulk shear and longitudinal waves [41]. In the shear vertical wave motion, the particle displacement is parallel to the surface along the direction of wave propagation, while the particle displacement is normal to the surface in longitudinal wave motion. In 1965, White and Voltmer developed first SAW device with two ports of the interdigital transducer (IDT) as a transmitter and receiver of surface waves [42]. The IDT is a sequence of metal electrodes alternately connected to two bus bars as shown in Figure 2.4. When a voltage is applied to the one side of IDT, it generates a periodic electric field along
the IDT and results in a mechanical acoustic wave propagating on the substrate surface. The frequency \( f \) of the wave is defined as \[ \lambda / v \]
and
\[ \lambda = 2 \times p \]
where \( v \) is wave velocity, \( \lambda \) is the wavelength, and \( p \) is the gap between electrodes.

At the output, the receiving IDT acts in a reciprocal manner, converting incident waves to an output voltage. Any physical changes on the wave propagation path will be reflected in the output electric signal. Therefore, the SAW device can be designed to quantify any phenomenon which alters these properties.

The first application of Rayleigh wave SAW devices as sensors was in 1979 for gas detection [44] [45] [46]. However, Rayleigh wave SAW devices did not operate efficiently in contact with liquid medium; it was because particle displacement were normal to the surface of the device, which resulted in a strong radiation loss into the liquid. To overcome the high attenuation caused by the liquid environments, the particle displacement must be parallel to the surface of the device [47]. The first successful approach using SAW devices in contact with liquids was achieved in 1987 [48] [49]; these SAW devices operated with shear horizontal...
polarized waves (SH-SAW). The particles displacement in this mode is parallel to the device’s surface, and therefore the energy of acoustic waves is not easily dissipated into the liquid [50] and hence the device maintains a high sensitivity in liquids. Consequently SH-SAW devices are particularly well suitable for bio-detection, especially for “real-time” monitoring. In the most recent research, the sensitivity of SH-SAW can be improved by depositing a guiding layer on top of substrate. This guided SH device operates in a Love wave mode with the acoustic energy trapped within a thin waveguide layer. This result in an enhancement in the detection sensitivity compared with a conventional SAW device. They are therefore frequently employed to perform biosensing in liquid conditions [51].

For example, F. Josse et al. [52] [53] presented a SH-SAW sensor for chemical and biomedical detection in liquid. They demonstrated that the guided SH-SAW on 36° YX-LiTaO₃ substrates can be used for high-sensitivity sensor implementation in liquid environments. The SH-SAW device was operated at 103 MHz with the mass sensitivities of 1420 Hz/(ng/mm²).

2.2.2 Bulk Acoustic Wave (BAW) Devices

Quartz crystal is the most common bulk acoustic wave device. A QCM resonator consists of a quartz crystal disk arranged between two evaporated metal electrodes as shown in Figure 2.5. It was first presented by Dr. Cady in 1920s. He used the reverse piezoelectric effect to demonstrate a crystal oscillator, and the stabilized an oscillator at a steady frequency related to the quartz crystal’s natural period of vibration [54]. In 1959, Sauerbrey developed a first mass sensor based on quartz crystal [55]. He suggested that the increase of thickness of thin film will result
in the decrease of resonant frequency of quartz device. In 1964, King used the quartz to develop the first gravimetric sensor for detecting the adsorption of gases [56].

The QCM typically operates in a shear thickness mode (TSM), where its resonance frequency can be tuned by varying the thickness of the piezoelectric thin film. The first resonant frequency for the QCM resonator occurs when the thickness of piezoelectric is half the acoustic wavelength. The relation between the thickness of the piezoelectric layer and the resonant frequency can be expressed as [57]

\[ f = n \frac{v_a}{2d}, \ n=1, 3, 5 \ldots \]  

(2.19)

where \( f \), \( v_a \), and \( d \) are the resonant frequency, acoustic velocity, and thickness of the piezoelectric layer, respectively. For example, the thickness of the QCM plate for 5 MHz device is 300 µm [58] and for 35 MHz device is 1 µm [59]. For the mass sensing applications, a shift in the resonant frequency of the QCM (\( \Delta f \)) can be

![Figure 2.5: Circular quartz resonator of thickness d coated with electrodes.](image)
attributed to the mass loaded ($\Delta m$) on the surface of sensor which can also be defined by the Sauerbrey equation [60].

$$\Delta f = \frac{-2f_0^2 \Delta m}{A\sqrt{\rho_q \mu_q}} \tag{2.20}$$

where $f_0$ is the fundamental resonant frequency, $A$ is the piezoelectrically active area defined by the two electrodes, $\rho_q$ is the density of quartz, and $\mu_q$ is the shear modulus.

Currently, QCM devices are widely used as sensors in the field of biochemistry and biotechnology. The ability of QCM to operate in liquids has been demonstrated in the number of applications including the characterization of different type of molecular interactions such as: proteins [61], bacteriophages [62], bacteria [63], viruses [64], and cells [65]. Recently it has been applied to detect DNA strands [66].

### 2.2.3 Thin Film Bulk Acoustic Wave Resonator (FBAR) Devices

The operating frequency of QCM devices depends on the acoustic wave velocity and the thickness of the device as given in (2.19). To increase the resonance frequency of the QCM further, the quartz plate thickness should be reduced more, but this makes the plate very fragile and difficult to handle. On the other hand, thin film bulk acoustic wave resonators (FBAR) are more suitable for high frequency applications because they allow the implementation of BAW devices from tens of micrometers to tens of nanometers, which results in the operating frequencies from several hundred MHz to several GHz.

FBARs have been perceived as an excellent frequency control unit in communication systems due to their high operating frequency, high quality factor and demonstrated compatibility with integrated circuit processing [67]. A thin film bulk
resonator is formed by depositing a piezoelectric thin film between two electrodes on a substrate. Several techniques have been used to isolate the FBAR structure from the substrate, including conventional FBAR and solidly mounted FBAR (SMFBAR). The conventional FBAR has inherently better energy constraint due to the large acoustic impedance between solid and air which will maximally reflect the acoustic wave from the air-solid boundary and thus the energy loss is minimized. Three main types of conventional FBARs have been developed: back etching type, cavity gap and bridge type [68]. The structure of back etching type is shown in Figure 2.6(a). The cavity is etched from back side and through the whole substrate using deep-RIE technology [69]. The membrane material can be silicon, doped silicon, silicon dioxide, or diamond. However, most devices would like to choose a low stress membrane such as silicon nitride (Si$_3$N$_4$) [70] [71].

The resonant layer is deposited on top of the membrane. In this way, both sides of a resonant layer are connected with air directly; therefore, the large mismatch of acoustic impedance between air and solid is present. This large difference reflects most of the acoustic wave and reduces the acoustic energy leakage. However, the fabrication process is complicated which requires photolithography and processing on the back side of the substrate, which must be highly accurate. Moreover, the disadvantage of this type of structure is the back etching process, which might not be compatible with monolithic fabrication of readout or other electronic circuits.

The cavity type of FBAR is shown in Figure 2.6(b). To achieve this structure, first, the cavity is formed and filled with a sacrificial layer. Second, the substrate surface is polished using chemical mechanical polishing technology. Next, the bottom electrode layer is deposited follow by the deposition of the piezoelectric layer and top electrode layers. Finally, the sacrificial layer is removed to form the cavity.
Figure 2.6: FBAR cross-section. (a) backside substrate etch, (b) air cavity type (c) bridge type FBAR.

Figure 2.6(c) shows a bridge type FBAR that contrasts with back-etching type and cavity type FBAR structures in that it is formed on a flat substrate and does not need a cavity. In this structure, the sacrificed layer is deposited before the sputtering of the piezoelectric layer, which is used to form a gap between the bottom electrode and the substrate. After the fabrication process of the top resonator material, the sacrificial layer is removed to form a structure, and the resonator active region is suspended in the air.

FBARs are fabricated by etching the support layer in order to create an air boundary on both sides of the piezoelectric film. The large acoustic impedance
between solid and air would reflect most of acoustic wave energy and constrain the energy inside of piezoelectric layer, which results in a higher quality factor (Q) and thus improves the sensitivity of the device.

2.2.4 Solidly Mounted FBAR (SMFBAR) Devices

The conventional FBAR devices provide a better quality factor (Q) due to the large acoustic impedance between the solid structure and air. However, in order to create an air-gap, the etching step is difficult to achieve and requires additional and expensive etching steps. The alternative approach to build a FBAR device is represented by the solidly mounted FBAR, which was first reported by Newell in 1965 [72]. Since the piezoelectric layer is solidly mounted on the substrate, it is necessary to deposit some kind of materials which can isolate the piezoelectric layer from the substrate in order to obtain a high quality factor of resonance. The solution to this problem is to deposit a Bragg reflector (also known as acoustic mirror) right under the piezoelectric layer as shown in Figure 2.7. The type of device is called solidly mounted thin film bulk resonator (SMFBAR).
Newell discovered that the quarter wavelength sections of materials with large impedance mismatch can effectively reflect acoustic wave and give partial isolation. The greater the impedance mismatched of the reflectors, the better the isolated efficiency can be obtained. At the interface of each layer, a part of the acoustic wave energy is reflected. The number of layers in the Bragg reflector needed for complete wave reflection is determined by their acoustic impedance ratio \[73\]. The acoustic impedance of material is defined as \[74\]:

\[Z_{\text{Acoustic}} = \sqrt{\rho \cdot E}\]  \hspace{1cm} (2.21)

where \(\rho\) is density and \(E\) is the Young’s modulus of material. The acoustic impedance of the materials which are frequently employed to fabricate as Bragg reflector are shown in Table 2.1. All listed materials are compatible with CMOS integrated circuit technology. It can be seen that tungsten (W) has the highest acoustic impedance, and silicon dioxide (SiO\(_2\)) has the lowest acoustic impedance with values of 2809 kg/m\(^2\)/s and 403 kg/m\(^2\)/s, respectively.
SMFBARs have been developed for liquid sensing applications in a number of studies. Gabl et al. [75] presented a biosensor system based on 2 GHz longitudinal mode for DNA and molecules detection as illustrated in Figure 2.8. The detection principle of these sensors is label-free and relies on a resonance frequency shift caused by mass loading of an acoustic resonator. The report shows that the sensor was able to detect protein as well as DNA molecules, with a mass sensitivity being 2500 times higher than by using 20MHz QCM with 25 ng/cm² of the mass resolution. The research shows that based on the simplicity of the label-free detection principle, the SMFBAR sensor is capable of be applying in different biosensing applications.

<table>
<thead>
<tr>
<th>Material</th>
<th>Density (kg/m³)</th>
<th>Young’s Modulus (Gpa)</th>
<th>Acoustic Impedance (kg/m²/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>2700</td>
<td>74.14</td>
<td>447</td>
</tr>
<tr>
<td>Au</td>
<td>19280</td>
<td>80</td>
<td>1242</td>
</tr>
<tr>
<td>Pt</td>
<td>21140</td>
<td>170</td>
<td>1896</td>
</tr>
<tr>
<td>Ag</td>
<td>10500</td>
<td>83</td>
<td>934</td>
</tr>
<tr>
<td>W</td>
<td>19250</td>
<td>410</td>
<td>2809</td>
</tr>
<tr>
<td>Cr</td>
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<td>140</td>
<td>1003</td>
</tr>
<tr>
<td>Ti</td>
<td>4510</td>
<td>110</td>
<td>704</td>
</tr>
<tr>
<td>Cu</td>
<td>8960</td>
<td>128</td>
<td>1071</td>
</tr>
<tr>
<td>SiO₂</td>
<td>2197</td>
<td>74</td>
<td>403</td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>4000</td>
<td>350</td>
<td>1183</td>
</tr>
<tr>
<td>AlN</td>
<td>3300</td>
<td>300</td>
<td>995</td>
</tr>
<tr>
<td>ZnO</td>
<td>4680</td>
<td>210.9</td>
<td>1094</td>
</tr>
</tbody>
</table>
2.3 Piezoelectric Materials

Different piezoelectric materials have different properties and those properties can have significant impact on device performance therefore, it is important to select suitable material for a particular application. Typically, single crystal materials, such as quartz, lithium tantalate (LiTaO$_3$) and lithium niobate (LiNbO$_3$), have been the mainstream material used for bulk resonators [76] [77] [78]. Single crystals are suitable for bulk resonators. The single crystal bulk resonator provides high performance in terms of repeatability, quality factor and longitudinal drift. This is due to material properties such as material uniformity, low material defect rate, and high material stability [79]. However, these materials are relative expensive and difficult to grow film epitaxial as well as less easily integrated with electronic circuits [80].

In contrast, the piezoelectric thin films are piezoelectric materials that can be grown in thin film form on a variety of substrates and can be integrated into Micro-Electro-Mechanical Systems (MEMS) and microelectronic processes [81] [82].

Figure 2.8: Schematic cross-section of a sensor cell of the novel integrated bio-sensor array [75].
Aluminum Nitride (AlN) and Zinc Oxide (ZnO) are the most common materials for piezoelectric film. Both AlN and ZnO belong to the hexagonal wurtzite (6mm) crystal class in which the c-axis, for the (002) oriented AlN and ZnO, is oriented normal to the surface as shown in Figure 2.9 [78].

![Diagram of hexagonal unit cell with (002) crystal plane](image)

Figure 2.9: Schematic representation of the hexagonal unit cell showing (002) crystal plane, with the normal to this plane being equivalent to the substrate normal.

Due to symmetry in the hexagonal AlN and ZnO crystal, the physical parameters and physical constants of stiffness $c$, piezoelectric-stress coupling $e$, and electrical permittivity $\varepsilon$ can be defined as the following matrices.

\[
c = \begin{bmatrix}
c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\
c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\
c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & c_{66}
\end{bmatrix}
\] (2.22)
where $c_{66} = 0.5 \times (c_{11} - c_{12})$ and the values of each independent parameters of AlN and ZnO are given in Table 2.2 [83] [84] [85] [86].

In terms of selecting a suitable piezoelectric material for thin film bulk acoustic wave device, the acoustic wave velocity and the electromechanical coupling coefficient are major factors for consideration. The first important requirement for the thin film acoustic wave device is high acoustic wave velocity. As shown in (2.19), the operating frequency is proportional to the acoustic velocity. Devices with a higher wave velocity material can easily achieve operating frequencies in the GHz range. Another important requirement for the device is a high electromechanical coupling coefficient, which is the parameter defined as the conversion efficiency between electrical and mechanical acoustic energy in piezoelectric materials. The electromechanical coupling coefficient can be expressed as:

$$K = \sqrt{\frac{e^2}{\varepsilon c}}$$  (2.25)

Here $e$, $\varepsilon$ and $c$ are the piezoelectric-stress coupling, electrical permittivity and stiffness, respectively, as described above. As one of the key goals of the project, a high electromechanical coupling coefficient is needed. Therefore, the ZnO has been selected and used in this project.
This chapter introduces piezoelectricity, piezoelectric effect and acoustic wave devices. It provides a brief introduction of piezoelectric effect and an overview of the different acoustic wave devices that are suitable for a wide variety of biosensing applications. A brief discussion about the different types of acoustic wave was then presented. The following chapter deals with the modeling and simulation of thin film bulk acoustic wave devices.
For many engineering problems, a mathematical model is developed to represent all the important characteristics of the physical properties. Currently, many software packages are available for the design and testing of various electronic components. This chapter will give a brief overview of the different modeling techniques used for the design and simulation of typical FBAR and SMFBAR devices. In section 3.1, the first discussed model will be the one-dimensional Mason's equivalent circuit with the transmission line model. In this model, the frequency response of the devices is computed by multiplying the transmission matrices corresponding to each layer in the thin film acoustic wave resonator. The modules and the simulation results were performed using MATLAB™. The goal in describing the Mason's model is not to give details on how the devices are used but to illuminate the assumptions on the frequency response of the device. In section 3.2, the use of three-dimensional finite element modeling and simulation method to obtain a more accurate analysis in terms of impedance response and the particle vibration will be described. This three-dimensional finite element analysis was performed using CoventorWare™.

3.1 One-dimensional Modeling and Simulation

In order to efficiently and properly analyze the acoustic wave devices, it is necessary to have reasonable models. Various one-dimensional models have been proposed in the past. The most well known models are represented by Mason and Butterworth-Van Dyke (BVD) [32]. Both types of modeling can be used for device design, layout, and sensitivity analysis.
The BVD model consists of an inductance, capacitance and resistance, corresponding respectively to inertia, compliance and damping of the mechanical system [87] as shows in Figure 3.1. The serial resonant frequency \( f_s \) and parallel resonant frequency \( f_p \) are defined as [87]:

\[
f_s = \frac{1}{2\pi \sqrt{L_r C_r}} \quad (3.1)
\]

\[
f_p = \frac{1}{2\pi} \left[ \frac{1}{L_r} \left( \frac{1}{C_r} + \frac{1}{C_s} \right) \right]^{1/2} \quad (3.2)
\]

where, \( L_r \) and \( C_r \) are motional inductor and capacitor, respectively. \( R_s \) and \( R_r \) are series resistor and comprises resistor, respectively. \( C_s \) is a substrate capacitor.

![Figure 3.1: Modified Butterworth Van Dyke (MBVD) model.](image)

**3.2 Mason’s Model**

Although the BVD model gives an accurate representation of the resonator, it can’t be simply used to analyze multi-layer structure devices. Apart from the BVD model, the conventional Mason’s model is more accurate and always valid for any one-dimensional multi-layer resonators and transducers [88]. The Mason model is a transmission line representation of the physically based one-dimensional assumptions. Figure 3.2 shows the Mason’s equivalent circuit for a single piezoelectric layer. A piezoelectric layer can be seen as a three-port component where one is the electric
port with voltage and current, and the other two ports are the mechanical ports with the force \( F \) and the acoustic velocity \( u \). The equations for the piezoelectric layer can be described as [89]:

\[
F_1 = \frac{Z_0}{j\sin(kd)}(u_1 - u_2) + jZ_0 \tan\left(\frac{kd}{2}\right)u_1 + \frac{h}{j\omega}I \\
F_2 = \frac{Z_0}{j\sin(kd)}(u_1 - u_2) - jZ_0 \tan\left(\frac{kd}{2}\right)u_2 + \frac{h}{j\omega}I
\]  

(3.3) \hspace{2cm} (3.4)

\[
\frac{V}{I} = \frac{h}{j\omega}\left(u_1 / I - u_2 / I\right) + \frac{1}{j\omega C_0}
\]

(3.5)

\[
k = \omega / v \quad \text{and} \quad h = e / \varepsilon^s
\]

(3.6)

where \( F_1 \) and \( F_2 \) represents the force from top and bottom surface of the piezoelectric layer, where \( u_1 \) and \( u_2 \) are the acoustic velocity for the top and bottom surface plane of the layer respectively, \( V \) and \( I \) are external electric voltage and the electric current, respectively. In addition, \( v, \varepsilon^s \) and \( e \) are the longitudinal velocity in piezoelectric layer, the permittivity of piezoelectric material under the strain condition and the piezoelectric coefficient respectively, \( C_0 = \varepsilon^s A / d \) is the static capacitance of the layer with the surface area \( A \), and \( Z_0 = A \rho v \) is the acoustic impedance of piezoelectric layer with the material density \( \rho \). The superscript \( s \) indicates that the constants are evaluated at constant strain.
In the ideal condition, a single piezoelectric layer surrounding with air and has mechanical free boundary condition on both sides of surface. Thus forces $F_1$ and $F_2$ can be considered to be zero. After the conversion, equations (3.1) and (3.2) can be written as:

$$0 = Z_0 \left( \frac{u_1}{j \tan(kd)} - \frac{u_2}{j \sin(kd)} \right) + \frac{h}{j \omega} I $$

(3.7)

$$0 = Z_0 \left( \frac{u_1}{j \sin(kd)} - \frac{u_2}{j \tan(kd)} \right) + \frac{h}{j \omega} I $$

(3.8)

Equations (3.7) and (3.8) can also be expressed as:

$$\begin{bmatrix}
-\frac{h}{j \omega} I \\
-\frac{h}{j \omega} I
\end{bmatrix} = \begin{bmatrix}
\frac{Z_0}{j \tan(kd)} & -\frac{Z_0}{j \sin(kd)} \\
\frac{Z_0}{j \sin(kd)} & -\frac{Z_0}{j \tan(kd)}
\end{bmatrix} \begin{bmatrix}
u_1 \\
u_2
\end{bmatrix}$$

(3.9)

The $u_1$ and $u_2$ can be solved by inverting the coefficient matrix

$$\begin{bmatrix}
u_1 \\
u_2
\end{bmatrix} = \begin{bmatrix}
\frac{Z_0}{j \tan(kd)} & -\frac{Z_0}{j \sin(kd)} \\
\frac{Z_0}{j \sin(kd)} & -\frac{Z_0}{j \tan(kd)}
\end{bmatrix}^{-1} \begin{bmatrix}
-\frac{h}{j \omega} I \\
-\frac{h}{j \omega} I
\end{bmatrix}$$

(3.10)

Solving for $u_1/I$ and $u_2/I$, we can get

Figure 3.2: Mason model equivalent circuit of a piezoelectric layer.
\[
\frac{u_1}{I} = \frac{u_2}{I} = -h \cdot \frac{1}{j\omega Z_0 \left( j\tan(kd) \right) + Z_0 \left( j\sin(kd) \right)}
\]  
(3.12)

By substituting \(u_1/I\) and \(u_2/I\) to (3.5), the input impedance of the single piezoelectric layer \(Z_{in}\) can be written as

\[
Z_{in} = \frac{V}{I} = \frac{-2h}{j\omega^2 Z_0} \left( \frac{1}{1/\tan(kd) + 1/\sin(kd)} \right) + \frac{1}{j\omega C_0}
\]  
(3.13)

Using the trigonometric identity

\[
\frac{1}{\tan(kd)} = \frac{1}{\sin(kd)} + \tan\left(\frac{kd}{2}\right)
\]  
(3.14)

The impedance of the single piezoelectric can be expressed as follow:

\[
Z_{in} = \frac{V}{I} = \frac{1}{j\omega C_0} \left( 1 - k_i^2 \frac{\tan(kd/2)}{kd/2} \right)
\]  
(3.15)

where \(k_i^2 = \frac{\varepsilon^2}{ce^5}\) is the electromechanical coefficient of the piezoelectric film.

### 3.2.1 Single ZnO Structure

Figure 3.3 shows the impedance response of a single ZnO thin film with the material properties listed in Table 3.1. It can be seen that the resonance of a signal ZnO thin film is observed at the frequency of 3.64 GHz when the thickness is 800 nm. This result is close to the theoretical resonant 3.76 GHz as defined in (2.19). By changing the thickness of the ZnO layer, the device can operate in various frequencies. For example, as shown in Figure 3.4, the resonant frequency of 2.64 GHz, 2.91 GHz, 3.23 GHz, 3.64 GHz and 4.16 GHz can be obtained when the thickness of ZnO is 1100 nm, 1000 nm, 900 nm, 800nm and 700 nm, respectively. The results show that the resonance frequency will decrease with the increase of the
thickness of the ZnO film. In addition, the resonant frequency of the ZnO film layer is proportional to the thickness of ZnO layer as illustrated in Figure 3.5, and the result is matched with the theoretical definition as described in (2.19).

Table 3.1: Parameter for the simulation

<table>
<thead>
<tr>
<th>Material</th>
<th>ZnO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Film Thickness ((d))</td>
<td>800 nm</td>
</tr>
<tr>
<td>Density ((\rho))</td>
<td>100 (\mu m^2)</td>
</tr>
<tr>
<td>Electromechanical coupling coefficient ((k_t^2))</td>
<td>8%</td>
</tr>
<tr>
<td>Acoustic velocity</td>
<td>6030 m/s</td>
</tr>
<tr>
<td>Sensing Area</td>
<td>100 (\times) 100 (\mu m^2)</td>
</tr>
</tbody>
</table>

Figure 3.3: The impedance response of a single ZnO layer with the thickness of 800 nm.
3.2.2 FBAR Structure

In reality, the FBAR resonator is more than one layer in a structure. It consists of electrode layers and membrane layer as shown in Figure 2.6(a). The loading effect
from those layers has to be considered. Hence, the multi-layer transformation matrix approach is adopted to obtain the overall impedance of multiple-layer resonator.

Based on the Mason’s model as shown in Figure 3.2, the transformation matrix of a piezoelectric layer related to the input voltage and current with the stress and particle velocity can be expressed as [90]

\[
\begin{bmatrix}
V_i \\
I_i
\end{bmatrix} = \begin{bmatrix}
A_p & B_p \\
C_p & D_p
\end{bmatrix} \begin{bmatrix}
F \\
u
\end{bmatrix} \cdot A^i
\]

(3.16)

\[
A_p = \begin{bmatrix}
A_p & B_p \\
C_p & D_p
\end{bmatrix} = \frac{1}{\phi H} \begin{bmatrix}
1 & j\phi^2 / 2C_0 \\
j\phi C_0 & 0
\end{bmatrix} . A^i
\]

(3.17)

\[
H = \cos \gamma - 1 + j\zeta \sin \gamma
\]

(3.18)

\[
A^i = \begin{bmatrix}
A' & B' \\
C' & D'
\end{bmatrix} = \begin{bmatrix}
\cos \gamma + j\zeta_{top} \sin \gamma & Z_0 (\zeta_i \cos \gamma + j \sin \gamma) \\
j \sin \gamma / Z_0 & 2(\cos \gamma - 1) + j\zeta_{top} \sin \gamma
\end{bmatrix}
\]

(3.19)

where \( \phi = k(Z_0 / \omega C_0 / \pi)^{1/2} \) is the transformer ratio in Mason’s equivalent circuit, \( Z_{top} \) represents the acoustic impedance from top of piezoelectric material. \( Z_0 \) and \( C_0 \) are the acoustic impedance of a piezoelectric layer and clamped capacitance, respectively. \( \gamma = \omega d / v \) is the phase delay of the acoustic wave in the piezoelectric layer where \( d \) is the thickness of layer and \( v \) is the acoustic velocity of the layer.

For a non-piezoelectric layer such as electrodes, the equivalent circuit is illustrated in Figure 3.6, which has input and output variables \( F_n, u_n \) and \( F_{n+1}, u_{n+1} \) are related by the transformation matrix:

\[
\begin{bmatrix}
F_n \\
u_n
\end{bmatrix} = \begin{bmatrix}
A_n & B_n \\
C_n & D_n
\end{bmatrix} \begin{bmatrix}
F_{n+1} \\
u_{n+1}
\end{bmatrix}
\]

(3.20)

where
\[
\begin{bmatrix}
A_n & B_n \\
C_n & D_n
\end{bmatrix} = \begin{bmatrix}
\cos \gamma_n & jZ_n \sin \gamma_n \\
\frac{j \sin \gamma_n}{Z_n} & \cos \gamma_n
\end{bmatrix}
\]  \hspace{1cm} (3.21)

where the subscript \( n \) represents the various non-piezoelectric layers. For example, the impedance for top and bottom electrode can be written as:

\[
Z_{top} = \frac{F_{top}}{u_{top}} = jZ_{top} \tan \gamma_{top}
\]  \hspace{1cm} (3.22)

\[
Z_{bot} = \frac{F_{bot}}{u_{bot}} = jZ_{bot} \tan \gamma_{bot}
\]  \hspace{1cm} (3.23)

![Mason model equivalent circuit of a non-piezoelectric layer.](image)

Figure 3.7 shows the matrix model for a typical FBAR device which consists of top electrode, ZnO thin film and bottom electrode. \( A_0 \) and \( A_1 \) represent the top and bottom electrode layers, respectively, and \( B \) represents a piezoelectric layer. As described in (3.16), the electric pair \( V \) and \( I \) can be expressed as:

\[
\begin{bmatrix}
V \\
I
\end{bmatrix} = A_p \begin{bmatrix}
F_{bot} \\
u_{bot}
\end{bmatrix}
\]  \hspace{1cm} (3.24)

where \( A_p \) is the same as defined in (3.17) and \( \begin{bmatrix} F_{bot} \\ u_{bot} \end{bmatrix} \) is defined in (3.20).
By substituting equations from (3.16) to (3.21) into (3.24), we can obtain the acoustic impedance of a typical FBAR device as

\[ Z_{\text{total}} = \frac{V}{I} = \frac{1}{j \omega C_0} \left[ 1 - \frac{k_i^2}{\gamma} \left( z_{\text{top}} + z_{\text{bot}} \right) \sin \gamma + j 2 \left( 1 - \cos \gamma \right) \right] \]  

(3.25)

where \( z_{\text{top}} = Z_{\text{top}}/Z_0 \) and \( z_{\text{bot}} = Z_{\text{bot}}/Z_0 \) are the normalized acoustic impedance of the top electrode layer and the bottom electrode. Equation (3.25) can then be used to calculate the impedance response of a typical FBAR with various thickness of electrode. As it can be seen in Figure 3.8, the resonant frequency of device was decreased from 3.53 GHz to 3.34 GHz to 3.17 GHz to 2.98 GHz when the thickness of electrodes was increased from 50 nm to 100 nm to 150 nm to 200 nm, respectively. It can be seen that the resonance frequency is decreased with the increase of the thickness of the electrodes, and the mass of electrode added on the structure can be calculated using the Sauerbrey equation (2.1). As shown in Figure 3.9, the calculated mass is increased from 0.926 ng to 1.91 ng, to 2.95 ng, and to 4.05 ng when the thickness of electrode increased from 50 nm, to 100 nm, to 150 nm, and to 200 nm, respectively. The mass of electrode is increased about 1 ng per 50 nm thick electrode. This result closely approximates to the theory which is defined as
where the \( v \) is the volume of the element. For this example, the density of the electrode is 2300 kg/m\(^3\) and the volume of the electrode is 500 \( \mu \)m\(^3\). The calculated mass of the electrode with the thickness of 50 nm is 1.15 ng which is close to the simulation results. The parameters used in this simulation are listed Table 3.2.

Figure 3.8: The frequency response for the typical FBAR device with various thickness of electrode layer.
3.2.3 SMFBAR Structure

The same method is adopted to analyze a SMFBAR device. The schematic diagram of SMFBAR is shown in Figure 3.10, and the corresponding transfer matrix model is shown in Figure 3.11.
By using the method described above, the transformation matrix for SMFBAR device can be express as follows:

\[
\begin{bmatrix}
V \\
I
\end{bmatrix} = \begin{bmatrix}
A_{ZnO} & B_{ZnO} \\
C_{ZnO} & D_{ZnO}
\end{bmatrix}
\begin{bmatrix}
F \\
u
\end{bmatrix}
\]  \hspace{1cm} (3.27)

and

\[
\begin{bmatrix}
F \\
u
\end{bmatrix} = \begin{bmatrix}
A_{bot} & B_{bot} \\
C_{bot} & D_{bot}
\end{bmatrix}
\begin{bmatrix}
A_{SiO_2} & B_{SiO_2} \\
C_{SiO_2} & D_{SiO_2}
\end{bmatrix}
\begin{bmatrix}
A_{w} & B_{w} \\
C_{w} & D_{w}
\end{bmatrix}
\begin{bmatrix}
A_{SiO_2} & B_{SiO_2} \\
C_{SiO_2} & D_{SiO_2}
\end{bmatrix}
\begin{bmatrix}
A_{bot} & B_{bot} \\
C_{bot} & D_{bot}
\end{bmatrix}
\begin{bmatrix}
F \\
u
\end{bmatrix}
\]  \hspace{1cm} (3.28)
Using (3.27), we can obtain the electric impedance of a SMFBAR device. Figure 3.12 shows the impedance response of a SMFBAR device with the properties listed in Table 3.1 and Table 3.2. It can be seen that the first resonance of a SMFBAR device is observed at the frequency of 1.34 GHz.

When compared to the single ZnO layer, the frequency drops from 3.64 GHz to 1.34 GHz. This decrease of the frequency is because of the mass loading of the Bragg reflector.

![Figure 3.12: The frequency response for the SMFBAR device.](image)

### 3.3 Finite Element Modeling and Simulation

Equivalent circuit models provide a good starting point for the study and the design of acoustic wave devices. The results obtained in the previous section allow the determination of the primary design parameters such as the resonant frequency of the device. However, it makes several approximations and assumptions such as wave velocity, acoustic impedance and capacitance to convert the acoustic properties into electrical representations. Although on-dimensional equivalent circuit models provide
a fast and relatively accurate analysis of the performance characteristics, it is always desirable to know the actual electromechanical interactions and the fundamental physics of acoustic wave generation and propagation. Therefore, a comprehensive finite element analysis method was used to analyze the acoustic wave devices. In this dissertation, I used CoventorWare™ to analyze a three-dimensional structure of SMFBAR devices.

CoventorWare™ is a powerful modeling tool for MEMS devices. It has varied capabilities including process flow design, two-dimensional mask creation, three-dimensional model generation and device analysis for MEMs and microfluidics applications. The software provides DESIGNER, and ANALYZER modules to approach the MEMS Design. The sequence of steps that were followed in creating three-dimensional model of the FBAR devices is described below.

First, the properties for the materials to be used in the structure were created in the material properties database (MPD). The MPD includes the material properties of the most commonly used materials. The properties associated with the materials include strength, density, conductivity and thermal characteristics. For the piezoelectric materials, the most critical properties to be specified are stiffness matrix [C], piezoelectric stress coupling matrix [e], electrical permittivity matrix [ɛ] and density [ρ]. Typically, the elastic properties of piezoelectric material are given in the compliance matrix format in SI units as described in (2.8). In this format, the coefficients are described in conventional crystallographic order, in which 1 = xx, 2 = yy, 3 = zz, 4 = yz, 5 = zx and 6 = xy. However, the coefficients described in CoventorWare™ follow the conventional FEM format, i.e., 1 = xx, 2 = yy, 3 = zz, 4 = xy, 5 = zx and 6 = yz [91]. Therefore the properties of ZnO materials used in the CoventorWare™ are:
\[
c = \begin{bmatrix}
20.97 & 12.11 & 10.51 & 0 & 0 & 0 \\
12.11 & 20.97 & 10.51 & 0 & 0 & 0 \\
10.51 & 10.51 & 21.09 & 0 & 0 & 0 \\
0 & 0 & 0 & 4.43 & 0 & 0 \\
0 & 0 & 0 & 0 & 4.24 & 0 \\
0 & 0 & 0 & 0 & 0 & 4.24 \\
\end{bmatrix} \times 10^4 \mu N / \mu m^2
\] (3.29)

\[
e = \begin{bmatrix}
0 & 0 & 0 & 0 & -11.34 & 0 \\
0 & 0 & 0 & -11.34 & 0 & 0 \\
-5.43 & -5.43 & 11.67 & 0 & 0 & 0 \\
\end{bmatrix} \times pC / N
\] (3.30)

\[
e = \begin{bmatrix}
8.55 & 0 & 0 \\
0 & 8.55 & 0 \\
0 & 0 & 8.55 \\
\end{bmatrix}
\] (3.31)

\[
\rho = 5.68 \times 10^{-15} kg / \mu m^3
\] (3.32)

The material properties for the SiO$_2$ and W layers are listed in Table 3.2.

Once the material properties are defined in the MPD, the fabrication steps is then specified in the process editor. Figure 3.13 shows the screenshot of the process editor showing the fabrication steps. Fabrication started with the deposition of a Bragg reflector on top of the silicon substrate. The thickness of W and SiO$_2$ are set as 303 nm and 381 nm respectively. After that, a 50 nm bottom electrode is deposited to be followed by 800 nm ZnO layer and 50 nm of top electrode layer. After the fabrication process is defined, the two-dimensional mask patterns for the SMFBAR device is drawn using the layout editor, as shown in Figure 3.14. Here, the SMFBAR device was designed with a surface area of 120×120 μm$^2$ and an active area of 100×100 μm$^2$. 
Figure 3.13: Fabrication sequence in the Process Editor of CoventorWare™.

Figure 3.14: Mask layout of SMFBAR device in the Layout Editor. The area of active region is 100 μm × 100 μm.
The three dimensional structure of SMFBAR device is then built based on the layout masks, fabrication process and material properties defined in the previous section as shown in Figure 3.15. After that, the three-dimensional model needs to be meshed for FEM analysis. Since the device was designed in a square shape, a Manhattan parabolic mesh method is applied with the element size of 10 μm, 10 μm and 0.15 μm in X, Y and Z directions, respectively. While in the Preprocessor, it is necessary to name the patches on which boundary conditions can be applied. For example, the interface between ZnO and top electrode and the interface between ZnO and bottom electrode have to be named appropriately. The three dimensional structure was now ready for analysis.

![Meshed three-dimensional view of the SMFBAR device in Preprocessor.](image)

Figure 3.15: Meshed three-dimensional view of the SMFBAR device in Preprocessor.

Once the three-dimensional structure was modeled using Designer, the analysis is then run using the Analyzer module in CoventorWare™. The approach
CoverntorWare™ used to analyze the piezoelectric material is based on the constitutive equations as described in Chapter 2.2.1.

Figure 3.16 and Figure 3.17 show the simulation of particle displacement of piezoelectric material in SMFBAR device. The excited longitudinal mode caused a large particle movement in the $z$ axis with the maximum movement of 3 nm at the resonant frequency of 1.32 GHz. Although the device is operating in the longitudinal mode, it can be seen that part of particles are moving in the $x$ and $y$ direction. The reason for this is that some portion of the electric field was laterally orientated at the edge of the top electrode, and also that the electric field will excite a small shear mode in the $x$-$y$ plane. The result of impedance response of device is shown in Figure 3.18. It can be seen that the SMFBAR device is resonated at the frequency of 1.316 GHz. This simulated result was in good agreement with the one-dimensional simulation as shown in Section 3.1.

![Figure 3.16: The particle displacement of piezoelectric material in the longitudinal mode.](image-url)
Figure 3.17: The particle displacement of piezoelectric material in the longitudinal mode. The particle is move in z direction.

Figure 3.18: The impedance response of SMFBAR device.
3.4 Summary

This chapter describes the design of film bulk acoustic wave device and gives a detail account of the modeling and simulation using a one-dimensional equivalent circuit model and a three-dimensional finite element model. When it comes to modeling, the Mason’s model approach in Matlab requires an in-depth understanding of the device physics as well as the mathematics involved. It also requires derivation of the frequency response of the devices using matrix manipulation. Comparing to the Mason’s model, CoventorWare modeling is easier and provides more analysis functions. Only the design parameters have to be known in order to be able to perform the three-dimensional model. However, it requires the understanding of the optimization of the mesh element sizes and bounding condition setup in order to be able to obtain accurate results.

In terms of computational time, Matlab only takes few minutes compared to a few days for CoventorWare. Therefore, in my research, I used Matlab to obtain the initial information such as resonant frequency and impedance response of the device. Then, I used CoventorWare™ to obtain the detail information such as particle displacement in the frequency range which was obtained in Matlab. The next Chapter will discuss the method of generating shear acoustic wave. It also present a modeling and simulation of shear mode SMFBAR device.
CHAPTER 4

SHEAR MODE SMFBAR

The development of a novel acoustic wave sensor for liquid sensing applications required two primary problems to be solved. The most important is the identification of an appropriate acoustic mode being excited in the structure. As described in previous sections, the propagation of acoustic wave in a solid material can take several forms or modes. In general, these waves can be either longitudinal, shear or a combination of the two. For the purpose of developing a sensor for liquid sensing applications, it is necessary to have a shear acoustic wave. The second is the electromechanical coefficient of the devices. The electromechanical coupling coefficient of piezoelectric layer is an important property for the design of a resonator; the higher the electromechanical coupling coefficient of a sensor, the more the sensitivity to particles increases. Therefore, the research is aimed to develop an acoustic wave sensor for liquid sensing applications based on SMFBAR technology. The research design and methodology for this development is proposed in this chapter.

Section 4.1 presents the c-axis inclined structure to generated shear acoustic wave. The section provides the method to find the maximum electromechanical coupling coefficient of shear mode. Section 4.2 presents the lateral field excitation structure to generate the shear acoustic wave. Section 4.3 presents the design of lateral filed excitation SMFBAR. This section provides the method to improve the performance of Lateral Field Excitation LFE SMFBAR such as quality factor.
4.1 Shear Acoustic Wave with Inclined ZnO Thin Film

The first approach involves the growth of inclined c-axis oriented thin film. Several studies have shown that the different preferential orientation of piezoelectric thin film will form the different acoustic properties such as the propagation behavior of the acoustic wave and the electromechanical coupling coefficient of piezoelectric material [92] [93].

In order to characterize these two properties in a rotating ZnO thin film, the transformations of dielectric, piezoelectric stress and dielectric constants from one orientation to another orientation should be considered. In this dissertation, the c-axis of the ZnO thin film is defined to lie in the x, y plane. Two coordinate systems xyz and x'y'z' are correspondingly defined as the old coordinate axes and new coordinate axes respectively as shown in Figure 4.1.

Figure 4.1: The ZnO piezoelectric thin layer with the rotation about y axis.
For a clockwise rotation of the coordinate axes about the y-axis, the transformation matrices corresponding to the rotation \( \theta \) can be defined as [94]:

\[
c' = M \cdot c \cdot M'
\]
\[
e' = a \cdot e \cdot a'
\]
\[
e' = a \cdot e \cdot a'
\]
\[
a = \begin{bmatrix}
\cos \theta & 0 & \sin \theta \\
0 & 1 & 0 \\
-\sin \theta & 0 & \cos \theta
\end{bmatrix}
\]

where \( c', e' \) and \( \varepsilon' \) are new material properties of dielectric, piezoelectric stress, and dielectric constant respectively. The matrices \( a \) and \( M \) are the transformation matrix and Bond stress transformation matrix, respectively. The acoustic velocity and the electromechanical coupling coefficient of ZnO can be calculated by substituting the new material properties into the general equation of motion for piezoelectric materials given by Foster [92].

\[
v^{(L,S)} = \left[ \frac{\varepsilon_{33} + \varepsilon_{55}}{2\rho} \pm \sqrt{\left( \frac{\varepsilon_{33} + \varepsilon_{55}}{2\rho} \right)^2 + \left( \frac{\varepsilon_{35}}{\rho} \right)^2} \right]^{1/2}
\]

\[
k_L^2 = \frac{(e_L)^2}{\varepsilon'_{33} \rho \left( v^{(L)} \right)^2}
\]

\[
k_S^2 = \frac{(e_S)^2}{\varepsilon'_{33} \rho \left( v^{(S)} \right)^2}
\]
where \( v^{(L)} \) and \( v^{(S)} \) are the acoustic velocities in longitudinal and shear modes, respectively, \( c_{33}, c_{55} \) and \( c_{35} \) are elastic constants, \( \varepsilon_{33} \) is a dielectric constant, and \( k_{L}^2 \) and \( k_{S}^2 \) are the electromechanical coupling coefficients of longitudinal and shear modes, respectively. The material properties of ZnO thin film are calculated and shown in Figure 4.2 which can be seen that the electromechanical coupling coefficient, and the acoustic velocity of ZnO are tilted dependent.

The maximum electromechanical coupling coefficient of the shear and the longitudinal waves occur as the ZnO thin film is tilted with the angle of 34° and 0°, respectively, while the corresponding acoustic velocity is calculated as 3264 m/s and 6424 m/s, respectively. The pure shear wave can be excited at an angle of 42° and 90° while the pure longitudinal wave can be excited at an angle of 0° and 64°. In order to design an acoustic sensor with high sensitivity and performance for liquid sensing applications, the large electromechanical coupling coefficient of shear mode is desired.

The general approach to analyzing the vibration behavior of the SMFBAR device is given by the transmission line model based on the Mason’s equivalent circuit as described in Chapter 3 section 1. The SMFBAR structure used in this study is illustrated in Figure 3.10, in which the single piezoelectric layer (ZnO) and non-piezoelectric layers (electrodes, SiO₂ and W) are treated as a three-port (one electrical port and two mechanical ports) and two-port components, respectively.
The transmission line model for ZnO layer is illustrated in Figure 3.11. The ZnO thin film is tilted with the angle of 34° due to the maximum electromechanical coupling coefficient of shear wave as described in above section. As shown in Figure 4.2, with 34° tilted ZnO thin film, both shear and longitudinal waves are excited. The
consideration of the acoustic impedance for both shear and longitudinal waves are required and can be written:

\[
Z_{(S,L)} = \frac{1}{j\omega C_0} \left( 1 - k_r^2 \frac{\tan(k_r d / 2)}{k_r d / 2} \right)
\]  
(4.9)

On the other hand, the transmission line model for other non-piezoelectric layers such as electrodes, SiO\(_2\) and W can be described as a two-by-two transfer matrix:

\[
A_{n(S,L)} = \begin{bmatrix} \cos k_n(S,L) & jZ_n \sin k_n(S,L) \\ j\sin k_n(S,L) / Z_n(S,L) & \cos k_n(S,L) \end{bmatrix}
\]  
(4.10)

where \(Z\) is the acoustic impedance for each of non-piezoelectric layer \(n\). By implementing this transformation matrix into Mason’s model, the acoustic impedances describing the layer assemblies on left (top electrode) and right (bottom electrode and Bragg reflector) side of ZnO thin film are described as:

\[
Z_{\text{top}} = \prod_{n=1}^{N} A_n \begin{bmatrix} F_{\text{top}} \\ u_{\text{top}} \end{bmatrix}
\]  
(4.11)

\[
Z_{\text{bot}} = \prod_{m=1}^{M} A_m \begin{bmatrix} F_{\text{bot}} \\ u_{\text{bot}} \end{bmatrix}
\]  
(4.12)

where \(n\) and \(m\) are the layer number, \(N\) and \(M\) are the number of layers on top and bottom of the piezoelectric layer, respectively. \(F\) and \(u\) are the boundary condition of force and the displacement velocity, respectively. For the unperturbed condition, both of surfaces are considered as stress-free boundaries (\(F=0\)). By solving the equation (4.11) and (4.12), the total acoustic impedance of the SMFBAR device with a \(c\)-axis-tilted piezoelectric layer is given by:

\[
Z_{(L)} = \frac{k_r^2}{\gamma_{(L)}} \left[ \frac{(z_{\text{top}} + z_{\text{bot}}) \sin \gamma_{(L)} + j(1 - \cos \gamma_{(L)})}{(z_{\text{top}} + z_{\text{bot}}) \cos \gamma_{(L)} + j(1 + z_{\text{top}} z_{\text{bot}}) \sin \gamma_{(L)}} \right]
\]  
(4.13)
\[
Z_{(S)} = \left[ \frac{k^2}{\gamma_{(S)}} \right] \frac{(z_{\text{top}} + z_{\text{bot}})\sin\gamma_{(S)} + j2(1-\cos\gamma_{(S)})}{(z_{\text{top}} + z_{\text{bot}})\cos\gamma_{(S)} + j(1+z_{\text{top}}z_{\text{bot}})\sin\gamma_{(S)}}
\]

(4.14)

\[
Z_{in} = \frac{V}{I} = \frac{1}{f\omega C_0} [1 - (Z_{(S)} + Z_{(L)})]
\]

(4.15)

\[
z_{\text{top}} = \frac{Z_{\text{top}}}{Z_0}
\]

(4.16)

\[
z_{\text{bot}} = \frac{Z_{\text{bot}}}{Z_0}
\]

(4.17)

\[
Z_0 = S\rho(v_s + v_L)
\]

(4.18)

where \(Z_0\) is the total acoustic impedance of piezoelectric layer with both shear and longitudinal waves. \(S\) and \(\rho\) are the active area and the density of piezoelectric layer respectively.

The resonant frequency of shear and longitudinal modes were also observed in three-dimensional simulation. As the device is operated in the shear mode, the particle vibration is parallel to the surface with the maximum displacement magnitude of 0.84 nm at resonance frequency of 425 MHz (See Figure 4.3(a)). In longitudinal mode, the particle vibration is perpendicular to the device surface with the maximum displacement magnitude of 0.66 nm at resonance frequency of 687 GHz (See Figure 4.3(b)). By comparing the results from one-dimensional Mason’s model simulation and three-dimensional finite element simulation, it can be seen that both simulations have close results as can be seen from Figure 4.4. The parameters that are used in this simulation are listed in Table 4.1.
Figure 4.3: Particle displacement of SMFBAR device in resonant frequency of (a) shear mode and (b) quasi-longitudinal mode.
Table 4.1: The resonance frequency of the SMFBAR device with both shear and longitudinal modes

<table>
<thead>
<tr>
<th>Thickness (nm)</th>
<th>Top Electrode</th>
<th>ZnO</th>
<th>Bottom Electrode</th>
<th>W</th>
<th>SiO2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m³)</td>
<td>2700</td>
<td>5680</td>
<td>2700</td>
<td>2197</td>
<td>1925</td>
</tr>
<tr>
<td>Acoustic Velocity (m/s)</td>
<td>5240</td>
<td>6200 (L) 3500(S)</td>
<td>5240</td>
<td>5802</td>
<td>4615</td>
</tr>
</tbody>
</table>

(L) represents the acoustic velocity in longitudinal mode and (S) represents the acoustic velocity in the shear mode.

Figure 4.4: The resonance frequency of the SMFBAR device with both shear and longitudinal modes.
4.2 Shear Acoustic Wave with Lateral Field Excitation Structure

Another approach to have a shear acoustic wave in SMFBAR device is regarding to the lateral field excitation (LFE) method. Figure 4.5 shows the lateral structure of SMFBAR device.

![Diagram of Lateral Field Excitation (LFE) SMFBAR](image)

Figure 4.5: The schematic diagram of the Lateral field excitation (LFE) SMFBAR with c-axis oriented ZnO thin film.

In the LEF FBAR, both signal and ground electrodes are set on a top piezoelectric thin film. When an electric field is applied between these electrodes, a bulk acoustic wave is generated in shear mode with a polarization in the y direction. This phenomenon can be described by the piezoelectric Christoffel equation, which is defined as [95]:

\[
k^3 \left( l_{ik} \left( c_{KL} \frac{1}{l_{ij}} + \frac{1}{l_{ilj}} \right) l_{il} \right) v_j = \rho \omega^2 v_i
\]

where \( k \) is the wave number, \( \omega \) is frequency, \( v_j \) represents particle polarization direction vector, \( c_{KL} \) is the stiffness matrix of piezoelectric material, and \( l_{il} \) is the matrix for describing the arbitrary propagation direction from the propagation vector \( I \).
\[
I_{il} = \begin{bmatrix}
I_x & 0 & 0 & 0 & I_y & I_z \\
0 & I_y & 0 & I_z & 0 & I_x \\
0 & 0 & I_z & I_y & 0 & I_x
\end{bmatrix}
\] (4.20)

\[
I = I_x \hat{i} + I_y \hat{j} + I_z \hat{k}
\] (4.21)

In this structure, the electric field is applied in the x-axis through the bulk of piezoelectric material, and since the c-axis is orientated normal to the surface [86], the wave propagation is perpendicular to the electric field in the z direction. Therefore, the propagation vector in the \( I_x \) and \( I_y \) directions is one, and in the \( I_z \) direction is zero. By substituting these values to (4.21), the Christoffel equation can be obtained as:

\[
k^2 = \begin{bmatrix}
 c_{44} + \frac{\epsilon_{15}^2}{\epsilon_{11}^2} & 0 & 0 \\
 0 & c_{44} + \frac{\epsilon_{15}^2}{\epsilon_{11}^2} & 0 \\
 0 & 0 & c_{33}
\end{bmatrix}
\begin{bmatrix}
v_x \\
v_y \\
v_z
\end{bmatrix} = \rho \omega^2
\begin{bmatrix}
v_x \\
v_y \\
v_z
\end{bmatrix}
\] (4.22)

and

\[
v_{ac} = \sqrt{\frac{c_{44} + \frac{\epsilon_{15}^2}{\epsilon_{11}^2}}{\rho}}
\] (4.23)

Using parameter values for ZnO listed in (3.21) to (3.24), the theoretical acoustic velocity for the piezoelectrically stiffened thickness shear mode is approximately 2841 m/s. This calculated acoustic velocity is an approximate figure and not an absolute value from which to evaluate an experimentally obtained mode. The theoretical piezoelectric coupling constant for the ZnO LFE resonator is given by

\[
k^2 = \frac{\epsilon_{15}^2}{c_{44} \epsilon_{11}}
\] (4.24)

### 4.3 Summary

This chapter describes the design of shear mode bulk acoustic wave device and gives a detailed account of the modeling and simulation of shear mode bulk
acoustic wave using two different tools namely Matlab\textsuperscript{TM} and Coventor\textsuperscript{TW}. The theoretical analysis for the c-axis inclined structure and the lateral field excitation structure has been presented. Both structures can excite the shear acoustic wave; however, the fabrication process of c-axis inclined structure is more complicate since the substrate has to be rotated in a certain degree. With these results, the theory and simulation of longitudinal, shear, and LFE structure have been performed. In the next chapter, it is explained that LFE structure has been chosen due to the fabrication feasibility. In addition, the design fabrication and characterization of the LFE SMFBAR device is presented.
CHAPTER 5

DESIGN AND FABRICATION OF LATERAL FIELD EXCITATION SMFBAR DEVICE

Multiple LFE SMFBAR devices with a resonant frequency of 500 MHz were designed using COMSOL™ platform and fabricated on a silicon wafer. The fabrication was performed by the Institute for Electronics and Nanotechnology (IEN) in Georgia Institute of Technology. This chapter describes in detail the design, fabrication and characterization of the LFE SMFBAR devices. The performance of the LFE SMFBAR devices with liquid loading is also presented.

5.1 Design of Lateral Field Excitation SMFBAR Device

The goal of this dissertation is to develop a bulk acoustic wave sensor for liquid based sensing applications. The FBAR structure does not support liquid media sensing. This is due to the fact that the piezoelectric layer of the FBAR is suspended in air and the weight of the liquid causes deformation of the sensing layer, resulting in an inaccurate measurement. The SMFBAR structure is more suitable for liquid sensing because the SMFBAR can fully support the weight of liquid since the piezoelectric layer is solidly attached on top of alternating layers. In addition, as described in Chapter 4, both c-axis inclined method and lateral field excitation method can excite a shear acoustic wave. However, the fabrication process of c-axis inclined method was relatively more complicated than the lateral field excitation method. Therefore, in this study, the lateral excitation method with SMFBAR structure was chosen.
The three-dimensional structure of the lateral field excitation SMFBAR is shown in Figure 5.1. Figure 5.2 shows three different electrode designs which were employed to excite the shear acoustic wave. Design 1 depicts a typical lateral field excitation structure where the two electrodes are parallel and placed on top of a ZnO thin film layer. The dimension of the electrodes is 280 μm × 7500 μm, separated by a gap of 40 μm. Design 2 consisted of 44 pairs of electrodes, where the spacing between two electrodes was 40 μm and the overlap length was 700 μm. Design 3 consisted of 3 pairs of electrodes with 40 μm separation and an overlap length of 3432 μm. In this study, the devices were designed with a resonant frequency in the range of 520 MHz and electrode thickness of 150 nm, 2500 nm, 1780 nm and 2240 nm for Au, ZnO, W and SiO₂, respectively. The overall dimension of each device was 12260 μm × 11900 μm.

Figure 5.1: The three dimensional structure of LFE SMFBAR device.
The performance analysis of the devices in terms of resonant frequency and particle displacement was carried out using COMSOL™ platform. The sequence of steps that were followed for designing and simulating two-dimensional model of the LFE SMFBAR devices is described below.

Figure 5.2: SMFBAR device with three designs (a) design 1, (b) design 2 and (c) design 3.
Initially, a new two-dimensional model of the LFE SMFBAR device was created using the Model Wizard in COMSOL™. In this model, the dimension and thickness of layers (silicon substrate, SiO₂, W, ZnO and electrode layers) was assigned using the Geometry Module as shown in Figure 5.3. The thickness of the electrodes, ZnO, W and SiO₂ were set as 150 nm, 2500 nm, 1780 nm and 2240 nm, respectively.

Figure 5.3: The two-dimensional structure in COMSOL™.

Next, the properties for the materials to be used in the structure were entered into the Material Module. The material database in COMSOL includes the material properties of the most commonly used materials. However, the pre-defined material properties such as ZnO were slightly different from the properties that we used in
Chapter 3. Therefore, in order to have a consistent analysis, the material properties of ZnO were re-assigned as provided in (3.29), (3.30), (3.31) and (3.32).

Following the structure design and material properties setup, the two-dimensional model was meshed using the Mesh function in COMSOL™. The Free Triangular method was chosen since it could effectively model both the isotropic and anisotropic behavior of the material. The Free Triangular method could automatically mesh the entire structure with nine different mesh sizes such as extremely coarse, extra coarse, coarse, normal, fine, finer, extra fine and extremely fine. In order to achieve an accurate result, the extremely fine mesh size was chosen. Figure 5.5 shows the meshed LFE SMFBAR structure. The total elements for the entire two-dimensional structure were reported to be 203,205.

Figure 5.4: Material properties setup in COMSOL™.
Once the two-dimensional structure was modeled and meshed, a frequency analysis was performed using the Study Function in COMSOL™. The approach that COMSOL™ used to analyze the piezoelectric material was based on the constitutive equations as described in Chapter 2, Section 2.1. The frequency was swept from 400 MHz to 600 MHz with a step size of 400 Hz. The impedance response of the three designs is shown in Figure 5.6. The resonant frequency of design 1, design 2 and design 3 were registered at 528 MHz, 528.6 MHz and 522.8 MHz, respectively. It was noted that although these three designs have different electrode configurations (electrode size and overlapping length), the resonant frequencies of three designs were

Figure 5.5: Meshed two-dimensional view of shear mode SMFBAR in COMSOL™.
close to 525 MHz, which means that the resonant frequency of the LFE SMFBAR device was mainly determined by the thickness of the piezoelectric layer.

Figure 5.6: The frequency response of (a) design 1, (b) design 2, and (c) design 3.

Figure 5.7 shows the particle displacement for design 1, design 2 and design 3 configurations. It can be seen that the particles were moving parallel to the surface in the x plane for all designs, which shows shear acoustic wave excitation. It is important
to note that most of the particle displacement is confined to the surface of the devices. It shows the designed alternative W and SiO$_2$ layers reflect the acoustic wave back to piezoelectric layer efficiently. This leads to limited acoustic energy loss and increased the quality factor for devices [96].

Figure 5.7: The particle displacement of (a) design 1, (b) design 2, and (c) design 3.
5.2 Photo-mask Design

Following the design and simulation, the photomask was designed using the Layout Editor in CoventorWare™. Figure 5.8 shows the mask layout of the entire wafer, where the mask consists of thirteen devices of design 1, twelve devices of design 2, and twelve devices of design 3. Following the mask design, a 5” × 5” chrome/sodalime photo-mask was manufactured by Photo Sciences Inc.

![Figure 5.8: Photo-Mask of three designs.](image)

5.3 Device Fabrication

In this study, the fabrication of a highly c-axis orientated ZnO thin film is required in order to excite the shear acoustic wave. In the past few years, several deposition techniques have been developed and studied to fabricate a highly c-axis
oriented ZnO, such as chemical vapour deposition CVD [97] [98], pulsed-enhanced chemical vapour deposition PECVD [99], electron beam (E-beam) [100] [101], pulse laser deposition PLD [102], reactive DC sputtering [103] and RF magnetron sputtering technique. Among these techniques, the RF magnetron sputtering is reported as the best method to grow a highly c-axis oriented ZnO thin film [104] [105] [106] [107]. This is because in the RF magnetron sputtering process, the film formation can be done at a relatively low temperature and low vacuum level which results in the good adhesion of the films on the substrates and yields uniform crystal films [108] [109]. In addition, parameters such as RF power [110], gas ratio [111], pressure and target-to-substrate spacing affect the quality of the film [112]. For these reasons, in this study, the c-axis oriented ZnO thin film was deposited based on Corso’s method [113].

The fabrication process of the SMFBAR devices is shown in Figure 5.9. This process started by cleaning 4” diameter of a silicon wafer. Then the alternating W and SiO₂ reflector layers were deposited using the Unifilm PVD-300 sputtering system. The tungsten was deposited using 0.86 V DC power, 100% Argon gas and 5×10⁻³ Torr pressure. The SiO₂ was deposited using RF sputtering, an Argon to Oxygen gas ratio of 98 : 2 and 5.02×10⁻³ Torr pressure. After additional alternate W and SiO₂ layers, a ZnO layer was then deposited using RF sputtering, an Argon to Oxygen gas ratio of 97.5 : 2.5, and 5.03×10⁻³ Torr pressure. A layer of photoresist was then spun on the top of ZnO thin film layer. The photoresist was then patterned by exposure to ultraviolet light through a mask in such a way as to create a positive image of the electrodes after developing. After the photoresist deposition, a 120 nm of Au was deposited on top of a 30 nm seeding layer of Cr to create the electrodes using an e-
beam evaporator. To finish the process, the photoresist was removed through a lift-off process. The parameters for fabricating all layers are outlined in Table 5.1.

Figure 5.9: The fabrication process. (a) the clean silicon wafer. (b) Alternative W and SiO$_2$ reflector layers are deposited using the Unifilm PVD-300 sputtering system. (c) The highly c-axis oriented ZnO layer was then deposited on top of the alternative layer. (d) The layer of photoresist was then spun on the top of ZnO thin film layer. (e) The photoresist was then patterned by exposure to ultraviolet light through a mask. (f) 120 nm of Au was deposited on top of a 30 nm seeding layer of Cr to create the electrodes. (g) The process was completed by removing photoresist through the lift-off process.
Table 5.1 Sputtering parameters for respective layers using a sputterer

<table>
<thead>
<tr>
<th>Parameter</th>
<th>W</th>
<th>SiO₂</th>
<th>ZnO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Layer thickness</td>
<td>1.78 µm</td>
<td>2.24 µm</td>
<td>2.5 µm</td>
</tr>
<tr>
<td>Temperature</td>
<td>Ambient</td>
<td>Ambient</td>
<td>325°C</td>
</tr>
<tr>
<td>Pressure</td>
<td>5×10⁻³</td>
<td>5.02×10⁻³</td>
<td>5.03×10⁻³</td>
</tr>
<tr>
<td>Argon:Oxygen Ratio</td>
<td>100:0</td>
<td>98:2</td>
<td>97.5:2.5</td>
</tr>
<tr>
<td>Power</td>
<td>0.86 DC</td>
<td>218 RF</td>
<td>135 RF</td>
</tr>
</tbody>
</table>

Device fabrication was performed at the IEN at Georgia Institute of Technology

5.4 Results and Discussion

5.4.1 Fabrication Outcome

Three wafers were fabricated. Only one deemed to the best. After receiving the fabricated wafer, it was carefully inspected using an optical microscope and it was discovered that only 3 out of 37 fabricated devices were working. Figure 5.10 shows the photographs of the fabricated wafer. It can be seen that the top part of the wafer was peeled-off. This could be due to large intrinsic stresses built up between the ZnO layer and alternative layers W and SiO₂ in the middle of the wafer. Previous studies have shown that lattice mismatch between the substrate and ZnO film, and the thermal mismatch induced due to a difference in the thermal expansion coefficients of the substrate, and the ZnO film could result in the intrinsic stresses [114]. However, research has also shown that the intrinsic stresses can be reduced by adjusting the deposition temperature or the annealing time [115].
Another issue was related to the incomplete or unsuccessful lift-off process. As it can be seen from Figure 5.11, the incomplete lift-off process caused short circuits. Generally, the lift-off is performed in a solvent bath that dissolves the photoresist and lifts the metal off from the substrate. The lift-off process must be completed before removing the sample from the solvent. The incomplete lift-off process might be due to the removal of the wafer from the solvent too early and therefore, the metal fell into the gap between the electrodes.

Figure 5.10: The photograph of the fabricated wafer with the peel-off area.
Due to the fabrication issues described in above, an extremely low yield of fabrication was obtained. Fortunately, three working devices were identified in the wafer; two of design 1 and one of design 3 are in the bottom and right side of the wafer as shown in Figure 5.12.

Figure 5.11: Incomplete lift-off process discovered in (a) design 1 and (b) design 3.
5.4.2 Structure Analysis of ZnO Thin Film

As described above, in order to excite a shear wave, highly (002) oriented ZnO thin film was needed. In order to know the crystal orientation of ZnO thin film, the X-ray diffraction (XRD) study was carried out on the deposited ZnO layer. For this purpose, an X-ray diffractometer with the X-ray source of Cu Ka and wavelength of 1.541 nm was used. Figure 5.13 shows the XRD spectrum of the ZnO thin film. It can be seen that a strong peak at the 2θ angle of 34.47° was obtained, which corresponds to ZnO (002) the preferred orientation [116]. It was also noted that in addition to the main peak of ZnO (002), Au (111) peak at 20 angle of 38.5° [117], tungsten W (110) peak at 20 angle of 40.26° [118], SiO$_2$ (203) peak at 20 angle of 69.46° [119] and Si (400) peak at 20 angle of 69.64° [120] were observed with XRD intensities at least ten times lower than the main ZnO (002) peak. The result shows that the deposited ZnO thin film on the W/SiO$_2$ alternative layers has a highly (002) crystal orientation, which was necessary for generating a shear acoustic wave in the ZnO film.

The grain size of the ZnO layer could be calculated by the Debye-Scherrer formula [121]
where $\lambda$, $B$, and $\theta$ are the wavelength of the X-ray source, the full width at half maximum (FWHM) of the ZnO (002) diffraction peak, and the Bragg diffraction angle, respectively. In this measurement, the wavelength of the X-ray source was equal to 0.1541 nm and the FWM of the ZnO peak was calculated as 0.48°. Therefore, the calculated crystallite size of the ZnO thin film is 1.05 nm.

Figure 5.13: X-ray diffraction pattern of a shear mode SMFBAR sample. The main peak of ZnO (002), Au (111), W(110), SiO2 (203) and Si (400) Re observed at 34.47°, 38.5°, 40.26°, 69.46° and 69.64°, respectively.
5.4.3 Measurement Setup

From the XRD measurement, the device shows a highly c-axis oriented ZnO thin film, which is required for exciting shear acoustic wave. Next, the LFE SMFBAR devices were tested for their functionality. Figure 5.14 shows a photograph of the experimental set up for testing the LFE SMFBAR devices. The LFE SMFBAR was placed in a custom platform which would hold the device. A spring probe (potted with epoxy) with SubMiniature version A (SMA) Cable was mounted into the platform to probe electric signals from the LFE SMFBAR devices. The impedance response of the devices was observed using a network analyzer (Agilent 4395B) with a sweep frequency range up to 1.8 GHz. The measured data was acquired by means of a LabView™ program (National Instruments, Austin, TX). The following section discusses the results obtained from the measurement.

5.4.4 Device Electrical Characterization

From the simulation results, the LFE SMFBAR devices were expected to have a shear mode resonance of around 500 MHz. In order to monitor the shear mode resonance, the network analyzer was set for a frequency sweep from 470 MHz to 570 MHz, with a frequency resolution of 5 kHz. Figure 5.15 shows the resonant frequency of design 1 and design 3. The fundamental resonant frequency ($f_0$) of design 1 and design 3 were measured at 518 MHz and 514.5 MHz, respectively. The measured resonant frequencies of design 1 and design 3 were close to the simulation results of 528 MHz and 522.8, respectively.
The performance of the LFE SMFBAR devices were also defined by the quality factor (Q) and the effective electromechanical coupling coefficient ($k_{\text{eff}}^2$). The quality factor is a measurement of the energy loss in the system, and the effective electromechanical coupling coefficient defines the transformed ability of piezoelectric material. Both of parameters are defined as [122]

Figure 5.14: The photo of the experimental setup.
\[ Q = \frac{f}{2} \frac{\Phi_Z}{\partial f} \]  
\[ k_{\text{eff}}^2 = \frac{\pi}{2} \frac{f_p}{f_s} \approx \frac{\pi^2}{4} \frac{f_p - f_s}{f_p} \]

where \( \Phi_Z \) is the phase of impedance and \( f_p \) and \( f_s \) are the parallel and series resonant frequency, respectively.

Figure 5.15: The impedance response of (a) design 1 and (b) design 3 of the LFE SMFBAR device.
The parallel resonant frequency of design 1 and design 3 were measured at 524.5 MHz and 520 MHz, respectively. The series resonant frequency of design 1 and design 3 were measured at 518.5 MHz and 514.5 MHz, respectively. By substituting the center frequency into (5.2) and parallel resonant frequency and serial resonant frequency into (5.2), the effective coupling coefficients of design 1 and design 3 were calculated as 3.06% and 2.84% while the quality factor of design 1 and design 3 were 886 and 647, respectively. Comparing to the previous study presented by C.D. Corso et al. [47], the LFE SMFBAR devices designed in this study show better performance in terms of the effective coupling coefficients and the qualify factor. The effective coupling coefficients and qualify factor reported by C.D. Corsol were 0.88% and 550, respectively.

5.4.5 Device Electrical Characterization with Liquid Loading

As described above the LFE SMFBAR devices designed in this study had good performance in the air measurement. However, it was important to know the performance of the devices with liquid loading. For the measurement of the devices with liquid loading, 1 μL of distilled (DI) water was dropped on the sensing area of the devices using a manual micropipette as shown in Figure 5.16. Figure 5.17 shows the impedance response before and after application of water to the surface of design 1 and design 3 devices. As can be seen, a negative frequency shift occurred after water was applied to the surface of the devices with the decrement frequency of 4 MHz and 4.2 MHz for design 1 and design 3, respectively.

According to the Sauerbrey equation (2.20), it is reasonable to assume that the observed frequency shift indicates a mass loading on the surface of the device by the water.
Figure 5.16: The LFE SMFBAR device loaded with a drop of water.

Figure 5.17: (a) The impedance response and (b) the insertion loss of the design 3 LFE SMFBAR device.
The parallel resonant frequency of the design 1 and design 3 were measured at 521 MHz and 515.5 MHz, respectively. The series resonant frequency of the design 1 and design 3 were measured at 515 MHz and 510 MHz, respectively. By substituting the parallel resonant frequency and the serial resonant frequency into (5.3), the effective coupling coefficients of design 1 and design 3 were calculated as 3.08% and 2.6% while the quality factor of design 1 and design 3 were 436 and 213, respectively. The calculated quality factors and effective coupling coefficients are summarized in Table 5.2. It is worth noting that the quality factor of the designed LFE SMFBAR devices in this study was much higher than a previous study by M. Link et al. [123]. In the Link et al. study, the shear mode was excited through the inclined c-axis ZnO thin film with an angle of 18°. The device was operated in a high frequency of 849 MHz; however, the observed quality factor of the device was 192, with water loading. Based on the performance of the designed LFE SMFBAR devices, it is expected that these devices could be used as a platform for liquid based biosensor applications.

Table 5.2 The performance of the shear mode SMFBAR devices

<table>
<thead>
<tr>
<th>Sample</th>
<th>Medium</th>
<th>$f_s$(MHz)</th>
<th>$f_p$(MHz)</th>
<th>$K_{eff}^2$(%)</th>
<th>Q</th>
</tr>
</thead>
<tbody>
<tr>
<td>Design 1</td>
<td>Air</td>
<td>518.5</td>
<td>524.5</td>
<td>3.06</td>
<td>886</td>
</tr>
<tr>
<td></td>
<td>Water</td>
<td>515</td>
<td>521</td>
<td>2.84</td>
<td>436</td>
</tr>
<tr>
<td>Design 3</td>
<td>Air</td>
<td>514.5</td>
<td>520</td>
<td>2.84</td>
<td>647</td>
</tr>
<tr>
<td></td>
<td>Water</td>
<td>510</td>
<td>515.5</td>
<td>2.6</td>
<td>213</td>
</tr>
</tbody>
</table>
5.5 Summary

In this chapter, the design and fabrication of the shear mode SMFBAR devices were introduced and the detailed measurement results of these devices were presented. Due to the fabrication issues such as intrinsic stresses and incomplete lift-off process, the fabrication yield was very low. The impedance response of the LFE SMFBAR devices was characterized using a network analyzer and then the performance of the devices in terms of the qualify factor and effective electromechanical coupling coefficient were calculated. The results showed that the designed LFE SMFBAR devices have high effective electromechanical coupling coefficient and qualify factor with and without water loading, which indicated that the designed LFE SMFBAR devices were suitable for liquid based biosensing applications. The next chapter concludes the dissertation and provides with some suggestions for future work.
CHAPTER 6

CONCLUSION AND FUTURE WORK

6.1 Conclusion

The development of shear mode SMFBAR devices has been successfully demonstrated in this dissertation work with the accomplishment of both design and fabrication. Theoretical studies have also been conducted to design, optimize and characterize these shear mode acoustic devices. An experimental study has been conducted to fabricate and characterize the shear mode SMFBAR devices. The major accomplishments of this research are listed below:

- The theoretical method based on Mason’s model is developed to characterize the impedance response of the FBAR and SMFBAR devices.
- The two- and three-dimensional finite element model has been built to further analyze the particle displacement of the devices. The propagation direction of the acoustic wave and particle displacement at resonant frequency were visualized.
- The theoretical method for simulation of the inclined c-axis structure and lateral field excitation structure were presented.
- The maximum shear mode electromechanical coupling coefficient of inclined ZnO thin film has been found when the crystal orientation was rotate 34°.
- The LFE SMFBAR devices were successfully fabricated and tested. The devices were operated at 518 MHz and 514.5 MHz for design 1 and design 3, respectively. High quality factors of 886 and 647 were obtained in design 1 and design 3, respectively.

The LFE SMFBAR devices also performed very well with liquid loading. Quality factors of 436 and 213 were obtained for design 1 and design 3, respectively.
The results show that the LFE SMFBAR has potential for use in liquid based biosensing applications.

6.2 Future Work

Some suggestions for future work include the following:

1. To be able to use CoventorWare™ and COMSOL™ to successfully model shear mode SMFBAR devices with liquid loading in order to get better matching results between measured and simulated response.

2. To improve the fabrication process. The peel-off problem could be solved by reducing the intrinsic stresses. Several research reports have suggested that adjusting the deposition temperature and the annealing time could reduce intrinsic stresses.

3. To use the results from these experiments to successfully design and fabricate a second generation of LFE SMFBAR devices to perform these experiments in a continuous flow condition.

4. To develop a sensing system with a microfluidic flow cell and demonstrate the viability toward detection of various biomolecular substances.
APPENDIX A. MATLAB CODE TO SIMULATE THE FREQUENCY

function [Sc, Se, Sp] = Rotation_about_Y(Sc1,Se1,Sp1,beta)
% y Euler angle (in degree), counter-clockwise

%%% ---- Rotation Matrix----
% y Euler angle (in degree), counter-clockwise

R=zeros(3);
R(1,1)=cosd(beta);
R(1,3)=sind(beta);
R(2,2)=1;
R(3,1)=-sind(beta);
R(3,3)=cosd(beta);

A=zeros(3);
B=zeros(3);
C=zeros(3);
D=zeros(3);
A(1,1)=R(1,1)^2;
A(1,2)=R(1,2)^2;
A(1,3)=R(1,3)^2;
A(3,1)=R(3,1)^2;
A(3,2)=R(3,2)^2;
A(3,3)=R(3,3)^2;
A(2,1)=R(2,1)^2;
A(2,2)=R(2,2)^2;
A(2,3)=R(2,3)^2;
B(2,1)=R(2,2)*R(2,3);
B(2,2)=R(2,3)*R(2,1);
B(2,3)=R(2,1)*R(2,2);
B(1,1)=R(1,2)*R(1,3);
B(1,2)=R(1,3)*R(1,1);
B(1,3)=R(1,1)*R(1,2);
B(3,1)=R(3,2)*R(3,3);
B(3,2)=R(3,3)*R(3,1);
B(3,3)=R(3,1)*R(3,2);
C(1,1)=R(2,1)*R(3,1);
C(1,2)=R(2,2)*R(3,2);
C(1,3)=R(2,3)*R(3,3);
C(2,1)=R(3,1)*R(1,1);
C(2,2)=R(3,2)*R(1,2);
C(2,3)=R(3,3)*R(1,3);
C(3,1)=R(1,1)*R(2,1);
C(3,2)=R(1,2)*R(2,2);
C(3,3)=R(1,3)*R(2,3);

D(1,1)=R(2,2)*R(3,3)+R(2,3)*R(3,2);
D(1,2)=R(2,1)*R(3,3)+R(2,3)*R(3,1);
D(1,3)=R(2,2)*R(3,1)+R(2,1)*R(3,2);
D(2,1)=R(1,2)*R(3,3)+R(1,3)*R(3,2);
D(2,2)=R(1,3)*R(3,1)+R(1,1)*R(3,3);
D(2,3)=R(1,1)*R(3,2)+R(1,2)*R(3,1);
D(3,1)=R(1,2)*R(2,3)+R(1,3)*R(2,2);
D(3,2)=R(1,3)*R(2,1)+R(1,1)*R(2,3);
D(3,3)=R(1,1)*R(2,2)+R(1,2)*R(2,1);

M=[A,B*2;C,D];
N=[A,B;C*2,D];

%%% calculation
Sc=M*Sc1*(M');
Se=R*Se1*(M');
Sp=R*Sp1*(R');
end
Signal Layer of FBAR

% The code for single ZnO layer with adjustable inclined angle
%

clear all

beta=0; %Rotation angle

[Sd,vL,vS,kL,kS,Se,Sp] = Material_database_ZnO(beta);
[vLw,vSw,vLs,vSs,vLa,vSa] = Material_database();

fstep=6000;
f1=0.1*10^9;
f2=5*10^9;
f=(f1:(f2-f1)/fstep:f2);
Zin=zeros(size(f));
Z=zeros(size(f));
d= 0.8*10^(-6); %Thickness of ZnO layer
A=100e-6*100e-6; %Surface area
w=2*3.1415926*f; %Angular frequency
C0=(Sp(3,3)*A)/d; %Static capacitance
pcl=w/vL; %Propagation constant of longitudinal mode
pcs=w/vS; %Propagation constant of shear mode

%% ---- Impedance response with the function of frequency
for i=1:1:fstep+1
    ZL(i)=(kL*((tan((pcl(i)*d)/2))/((pcl(i)*d)/2)));
    ZS(i)=(kS*((tan((pcs(i)*d)/2))/((pcs(i)*d)/2)));
    Zin(i)=(1/(j*w(i)*C0))*(1-ZL(i)-ZS(i));
    Zin(i)=abs(Zin(i));
end
%% Plot figure
semilogy(f,Zin)
hold on
clear all

beta=34; %Rotation angle

[Sd,vL,vS,kL,kS,Sc,Se,Sp] = Material_database_ZnO(beta);
[vLw,vSw,vLs,vSs,vLe,vSe,Dw,Ds,De] = Material_database();

%%% ----Frequency setup--------
fstep=3000;
f1=0.3*10^9;
f2=0.75*10^9;
f1=(f1:(f2-f1)/fstep:f2);
%Zin=zeros(size(f));
Z=zeros(size(f1));
step=1;
for f=f1:(f2-f1)/fstep:f2

%%% ----Device's geometry
A=100e-6*100e-6; %Surface area
dz=800e-9; %Thickness of ZnO layer
dw=303e-9; %Thickness of W layer
ds=381e-9; %Thickness of SiO2 layer
de=150e-9; %Thickness of electrode layer

%%% ----Parameters used for the calculation------
w=2*3.1415926*f; %Angular frequency
C0=(Sp(3,3)*A)/dz; %Static capacitance
pcl=w/vL; %Propagation constant of longitudinal mode
pcs=w/vS; %Propagation constant of shear mode
PDzL=w*dz/vL; %Phase delay of ZnO (longitudinal mode)
PDzS=w*dz/vS; %Phase delay of ZnO (shear mode)
PDwL=w*dw/vLw; %Phase delay of W (longitudinal mode)
PDwS=w*dw/vSw; %Phase delay of W (shear mode)
PDsL=w*ds/vLs; %Phase delay of SiO2 (longitudinal mode)
PDsS=w*ds/vSs; %Phase delay of SiO2 (shear mode)
PDeL=w*de/vLe; %Phase delay of Au(longitudinal mode)
PDeS=w*de/vSe; %Phase delay of Au (shear mode)

Z0L=A*Sd*vL;
Z0S=A*Sd*vS;
ZwL=A*Dw*vLw; %Acoustic impedance of W (longitudinal mode)
ZwS=A*Dw*vSw; %Acoustic impedance of W (shear mode)
ZsL=A*Ds*vLs; %Acoustic impedance of SiO2 (longitudinal mode)
ZsS=A*Ds*vSs; %Acoustic impedance of SiO2 (shear mode)
ZeL=A*De*vLe; %Acoustic impedance of Au (longitudinal mode)
ZeS=A*De*vSe;  %Acoustic impedance of Au (shear mode)

M_wL=[cos(PDwL) j*ZwL*sin(PDwL); j*sin(PDwL)/ZwL*cos(PDwL)];  %Matrix for W (longitudinal mode)
M_wS=[cos(PDwS) j*ZwS*sin(PDwS); j*sin(PDwS)/ZwS*cos(PDwS)];  %Matrix for W (shear mode)
M_sL=[cos(PDsL) j*ZsL*sin(PDsL); j*sin(PDsL)/ZsL*cos(PDsL)];  %Matrix for W (longitudinal mode)
M_sS=[cos(PDsS) j*ZsS*sin(PDsS); j*sin(PDsS)/ZsS*cos(PDsS)];  %Matrix for W (shear mode)
M_eL=[cos(PDeL) j*ZeL*sin(PDeL); j*sin(PDeL)/ZeL*cos(PDeL)];  %Matrix for W (longitudinal mode)
M_eS=[cos(PDeS) j*ZeS*sin(PDeS); j*sin(PDeS)/ZeS*cos(PDeS)];  %Matrix for W (shear mode)

%% ----Matrix for Bragg Reflector and Top Electrode------
BRL=M_eL*M_sL*M_wL*M_sL*M_wL*[0;1];  %Acoustic impedance of BR (longitudinal mode)
BRS=M_eS*M_sS*M_wS*M_sS*M_wS*[0;1];  %Acoustic impedance of BR (shear mode)

zbotL=(BRL(1,1)/BRL(2,1))/Z0L;
zbotS=(BRS(1,1)/BRS(2,1))/Z0S;
% ----Impedance for the layer on top ZnO ------
ZtopL=j*ZeL*tan(PDeL);  %Impedance of top electrode (longitudinal mode)
ZtopS=j*ZeS*tan(PDeS);  %Impedance of top electrode (shear mode)

ztopL=ZtopL/Z0L;
ztopS=ZtopS/Z0S;
% % ---- Total Impedance ------

HL=cos(PDzL)-1+j*(ZtopL/Z0L)*sin(PDzL);
HS=cos(PDzS)-1+j*(ZtopS/Z0S)*sin(PDzS);
%A1L=[cos(PDzL)+j*(ZtopL/Z0L)*sin(PDzL)
Z0L*((ZtopL/Z0L)*cos(PDzL)+j*sin(PDzL));
% j*sin(PDzL)/Z0L 2*(cos(PDzL)-1)+j*(ZtopL/Z0L)*sin(PDzL)];
%A1S=[cos(PDzS)+j*(ZtopS/Z0S)*sin(PDzS)
Z0S*(ZtopS/ZOS)*cos(PDzS)+j*sin(PDzS));
% j*sin(PDzS)/Z0S 2*(cos(PDzS)-1)+j*(ZtopS/Z0S)*sin(PDzS)];

ZL=(kL/PDzL)*((ztopL+zbotL)*sin(PDzL)+j*2*(1-
-cos(PDzL)))/((ztopL+zbotL)*cos(PDzL)+j*(1+ztopL*zbotL)*sin(PDzL));
ZS=(kS/PDzS)*((ztopS+zbotS)*sin(PDzS)+j*2*(1-
-cos(PDzS)))/((ztopS+zbotS)*cos(PDzS)+j*(1+ztopS*zbotS)*sin(PDzS));

Z=(1/(j*w*C0))*(1-(ZL+ZS));
Zin(step)=abs(Z);
step=step+1;
end

%%% ---Plot Figure--------
semilogy(f1, Zin)
APPENDIX B. LIST OF PUBLICATIONS

B1. Journal Papers


B2. Conference Presentations


BIBLIOGRAPHY


[63] Y. S. Fung and Y. Y. Wong, "Self Assembled Monolayers as the Coating in a


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