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Temperature-Compensated and High-$Q$ Piezoelectric Aluminum Nitride Lamb Wave Resonators for Timing and Frequency Control Applications

by

Chih-Ming Lin

A dissertation submitted in partial satisfaction of the requirements for the degree of

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in

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in the

Graduate Division

of the

University of California, Berkeley

Committee in charge:

Professor Albert P. Pisano, Chair
Professor Liwei Lin
Professor Richard M. White
Professor Clark T.-C. Nguyen

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by

Chih-Ming Lin
Abstract

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Doctor of Philosophy in Mechanical Engineering

University of California, Berkeley

Professor Albert P. Pisano, Chair

The explosive development of wireless and mobile communication systems has lead to rapid technology innovation in component performance, complementary metal-oxide semiconductor (CMOS) compatible fabrication techniques, and system improvement to satisfy requirements for faster signal processing, cost efficiency, chip miniaturization, and low power consumption. The demands for the high-performance communication systems whose fundamentals are precise timing and frequency control have driven the current research interests to develop advanced reference oscillators and radio frequency (RF) bandpass filters. In turn a promising microelectromechanical systems (MEMS) resonator technology is required to achieve the ultimate goal. That is, micromechanical vibrating resonators with high quality factor (\(Q\)) and good frequency-temperature stability at high series resonance frequency (\(f_s\)) are the required fundamental components for a high-performance wireless communication system.

Recently, Lamb wave mode propagating in piezoelectric thin plates has attracted great attention for designs of the electroacoustic resonators since it combines the advantages of bulk acoustic wave (BAW) and surface acoustic wave (SAW): high phase velocity and multiple frequency excitation by an interdigital transducer (IDT). More specifically, the Lamb wave resonator (LWR) based on an aluminum nitride (AlN) thin film has attracted many attentions because it can offer the high resonance frequency, small temperature-induced frequency drift, low motional resistance, and CMOS compatibility. The lowest-order symmetric (S0) Lamb wave mode propagation in the AlN thin plate is particularly preferred because it exhibits a phase velocity close to 10,000 m/s, a low dispersive phase velocity characteristic, and a moderate electromechanical coupling coefficient. However, the uncompensated AlN LWR shows a first-order temperature coefficient of frequency (TCF) of approximately –25 ppm/°C. This level of the temperature stability is unsuitable for any timing application. In addition, the \(Q\) of the AlN LWR is degraded to several hundred while the IDT finger width is downscaled to a nanometer scale to raise the resonance frequency up to a few GHz.
This dissertation presents comprehensive analytical and experimental results on a new class of temperature-compensated and high-$Q$ piezoelectric AlN LWRs. The temperature compensation of the AlN LWR using the $S_0$ Lamb wave mode is achieved by adding a layer of silicon dioxide ($SiO_2$) with an appropriate thickness ratio to the AlN thin film, and the AlN/$SiO_2$ LWRs can achieve a low first-order TCF at room temperature. Based on the multilayer plate composed of a 1-$\mu$m-thick AlN film and a 0.83-$\mu$m-thick $SiO_2$ layer, a temperature-compensated LWR operating at a series resonance frequency of 711 MHz exhibits a zero first-order TCF and a small second-order TCF of $–21.5$ ppb/°C$^2$ at its turnover temperature, 18.05°C. The temperature dependence of fractional frequency variation is less than 250 parts per million (ppm) over a wide temperature range from $–55$ to 125°C. In addition to the temperature compensation at room temperature, the thermal compensation of the AlN LWRs is experimentally demonstrated at high temperatures. By varying the normalized AlN film thickness ($h_{AlN}/\lambda$) and the normalized $SiO_2$ film thickness ($h_{SiO_2}/\lambda$), the turnover temperature can be designed at high temperatures and the AlN LWRs are temperature-compensated at 214°C, 430°C, and 542°C, respectively. The temperature-compensated AlN/$SiO_2$ LWRs are promising for a lot of applications including thermally stable oscillators, bandpass filters, and sensors at room temperature as well as high temperatures.

The influences of the bottom electrode upon the characteristics of the LWRs utilizing the $S_0$ Lamb wave mode in the AlN thin plate are theoretically and experimentally studied. Employment of a floating bottom electrode for the LWR reduces the static capacitance in the AlN membrane and accordingly enhances the effective coupling coefficient. The floating bottom electrode simultaneously offers a large coupling coefficient and a simple fabrication process than the grounded bottom electrode but the transduction efficiency is not sacrificed. In contrast to those with the bottom electrode, an AlN LWR with no bottom electrode shows a high $Q$ of around 3,000 since it gets rid of the electrical loss in the metal-to-resonator interface. In addition, it exhibits better power handling capacity than those with the bottom electrode since less thermal nonlinearity induced by the self-heating exists in the resonators.

In order to boost the $Q$, a new class of the AlN LWRs using suspended convex edges is introduced in this dissertation for the first time. The suspended convex edges can efficiently reflect the Lamb waves back towards the transducer as well as confine the mechanical energy in the resonant body. Accordingly the mechanical energy dissipation through the support tethers is significantly minimized and the $Q$ can be markedly enhanced. More specifically, the measured frequency response of a 491.8-MHz LWR with suspended biconvex edges yields a $Q$ of 3,280 which represents a 2.6× enhancement in $Q$ over a 517.9-MHz LWR based on the same AlN thin plate but with the suspended flat edges. The suspended convex edges can efficiently confine mechanical energy in the LWR and reduce the energy dissipation through the support tethers without increasing the motional impedance of the resonator. In addition, the radius of curvature of the suspended convex edges and the AlN thickness normalized to the wavelength can be further optimized to simultaneously obtain high $Q$, low motional impedance, and large effective coupling coefficient ($k^2_{eff}$).
To further enhance the $Q$ of the LWR, a composite plate including an AlN thin film and an epitaxial cubic silicon carbide (3C–SiC) layer is introduced to enable high-$Q$ and high-frequency micromechanical resonators utilizing high-order Lamb wave modes. The use of the epitaxial 3C–SiC layer is attractive as SiC crystals have been theoretically proven to have an exceptionally large $f_s Q$ product due to its low acoustic loss characteristic at microwave frequencies. In addition, AlN and 3C–SiC have well-matched mechanical and electrical properties, making them a suitable material stack for the electroacoustic resonators. The epitaxial 3C–SiC layer not only provides the micromechanical resonators with a low acoustic loss layer to boost their $Q$ but also enhances the electromechanical coupling coefficients of some high-order Lamb waves in the AlN/3C–SiC composite plate. A micromachined electroacoustic resonator utilizing the third quasi-symmetric (QS$_3$) Lamb wave mode in the AlN/3C–SiC composite plate exhibits a $Q$ of 5,510 at 2.92 GHz, resulting in the highest $f_s Q$ product, $1.61 \times 10^{13}$ Hz, among suspended piezoelectric thin film resonators to date.
To my parents and Shing-Ting
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<tr>
<td>3C–SiC</td>
<td>Cubic Silicon Carbide</td>
</tr>
<tr>
<td>AC</td>
<td>Alternating Current</td>
</tr>
<tr>
<td>AKE</td>
<td>Akhiezer Effect</td>
</tr>
<tr>
<td>Al</td>
<td>Aluminum</td>
</tr>
<tr>
<td>AlN</td>
<td>Aluminum Nitride</td>
</tr>
<tr>
<td>Au</td>
<td>Gold</td>
</tr>
<tr>
<td>BAW</td>
<td>Bulk Acoustic Wave</td>
</tr>
<tr>
<td>BCC</td>
<td>Body-Centered Cubic</td>
</tr>
<tr>
<td>BF</td>
<td>Bright Field</td>
</tr>
<tr>
<td>BVD</td>
<td>Butterworth-Van Dyke</td>
</tr>
<tr>
<td>BW</td>
<td>Bandwidth</td>
</tr>
<tr>
<td>C</td>
<td>Capacitor</td>
</tr>
<tr>
<td>$C_0$</td>
<td>Clamped Capacitor</td>
</tr>
<tr>
<td>$C_m$</td>
<td>Motional Capacitor</td>
</tr>
<tr>
<td>CMOS</td>
<td>Complementary Metal-Oxide Semiconductor</td>
</tr>
<tr>
<td>CMP</td>
<td>Chemo-Mechanical Planarization</td>
</tr>
<tr>
<td>CMR</td>
<td>Contour-Mode Resonator</td>
</tr>
<tr>
<td>CMU</td>
<td>Clock Multiplying Unit</td>
</tr>
<tr>
<td>COM</td>
<td>Coupling-of-Modes</td>
</tr>
<tr>
<td>CVD</td>
<td>Chemical Vapor Deposition</td>
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<td>DC</td>
<td>Direct Current</td>
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<tr>
<td>ED</td>
<td>Electron Diffraction</td>
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<tr>
<td>FBAR</td>
<td>Film Bulk Acoustic Resonator</td>
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<tr>
<td>FCC</td>
<td>Face-Centered Cubic</td>
</tr>
<tr>
<td>FDD</td>
<td>Frequency Division Duplex</td>
</tr>
<tr>
<td>FEA</td>
<td>Finite Element Analysis</td>
</tr>
<tr>
<td>$f_s$</td>
<td>Series Resonance Frequency</td>
</tr>
<tr>
<td>$f_p$</td>
<td>Parallel Resonance Frequency</td>
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<tr>
<td>FPAR</td>
<td>Film Plate Acoustic Resonator</td>
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<tr>
<td>GaAs</td>
<td>Gallium Arsenide</td>
</tr>
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<td>Abbreviation</td>
<td>Description</td>
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<td>--------------</td>
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</tr>
<tr>
<td>GaPO$_4$</td>
<td>Gallium Orthophosphate</td>
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<tr>
<td>GHz</td>
<td>Gigahertz</td>
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<tr>
<td>GSM</td>
<td>Global System for Mobile Communications</td>
</tr>
<tr>
<td>HBAR</td>
<td>High-Overtone Bulk Acoustic Resonator</td>
</tr>
<tr>
<td>HR</td>
<td>High Resolution</td>
</tr>
<tr>
<td>ICP</td>
<td>Inductively Coupled Plasma</td>
</tr>
<tr>
<td>IDT</td>
<td>Interdigital Transducer</td>
</tr>
<tr>
<td>IF</td>
<td>Intermediate Frequency</td>
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<tr>
<td>IL</td>
<td>Insertion Loss</td>
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<tr>
<td>kHz</td>
<td>Kilohertz</td>
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<tr>
<td>L</td>
<td>Inductor</td>
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<td>LFE</td>
<td>Lateral-Field-Excited</td>
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<tr>
<td>LGT</td>
<td>Langatate</td>
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<tr>
<td>LiNbO$_3$</td>
<td>Lithium Niobate</td>
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<tr>
<td>LiTaO$_3$</td>
<td>Lithium Tantalate</td>
</tr>
<tr>
<td>$L_m$</td>
<td>Motional Inductor</td>
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<tr>
<td>LNA</td>
<td>Low Noise Amplifier</td>
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<td>LO</td>
<td>Local Oscillator</td>
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<td>LPCVD</td>
<td>Low Pressure Chemical Vapor Deposition</td>
</tr>
<tr>
<td>LSN</td>
<td>Low Stress Nitride</td>
</tr>
<tr>
<td>LTE</td>
<td>Long-Term Evolution</td>
</tr>
<tr>
<td>LTO</td>
<td>Low Temperature Oxide</td>
</tr>
<tr>
<td>LWR</td>
<td>Lamb Wave Resonator</td>
</tr>
<tr>
<td>MBE</td>
<td>Molecular Beam Epitaxy</td>
</tr>
<tr>
<td>MBVD</td>
<td>Modified Butterworth-Van Dyke</td>
</tr>
<tr>
<td>MEMS</td>
<td>Microelectromechanical systems</td>
</tr>
<tr>
<td>MHz</td>
<td>Megahertz</td>
</tr>
<tr>
<td>Mo</td>
<td>Molybdenum</td>
</tr>
<tr>
<td>MOCVD</td>
<td>Metal Organic Chemical Vapor Deposition</td>
</tr>
<tr>
<td>N$_2$</td>
<td>Nitrogen</td>
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</tbody>
</table>
Nb  Niobium
OCXO  Oven-Controlled Crystal Oscillator
OCVCXO  Oven-Controlled Voltage-Controlled Crystal Oscillator
OMR  Over-Moded Resonator
PAW  Plate Acoustic Wave
PCB  Printed Circuit Board
PECVD  Plasma Enhanced Chemical Vapor Deposition
PLL  Phase-Locked Loop
PML  Perfectly Matched Layer
ppb  Parts-Per-Billion
ppm  Parts-Per-Million
Pt  Platinum
PVDF  Polyvinylidene Flouride
PZT  Lead Zirconium Titanate
Q  Quality Factor
QA  Quasi-antisymmetric
$Q_p$  Quality Factor at the Parallel Frequency
QS  Quasi-symmetric
$Q_s$  Quality Factor at the Series Frequency
R  Resistor
RF  Radio Frequency
RIE  Reactive Ion Etching
$R_m$  Motional Resistor
SAW  Surface Acoustic Wave
Sc  Scandium
SCS  Single Crystal Silicon
SEM  Scanning Electron Micrograph
SHF  Super-High-Frequency
Si  Silicon
SiC  Silicon Carbide
SiO$_2$  Silicon Dioxide
<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>SiOF</td>
<td>Fluorine-Doped Silicon Oxide</td>
</tr>
<tr>
<td>SMA</td>
<td>Sub Miniature version A</td>
</tr>
<tr>
<td>SMR</td>
<td>Solidly Mounted Resonator</td>
</tr>
<tr>
<td>TCE</td>
<td>Temperature Coefficient of Elasticity</td>
</tr>
<tr>
<td>TCF</td>
<td>Temperature Coefficient of Frequency</td>
</tr>
<tr>
<td>TCP</td>
<td>Transformer Coupled Plasma</td>
</tr>
<tr>
<td>TCXO</td>
<td>Temperature-Compensated Crystal Oscillator</td>
</tr>
<tr>
<td>TCVCXO</td>
<td>Temperature-Compensated Voltage-Controlled Crystal Oscillator</td>
</tr>
<tr>
<td>TDD</td>
<td>Time Division Duplex</td>
</tr>
<tr>
<td>TE</td>
<td>Thickness Extension</td>
</tr>
<tr>
<td>TED</td>
<td>Thermoelastic Damping</td>
</tr>
<tr>
<td>TEM</td>
<td>Transmission Electron Microscopy</td>
</tr>
<tr>
<td>TeO₂</td>
<td>Tellurium Dioxide</td>
</tr>
<tr>
<td>TFE</td>
<td>Thickness-Field-Excited</td>
</tr>
<tr>
<td>Ti</td>
<td>Titanium</td>
</tr>
<tr>
<td>TMAH</td>
<td>Tetramethylammonium Hydroxide</td>
</tr>
<tr>
<td>TS</td>
<td>Thickness Shear</td>
</tr>
<tr>
<td>UHF</td>
<td>Ultra-High-Frequency</td>
</tr>
<tr>
<td>VCXO</td>
<td>Voltage-Controlled Crystal Oscillator</td>
</tr>
<tr>
<td>VHF</td>
<td>Very-High-Frequency</td>
</tr>
<tr>
<td>W</td>
<td>Tungsten</td>
</tr>
<tr>
<td>XO</td>
<td>Crystal Oscillator</td>
</tr>
<tr>
<td>XRD</td>
<td>X-Ray Diffraction</td>
</tr>
<tr>
<td>ZnO</td>
<td>Zinc Oxide</td>
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</table>
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CURRICULUM VITAE

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Chapter 1

Introduction

The signal processors in the communication systems usually including bandpass filters, reference oscillators, and mixers are used for up- and down-conversion in the receivers and transceivers. It is well-known that quartz resonators and surface acoustic wave (SAW) devices have been employed in oscillators and bandpass filters, respectively, for decades but the integration with complementary metal-oxide semiconductor (CMOS) circuits is still an unsolved problem due to the fabrication incompatibility of the piezoelectric bulk materials with the silicon (Si) wafers in nature. Film bulk acoustic resonators (FBAR) and FBAR-based bandpass filters are able to be fabricated on Si wafers and form one of the enabling technologies for radio frequency (RF) applications, but for the bulk acoustic wave (BAW) devices, it is challenging to enable multiple resonance frequencies on a single Si wafer. In the past eight years, plate acoustic wave (PAW) resonators (i.e. Lamb wave resonators) based on aluminum nitride (AlN) thin films offer resonance frequencies at several gigahertz (GHz), multiple frequencies on one chip, and microfabrication flows compatible with the CMOS circuits. The Lamb wave resonators (LWRs) can be served as frequency references in the electronic systems for frequency synchronization and clock sources as well as employed as GHz-range bandpass filters selecting the appropriate frequency ranges for the mobile phone radio to receive and transmit its communication signals, blocking out the other unwanted signals.

1.1 MEMS Resonators for Timing and Frequency Control Applications

The state of the art architectures for the analog RF front-end in wireless communication systems are based on super-heterodyne and direct conversion approaches. In the super-heterodyne architecture, a receiver usually utilizes frequency mixing or heterodyning to convert a received signal to a fixed intermediate frequency (IF), which is conveniently processed than the original radio carrier frequency. Figure 1–1 shows a block diagram of the super-heterodyne transceiver architecture where the bulky RF SAW filters and quartz crystal resonators are the main components for signal processing. The components are usually passive resonant mechanical structures that currently are unable to be integrated with the CMOS chips. Another approach is direct conversion architecture which mixes the RF carrier frequency directly to the baseband. This zero IF conversion approach
usually offers size miniaturization and reduction of components since it eliminates the use of bulky IF SAW filters [1], [2]. Despite this truth, the direct conversion architecture still needs the use of the off-chip bulky RF filters and oscillators.

With the emerging progress of microelectromechanical systems (MEMS) technology, mechanical structures with ability to shrink their features and mechanisms down to micro- and nano-scales can be fabricated on Si wafers [3]. In order to reduce the chip size, power consumption, and integration complexity, MEMS resonators and filters can be used to replace the current off-chip components because of their tiny size, integration with CMOS chips, and high quality factor ($Q$). With further development of interface circuitry, MEMS devices are able to provide substantial size and power reduction for timekeepers and frequency control functions in communication systems. The vibrating micromechanical resonators based on the polysilicon and piezoelectric thin films have now been demonstrated with their $Q$’s greater than 3,000 at the GHz-range resonance frequencies [4]–[7]. The high-$Q$ micromechanical vibrating resonators have also been embedded into oscillator circuits to achieve excellent phase noise performance, satisfying global systems for mobile communications (GSM) specifications of frequency reference oscillators [8]–[13]. It appears the replacement of the crystal resonator with the MEMS vibrating resonator and the integration of the MEMS resonator with the CMOS circuits on a single die will lead to a significant reduction in board complexity and bill-of-materials of electronic circuits [14].

In addition, as presented in Fig. 1–2, a novel RF frond-end channel-select architecture is proposed by Nguyen to eliminate the use of the RF low noise amplifiers (LNAs) and transistor mixers, thereby lowering the power consumption and enhancing linearity [15].

Figure 1–1. An example of the super-heterodyne transceiver using off-chip bulky SAW filters and quartz crystal resonators.
In the circuit of Fig. 1–2, the feature of the RF channel-select is the filter bank which would be perhaps the key to the greater performance, since it alone allows substantial simplification of circuits further down the receiving path. In particular, an RF channel-select filter bank is capable of eliminating not only out-of-band interferers but also out-of-channel interferers [16]. The RF channel-select filter bank is implemented with a multitude of narrowband filters, each paired with a switch to implement the frequency selection. For a narrowband filter, the insertion loss heavily depends on the resonator $Q$ while a small percent bandwidth is needed [17], [18]. All the above information reveals that temperature-compensated, high-$Q$, and low-impedance micromechanical resonators are essential to construct high-performance oscillators and narrowband filters.

1.1.1 Frequency References

Almost all electronic systems need a frequency reference source for keeping track of real time or setting precise clock frequency for digital data transmission. The performance of the electronic systems usually depends on the accuracy and stability of the timing clock and frequency reference. Therefore, the frequency references constitute a multi-billion dollar market in electronic industries today. For common consumer-type applications, two technologies are distinguished: electrical and mechanical reference oscillators. In the electrical reference oscillators, the frequency elements are integrated on the chip and comprise a network of resistors (R) and capacitors (C) or an inductor-capacitor (L-C) filter for clocking, logic, or frequency synthesizer applications [14]. In the mechanical reference oscillators, the frequency elements are essentially mechanical vibrating devices,
which provide the stable natural resonance frequencies. Over the past few decades, the mechanical reference oscillator (e.g., quartz crystal oscillator) has dominated the market and been widely used in many electronic systems.

Quartz is basically crystallized silicon dioxide ($\text{SiO}_2$) and belongs to $32$ symmetry group of the trigonal system. It intrinsically exhibits an intrinsic high quality factor ($Q$), making quartz resonators and oscillators widely used as the reference signal source in circuitry [19]. As depicted in Fig. 1–3, one-port quartz crystal has two deposited electrodes on each side of the slab. When a thickness vibration mode is excited in the quartz slab, the resonance frequency ($f_0$) of the vibration mode is determined by the acoustic wave velocity and the slab thickness. For the fundamental mode, the resonance frequency can be estimated by the wave synchronism expression,

$$f_0 = \frac{v_a}{\lambda} = \frac{v_a}{2d},$$  \hspace{1cm} (1.1)

where $v_a$ is the acoustic wave velocity, $\lambda$ is the wavelength, and $d$ represents the thickness of the crystal slab. The resonance frequency of the quartz resonator is typically specified from tens of kilohertz (kHz) to a few tens of megahertz (MHz). As shown in Fig. 1–3, high-order harmonic vibration modes also co-exist with the fundamental vibration mode in the crystal slab. Due to the reverse polarity of the two electrodes, only odd harmonic vibration modes can be excited in the quartz plate.

Crystal resonators are the most commonly used mechanical resonator in signal processing, due to their excellent temperature stability, long-term frequency stability, and manufacturability. Quartz has different elastic, piezoelectric, and dielectric properties according to the different orientations of the crystal cuts. Therefore, by slicing the quartz at various cuts with respect to its crystal axes, it is possible to obtain a variety of crystal resonators with different temperature characteristics. For example, as shown in Fig. 1–4, AT- and BT-cut quartz resonators operating in TS mode exhibit different frequency-temperature behaviors. The AT-cut quartz resonator has excellent frequency stability over a wide temperature range since its first- and second-order temperature coefficients of frequency (TCF) are both zero at room temperature and the frequency-temperature characteristic is only determined by a third-order function of temperature [19].

A common crystal oscillator (XO) is an electronic oscillator circuit that uses the primary mechanical resonance of the quartz crystal to create an electrical signal with a very precise frequency. The precise frequency is usually used to keep track of time, to

![Cross-sectional illustration of a quartz resonator and some of its vibration mode shapes.](Figure 1-3)
provide a stable timing clock signal for the digital integrated circuits, and to stabilize frequencies for the transmitters and receivers.

As shown in Fig. 1–5 (a), a crystal oscillator consists of a quartz crystal and a positive feedback transistor, and an output buffer amplifier. The crystal oscillator circuit sustains oscillation by taking a voltage signal from the quartz resonator, amplifying it, and then feeding it back to the crystal resonator. Figure 1–5 (b) shows a voltage-controlled crystal oscillator (VCXO) whose resonance frequency can be changed by applying direct current (DC) voltages to the VCXO. By employing a varactor diode, the oscillator is allowed to shift the resonance frequency by adjusting the effective capacitance. When the control voltage offsets the resonance frequency of the XO, it doesn't improve the resonance frequency accuracy over the temperature or supply voltage variations. The VCXO has a resonance frequency as accurate as the quartz crystal resonator contains. The budget for frequency errors in the RF systems is significantly less than those in lower frequency applications, and the oscillation frequency variations of low-cost XOs exceed the system

Figure 1-4. Frequency-temperature characteristics of AT- and BT-cut quartz resonators.

Figure 1-5. Illustrations of (a) XO and (b) VCXO [19].
requirements due to the temperature dependency.

Although quartz crystal resonators show excellent temperature stability, there are still drawbacks and fabrication limitations related to scaling for high-frequency applications. The material property of quartz crystal also limits the integration of frequency references and CMOS circuits on a single chip. By contrast, micromechanical vibrating resonators exhibit the extraordinary small size, high level of integration with CMOS chips, and low cost, opening exceptional possibilities for enabling miniature and precision oscillators at low cost. Moreover, it is expected that the MEMS-based oscillator has a superior phase noise performance and frequency stability compared to the electrical oscillator because the MEMS-based oscillator is based on the mechanically vibrating structure which usually exhibits a higher $Q$. That is to say, the MEMS vibrating resonators fill the gap between high-performance non-CMOS compatible technologies and low-performance CMOS compatible technologies.

1.1.2 Bandpass Filters

In wireless communication systems, the RF and IF bandpass filters are used to select the appropriate frequency ranges for the mobile phone radio to receive and transmit the communication signals and block out the other unwanted signals. Filtering the radio signals requires physical structures which are comparable to the wavelength of the carrier electromagnetic wave. However, the wavelength of an electromagnetic wave at 2 GHz in air is 15 centimeter which is too large for a mobile phone. Since the acoustic waves in solids typically show phase velocities of 3,000–12,000 m/s, the transformation of the electromagnetic waves to the acoustic waves can realize miniaturization of GHz range filters and the wavelength is reduced to micrometer range by the same fraction, allowing for realization of GHz range electroacoustic filters in the micrometer scale.

Figure 1–6 shows a common electrically coupled filter, a ladder filter configuration, employing resonators in both series and shunt branches [1], [2], [20]. All the resonators in the series branch have the same series and parallel resonance frequencies ($f_s$ and $f_p$). Similarly, the resonators in the shunt branch have the identical series resonance frequency differing from the series resonance frequency of the resonators in the series branch by $\Delta f$. A typical frequency response of the ladder filter is shown in Fig. 1–7. Of special interest

![Figure 1-6. Simple ladder filter with micromechanical resonators in the series and shunt branches [20].](image-url)
are the in-band insertion loss, 3dB bandwidth (BW), out-of-band rejection, and 20dB shape factor which is the ratio of the 20dB BW to 3dB BW. The center frequency of the ladder filter is usually equal to the \( f_s \) of the resonators in the series branch. The series branch has the lowest impedance while the resonators in the series branch are at resonance. In order to have unimpeded current flow in the series path, the resonators in the shunt branch are shifted by a specific frequency, \( \Delta f \), such that the \( f_p \) of the shunt resonators is equal to the \( f_s \) of the series resonators and the 3dB BW is usually set by the effective coupling coefficient (\( k^2_{\text{eff}} \)) of the series and shunt resonators. As a result, the circuit network has minimum current flow into ground via the shunt resonator elements. To minimize the insertion loss of the ladder filter, the shunt resonators should have high impedance at their parallel resonance frequency \( f_p \) and the series resonators have low impedance and high \( Q \) at their series resonance frequency \( f_s \).

The out-of-band rejection of the ladder filter is controlled by the capacitive voltage divider of the ladder circuit. More ladder resonator stages or higher static capacitance of the shunt resonators increase the out-of-band rejection but also increase the in-band insertion loss [1], [20]. More ladder stages of the filters and higher \( Q \)'s of the resonators sharpen the passband roll-off and improve the 20dB shape factor. However, the total number of the resonators employed in the series and shunt branches affects the insertion loss and overall size of the filter so high-\( Q \) resonators are desired to be used in the ladder filter. Fortunately the MEMS resonators simultaneously offer high \( Q \), small footprint, and CMOS compatible capability. It is expected that the bandpass filter based on the MEMS resonators has superior performance. In addition, for the filter bank in the channel-selection transceiver, the conventional off-ship and bulky filters are not suitable for cost and area effective implementation. The MEMS-based micromechanical filters would be one of the most promising technologies for the filter bank architecture.
1.2 Electrostatic Vibrating Resonators

The capacitively transduced resonators using various micromechanical structures, such as cantilevers or clamped-clamped beams, are driven by parallel-plate electrostatic forces [3], [21]. The capacitive transduction usually utilizes an electrostatic force across a sub-micron gap (usually smaller than 1 \( \mu \)m) to drive the micromechanical structure and then to sense the motional current. The \( Q \)'s of the electrostatic resonant structures are very low at atmospheric pressures because of the squeeze-film air damping in a sub-micron air gap, but the \( Q \)'s can be raised by orders of magnitude in vacuum [3]. In addition, the resonance frequency of the electrostatic vibrating resonator is determined by the lateral dimensions and able to achieve multiple frequencies on a single chip. However the large motional resistance (\( R_m \)) of the electrostatic resonant devices makes the interface with the 50-ohm RF system very difficult.

1.2.1 Electrostatic Comb-Drive Resonator

The first electrostatic vibrating comb-drive resonator was reported by Tang et al. in 1989 [22]. As shown in Fig. 1–8, the comb-drive resonator usually consists of a finger-supporting shuttle mass suspended several micron height above the substrate by folded flexures, which are anchored to a ground plane on the substrate. The ground plane should be in electrical contact with the suspended structure to prevent pulling in the structure. The electrostatic comb-driven and sensed lateral resonators offer numerous advantages over parallel-plate driven resonators. The most significant advantage is that the drive capacitance is linear with its displacement, resulting in a driving force independent on the vibration amplitude [22]. The resonance frequency of the comb-drive vibrating resonator is determined by material properties and lateral geometries [22], [23]. However, the resonance frequency of the vibrating comb-drive resonator is usually below 1 MHz due to the low spring constant of the long folded beam structure.

![Figure 1-8. Scanning electron micrograph (SEM) image of a capacitively transduced comb-drive resonator [22].](image-url)
1.2.2 Electrostatic Disk Resonator

Similar to the CMOS transistors, extending the resonance frequency of micromechanical resonators generally requires scaling of micromechanical structures. However, smaller dimension often coincides with smaller power handling and lower $Q$. In 2000, as shown in Fig. 1–9, Clark et al. proposed a new micromechanically vibrating disk resonator [24]. Based on the radial contour mode, the micromechanical disk structure can attain very high frequencies while retaining relatively large dimensions because the high stiffness of the disk structure. Particularly, the resonance motion of the contour mode is purely radial so the disk center is a motionless nodal point during vibration. The fundamental contour mode of the micromechanical resonator can offer a $Q$ as high as 23,000 at 193 MHz since energy losses to the substrate are minimized by anchoring the resonator at its center to reduce the mechanical motion [24], [25]. However, like the comb-drove resonator, the electrostatic disk resonator has a large motional resistance up to several thousand ohms, causing the impedance mismatch problem with the 50-ohm RF system.

1.3 Piezoelectric MEMS Resonators

Piezoelectricity was discovered by the brothers Curie in 1880 and received its name in 1881 from Hankel. In 1915, Langevin utilized a bulk acoustic wave transducer (steel-quartz-steel) in pulse echo experiments at a high frequency of 150 kHz for submarine detection in water. Cady followed up Langevin’s work and developed quartz crystal resonators for stabilizing the electronic oscillators in 1921 [26]. In fact, acoustic wave devices based on piezoelectric materials have been used in commercial applications for over 70 years [27].

Figure 1-9. SEM image of an electrostatic disk micromechanical resonator [24].
Generally speaking acoustic waves refer to surface acoustic waves, bulk acoustic waves, and plate acoustic waves, but are not limited to this category. Metal electrodes are used as transducers on the piezoelectric materials to convert electrical energy into mechanical displacement and vice versa, while employing different types of acoustic waves in solids. As their names suggest, SAW resonators take advantage of surface acoustic waves propagating on the top surface of the piezoelectric substrate, while BAW resonators employ bulk acoustic waves propagating in the thickness direction of the thin plate and LWRs employ Lamb waves propagating in the lateral direction of the thin plate. The most common piezoelectric substrate materials are quartz, lithium tantalate (LiTaO$_3$), and lithium niobate (LiNbO$_3$). Other piezoelectric materials with commercial potential include AlN, zinc oxide (ZnO), gallium arsenide (GaAs), silicon carbide (SiC), langasite (LGS), lead zirconium titanate (PZT), and polyvinylidene fluoride (PVDF). Each piezoelectric material has its specific advantages and disadvantages, such as temperature dependence, attenuation, electromechanical coupling, phase velocity, and cost [27].

1.3.1 Surface Acoustic Wave (SAW) Resonator

Extensive research work in the ultrasonic field continues in the 19th and 20th centuries after Rayleigh discovered surface acoustic waves propagating in solids in 1885 [28]. Although it remained a scientific curiosity with very few applications for a long time, the direct generation and detection of surface elastic waves through the piezoelectric effect led to a breakthrough in SAW devices after the invention of an interdigital transducer (IDT) by White and Voltmer in 1965 [29]. The interdigital finger width is usually equal to quarter wavelength ($\lambda$/4) and the interdigital electrode pitch ($\Lambda$) equals half wavelength ($\lambda$/2). SAW resonators and filters have been used for many electronic applications since then. One of the earliest SAW device applications was an intermediate frequency (IF) bandpass filter for television receivers, first developed in the 1970s [30].

SAW devices have been widely used as IF and RF filters in wireless transmission systems for several decades because of their small size, low cost, and great performance. They also have drawn much attention for dozens of sensing applications because most of acoustic energy of surface elastic waves is confined within one wavelength depth under the substrate surface, leading to high sensitivity. Figure 1–10 shows the configuration of a typical one-port SAW resonator consisting of one IDT and two grating reflectors at both sides on the piezoelectric substrate. SAWs can be generated by applying RF signals to the IDT and propagate on the surface of the substrate along the direction perpendicular to the transducer length. The generated SAWs would be reflected by the gratings at both sides, and consequently forms standing waves between the two sets of grating reflectors. The single IDT in the center is also used for receiving the reflected SAWs.

However, SAW phase velocities of common piezoelectric substrates, such as quartz, LiNbO$_3$, and LiTaO$_3$, are below 4,000 m/s so the center frequencies of SAW devices are usually limited to 3 GHz since strict shrinkage of the IDT finger widths is required for achieving higher resonance frequencies. In order to enable high-frequency SAW devices, a piezoelectric substrate with a high phase velocity is an alternative. It is well-known that diamond has the highest acoustic wave velocity among all materials because of its high Young’s modulus up to 1,143 GPa [31]; therefore, SAW devices fabricated on layered
structures including a piezoelectric thin film and a polycrystalline diamond layer on a Si substrate have been utilized for high-frequency applications [32]–[35].

1.3.2 Bulk Acoustic Wave (BAW) Resonator

For any material, there are three possible BAW propagation modes: longitudinal wave, shear horizontal (SH) wave, and shear vertical (SV) wave, where SH mode is polarized in the horizontal plane and SH mode is polarized in the vertical plane. In general, each mode has its different phase velocity and piezoelectric coupling coefficient due to the different polarization. Among the three BAW modes, the longitudinal acoustic wave has the highest phase velocity and it is sometimes called P-wave to stand for primary wave. BAW resonators employ the acoustic waves propagating through the bulk of a material. Generally the transduction of BAW requires the application of an alternating current (AC) electric field, applied to or in close proximity to, the surface of the piezoelectric plate using metal electrodes [36] and then acoustic waves propagate in longitudinal or shear modes. For quartz crystal resonators, thickness shear (TS) mode in the AT-cut quartz is the most common mode because it has the best temperature stability and efficient energy trapping underneath the coated electrodes on the crystal plate [37]. The resonance frequency of the AT-cut crystal resonator is determined by the plate thickness and the phase velocity of shear wave, rather than by the lateral dimensions of the thin plate.
However, due to difficult manufacture of the quartz crystal plate thinner than 20 µm by grinding, manufacturers have difficulty in producing crystals to reach a fundamental frequency over 80 MHz [19]. To produce a higher frequency for the oscillator, the quartz crystal resonator is often designed to operate at third, fifth, or seventh overtones because a thicker crystal plate is easier to manufacture than a crystal resonator utilizing the fundamental mode at the same resonance frequency. To achieve a GHz-range resonance frequency, a piezoelectric thin plate with a thickness less than 5 µm is needed. Therefore, instead of grinding the plate thickness of the quartz crystal, piezoelectric thin films grown on Si substrates by using reactive sputtering or metal organic chemical vapor deposition (MOCVD) have been successfully utilized to enable BAW resonators operating in ultra high frequency (UHF) and super high frequency (SHF) regions.

**Film Bulk Acoustic Resonator (FBAR)**

An FBAR or BAW resonator is normally operated in thickness extension (TE) mode, whose resonance frequency is determined by the thickness of the piezoelectric thin film and the phase velocity of the longitudinal wave rather than by the lateral dimensions of the piezoelectric plate. The FBAR using an external electrical field parallel to the normal of the piezoelectric plate is called thickness-field-excited (TFE) resonator as shown in Figs. 1–11 (a), (b), and (c) [36]. Figure 1–11 (a) presents the cross-sectional illustration of the FBAR which is sandwiched between top and bottom electrodes. The outer metal surfaces are against air so that the longitudinal wave reflects off the surfaces and the standing wave resonance is confined in the piezoelectric material body. As shown in Fig. 1–11 (b), the top and bottom metal electrodes are very close to the piezoelectric thin plate but not in contact with it. Small air gaps between the piezoelectric plate and metal electrodes ensure the voltage is applied to the piezoelectric body and the $Q$ is enhanced.

![Figure 1-11. Cross-sectional illustrations of various BAW resonators [36].](image)
since thin metal electrodes usually have too much electrical loss. However, the additional capacitances caused by the two air gaps also reduce the effective coupling $k_{\text{eff}}^2$.

Figure 1–11 (c) depicts an FBAR structure on another substrate whose thickness is often a number of wavelengths. Resonances occur at the frequencies where the total resonator thickness corresponds to the integral multiples of the half acoustic wavelength. This topology is usually called over-moded resonator (OMR) or high-overtone bulk acoustic resonator (HBAR). With a large number of half waves in the substrate layer, most of the acoustic energy is stored in the substrate so a high $Q$ over 70,000 has been demonstrated when an appropriate material, such as sapphire, is used as the substrate [38]. The lateral-field-excited (LFE) resonator, as shown in Fig. 1–11 (d), has both electrodes on the same plate face, leaving the opposing surface bare. An LFE BAW resonator is excited with the fringing electrical fields across the gap between the electrodes and operated in TS mode, whose resonance frequency is determined by the thickness of the piezoelectric plate and the shear wave velocity.

**Solidly Mounted Resonator (SMR)**

The solidly mounted resonator (SMR) in Fig. 1–12 is considerably different form than the BAW resonators described above. The piezoelectric layer is sandwiched between top and bottom electrodes but solidly mounted to the substrate so excellent acoustic isolation of the piezoelectric layer from the substrate is required if a high-$Q$ resonance is desired. In 1965, Newell described a reflector array which is nominally composed of quarter-wavelength-thick layers to provide acoustic isolation [39]. The reflector array is called a Bragg reflector which consists of many pairs of high and low acoustic impedance layers and is utilized to reflect acoustic waves back to the piezoelectric layer. If the substrate has relatively high acoustic impedance, the first layer on the top surface of the substrate
should have low acoustic impedance, the next layer, high acoustic impedance, and so on. Since AlN and most piezoelectric materials have moderately high acoustic impedance, the first layer under the piezoelectric thin film is of low acoustic impedance and SiO$_2$ is commonly used. As tungsten (W) has relatively high acoustic impedance, each following layer boundary has a higher reflection coefficient and then fewer layers are required. Thus a suitable sequence might be “SiO$_2$ and AlN” or “SiO$_2$ and W” on Si or sapphire substrates. The Bragg reflector diminishes the acoustic wave amplitude with the depth into itself [36], [38]. The number of the Bragg reflector layers required for a satisfactory reflection coefficient most depends on the acoustic impedances between layers. Since the SMR is constructed on the non-free-standing physical structure, it can provide better mechanical robustness and good power handling capacity.

1.3.3 Lateral Extension Mode Resonator

Except for the TS and TE modes, lateral extension mode in a thin plate is also utilized in the piezoelectric resonators [40]. Before 1937, many work focused on the development of the TS mode crystal resonators. In 1937, Hight and Willard described CT- and DT-cut crystal resonators operating in face shear mode that showed a zero TCF [41]. Later, in 1940, Mason proposed a new GT-cut crystal resonator operating in lateral extension mode which exhibits the best frequency-temperature behavior among all well-known crystal resonators [42]. Since then a great deal of research work has been devoted to contour-mode crystal resonators, including the shear mode and lateral extension mode [43]. Moreover, the vibration motion of the contour mode mostly occurs in plane so the resonance frequency of the contour-mode resonator (CMR) is determined by the lateral dimensions (e.g. length or diameter). As shown in Fig. 1–13, the resonance frequency of the lateral extension mode resonator is determined by its width or length rather than thickness. As a result, the CMRs are devoid of the main drawback of the FABRs and SMRs, namely incapacity of achieving multiple frequencies on a single chip.

In order to enable a high resonance frequency, Piazza and Pisano developed the AlN CMR since 2002 [1], [44]. Similar to the FBAR, as illustrated in Fig. 1–13, the resonant body of the CMR is made of a piezoelectric AlN thin plate sandwiched between top and bottom electrodes, and two quarter-wavelength long tethers are normally used to suspend the resonator in air [45]. Figure 1–14 shows the scanning electron micrograph (SEM) images of the rectangular and circular ring CMRs. The rectangular plate resonator can be

![Figure 1-13. Cross-sectional illustrations of (a) one-port and (b) two-port piezoelectric resonators operating with the lateral extension mode.](image-url)
excited in the length-extensional or width-extensional mode whereas the circular ring resonator is excited in the radial contour mode. As shown in Fig. 1–14 (b), notches were introduced in the circular ring structure to minimize the interference of the anchor on the vibration mode shape. Typically the AlN CMRs show their $Q$ of several thousands and low motional impedance at the very high frequency (VHF) range (30–300 MHz) [44], [45]. Unfortunately, with an increasing interest in the high resonance frequencies, scaling of the AlN CMRs causes a considerable increase on motional impedance which is usually in reciprocal proportion to the effective transduction area.

1.3.4 Lamb Wave Resonator (LWR)

In 1973, Toda first realized a Lamb wave device on a PZT ceramic plate [46]. Since then Lamb wave devices utilizing the lowest-order antisymmetric ($A_0$) mode propagation in ZnO thin plate were widely studied for sensing applications [47] as the $A_0$ mode has a phase velocity slower than the compressional wave velocity in most liquids. In this situation, the $A_0$ Lamb wave cannot radiate its energy into the surrounding liquid with the higher velocity [48]. Recently, Lamb wave modes propagating in the AlN thin plate have attracted great attention for the designs of electroacoustic resonators since it combines the advantages of BAW and SAW: high phase velocity and multiple-frequency excitation by an IDT. More specifically, the lowest-order symmetric ($S_0$) Lamb wave mode in an AlN thin plate is particularly preferred because it exhibits its phase velocity close to 10,000 m/s, a low dispersive phase velocity characteristic, and a moderate electromechanical coupling coefficient [49]–[58]. In addition, the AlN LWRs are able to simultaneously solve the high motional impedance issue faced by electrostatic resonators, the low resonance frequency limitation faced by piezoelectric contour-mode resonators, and the multiple frequency capability problem faced by piezoelectric BAW resonators.

In the past eight years, the AlN LWRs are being developed in two different topologies with respect to the Lamb wave reflection. As presented in Fig. 1–15 (a), like SAW resonators, the first topology is based on the reflection from periodic grating reflectors with an electrode width of quarter wavelength [49]–[52]. The second topology is based on the reflection from suspended free edges of the thin plate as depicted in Fig. 1–15 (b) [53]–[59]. Lamb wave modes can be generated by applying RF signals to the transducer.
and then propagate in the AlN thin plate. The generated Lamb waves are reflected by the periodic metal gratings or the suspended free edges at both sides of the piezoelectric thin plate, and consequently the standing waves form inside the thin plate. In general, Lamb wave conversion into the other modes does not occur while it propagates along a long periodic grating whereas Lamb waves would exhibit mode conversion upon reflection at the suspended free edges [60]. Mode conversion loss significantly depends on the wavelength, plate thickness, and Lamb wave mode. Fortunately, the lowest-order Lamb wave modes don’t exhibit mode conversion upon reflection at the suspended free edges and can be fully reflected [61].

1.4 Temperature Compensation Techniques

Quartz crystal resonators exhibit outstanding advantages, such as high $Q$ and excellent temperature stability; unfortunately the quartz crystals are often too large in size and hard to integrate with the CMOS circuitry, forming a bottleneck for the miniaturization of electronic systems. Although MEMS resonators show advantages of size and integration over quartz crystal resonators, further improvement in the frequency-temperature stability is strongly demanded, especially for the narrowband filters and reference oscillators.

1.4.1 Passive Temperature Compensation

Most materials, such as Si, AlN, or ZnO, become mechanically soft with an increasing temperature due to their negative temperature coefficients of elasticity (TCE); as a result, Si micromechanical resonators exhibit a first-order TCF of approximately $-31 \text{ ppm/}^\circ\text{C}$ [62]; AlN MEMS resonators, $-25 \text{ ppm/}^\circ\text{C}$ [58], [59]; ZnO MEMS resonators, $-60$
17 ppm/°C [36]. This level of temperature stability is unsuitable for any frequency reference application. It is well-known that quartz is the crystalline form of SiO$_2$ and becomes mechanically stiff with an increasing temperature because of the positive temperature dependence of stiffness constants (i.e. $C_{14}$ and $C_{66}$) and shows the existence of some temperature-insensitive cuts in quartz crystals [63]. An amorphous SiO$_2$ layer also shows positive TCEs [64] and a passive thermal compensation technique using a compensating layer of SiO$_2$ has been widely applied to various Si-based electrostatic MEMS resonators [62] and piezoelectric resonators [61], [65]–[69].

Figure 1-16 illustrates the passive temperature compensation technique for the SAW and BAW resonators. By adding a compensating thin film with an appropriate thickness, the first-order TCF can be reduced to zero at room temperature. Since the second-order TCEs of SiO$_2$ are not of positive temperature dependence [64], the second-order TCF would be still temperature dependent after passive temperature compensation. Except for SiO$_2$, tellurium dioxide (TeO$_2$) [70] and highly-doped Si [71], [72] layers were also used as the compensating material. Recently, fluorine-doped silicon oxide (SiOF) was found to have better temperature compensation efficiency than undoped SiO$_2$ films [73].

### 1.4.2 Active Temperature Compensation

Although AT-cut quartz resonators and temperature-compensated MEMS resonators are able to offer temperature stability lower than 100 ppm from –40°C to 85°C, which is still unsuitable for the reference oscillator application, the resonators must rely on additional temperature compensation techniques to achieve better frequency stability. One approach is to apply an electrostatic force to the resonator via a DC potential, causing a spring softening effect to adjust the resonance frequency [74], [75]. Another approach is to employ a temperature sensor to detect the temperature changes and a compensation circuitry to minimize the temperature-induced frequency drifts, typically in a range from fractions to hundreds of ppm.

Figure 1–17 (a) shows a temperature-compensated crystal oscillator (TCXO) as well as a temperature-compensated VCXO (TCVCXO), which employs a temperature sensor to sense the temperature variation and a temperature compensation circuitry to minimize oscillation frequency drifts caused by the temperature variations. As shown in Fig. 1–18, the TCXO is allowed for shifting the resonance frequency by adjusting the effective
capacitance via applying a correction voltage to the varactor diode and offer excellent temperature stability with low power consumption and short stabilization time.

In order to achieve a higher degree of frequency-temperature stability, for example, a complicated circuitry is implemented in a microcomputer compensated crystal oscillator (MCXO) or a thermostatically controlled oven is implemented in an oven-controlled crystal oscillator (OCXO), typically used for the highest precision frequency applications. Figure 1–17 (b) depicts an OCXO as well as an oven-controlled VCXO (OCVCXO),

![Figure 1-17. Illustrations of (a) TCXO / TCVCXO and (b) OCXO / OCVCXO [19].](image)

Figure 1-18. Principle of active temperature compensation of TCXOs.

![Figure 1-18. Principle of active temperature compensation of TCXOs.](image)
which employs a temperature sensor to sense the temperature variations and then uses a temperature-controlled oven. The temperature-controlled chamber is used to maintain the micromechanical resonator of the oscillator at a constant temperature for preventing changes in the oscillation frequency due to variations in ambient temperature. The OCXO usually achieves the highest frequency stability among the XO family. Since the crystal resonator and associated circuitry are heated to the upper turning point of crystal and a narrow temperature window needs to be maintained, better frequency-temperature stability always accompanies larger power consumption and longer stabilization time. The frequency-temperature stability of the reference oscillators is usually characterized over the temperature range from 0°C to 70°C, (commercial grade), –40°C to 85°C (industrial grade), or –55°C to 125°C (military grade). Table 1–1 summarizes the performance of the XO, TCXO, MCXO, and OCXO. Of course, the active temperature compensation approaches can be used in micromechanical resonators as well.

### 1.5 Dissertation Outline

This dissertation is dedicated to the design issues of the temperature-compensated and high-\( q \) AlN Lamb wave resonators and laid out into seven chapters. Chapter 1 presents the background, research motivation, modern micromechanical resonator technologies, and common temperature compensation approaches.

Chapter 2 gives a comprehensive theoretical analysis of acoustic wave characteristics of Lamb wave modes propagating in the piezoelectric AlN membranes and composite plates. The \( S_0 \) Lamb wave mode in the AlN/SiO\(_2\) composite plate is particularly studied since the SiO\(_2\) layer can be potentially utilized to compensate the temperature-induced frequency drifts. The Lamb wave modes in a multilayer plate composed of AlN thin film and cubic silicon carbide (3C–SiC) layer is also discussed since SiC crystals have been theoretically proven to have an exceptionally large \( f_s q \) product given their intrinsic low acoustic loss.

Chapter 3 describes the baseline microfabrication processes of the LWRs based on the AlN thin film and various composite plates. The characterization of the AlN thin film growth and the effect of the bottom electrode metallization on the AlN thin film quality are also experimentally studied herein.
Chapter 4 presents the experimental studies of the conventional AlN LWRs using the $S_0$ mode. A novel design of convex free edges is introduced to boost the $Q$ of the AlN LWR since the convex shape can efficiently confine the mechanical energy in the resonator and eliminate the energy loss through the support tethers. A 491.8-MHz LWR on a 1.5-$\mu$m-thick AlN thin plate utilizing the convex free edges yields a high $Q$ up to 3,280, presenting a 2.6× enhancement in $Q$ over a 517.9-MHz LWR utilizing suspended flat edges. Moreover, one-port AlN LWRs with the electrically open, grounded, and floating bottom surface conditions are theoretically and experimentally investigated. The use of the floating bottom electrode results in the lower static capacitance and enhances the effective coupling coefficient $k^2_{\text{eff}}$ of the AlN LWRs.

Chapter 5 details the frequency-temperature behaviors of the AlN/SiO$_2$ composite plate. Fine selection of the SiO$_2$ layer thickness for complete temperature compensation of the AlN LWRs at room temperature will be studied in details. A well temperature-compensated AlN/SiO$_2$ LWR exhibits a zero first-order TCF and a second-order TCF of $-21.5$ ppb/°C$^2$ at the turnover temperature, 18.05°C. In addition, a novel temperature compensation approach for the AlN LWR operating at high temperature is also presented herein. Based on the different thickness ratios of the AlN thin film to the SiO$_2$ layer, complete thermal compensation of the AlN/SiO$_2$ LWRs was experimentally demonstrated at 214°C, 430°C, and 542°C, respectively.

In Chapter 6, the AlN/3C–SiC composite plate is used to enable a high-frequency, high-$Q$, and low-impedance electroacoustic resonator utilizing the high-order Lamb wave modes. The experimental results show that the epitaxial 3C–SiC layer not only enhances the electromechanical coupling coefficient of the third quasi-symmetric (QS$_3$) Lamb wave mode but also boosts the $Q$. A one-port AlN/3C–SiC LWR utilizing the QS$_3$ mode exhibits a low motional impedance of 91 $\Omega$ and a high $Q$ of 5,510 at 2.92 GHz, showing the highest $f_cQ$ product (1.61×10$^{13}$ Hz) among the suspended piezoelectric thin film electroacoustic resonators reported to date. In addition, two-port Lamb wave resonators and filters based on the AlN/3C–SiC composite plate are also experimentally investigated in this chapter.

Finally Chapter 7 concludes the entire research works presented in this dissertation. Several potential research directions are presented as well.
Chapter 2

Propagation Characteristics of Lamb Waves in Piezoelectric Membranes and Composite Plates

Piezoelectric thin films, such as AlN, GaN, and ZnO, have been utilized in SAW filters as well as BAW resonators and filters for communication applications. There are two main factors for broad use of piezoelectric thin films: efficient electromechanical transduction and growth of high-quality piezoelectric thin films on a variety of substrates, such as Si, quartz, SiC, GaAs, and sapphire. With growing interests in high-frequency and high-$Q$ resonators for millimeter-wave circuit applications, the Lamb wave mode propagation in a piezoelectric thin plate has drawn great attention due to its high phase velocity. In this chapter, comprehensive theoretical studies of the lowest-order Lamb wave modes (i.e. $A_0$ and $S_0$ modes) in piezoelectric membrane and composite plates are presented. The phase velocities, electromechanical coupling coefficients, and dispersion characteristics of the Lamb wave modes will be discussed according to the theoretical results. The propagation properties of the Lamb waves in the piezoelectric media will be investigated and then employed in the designs of the AlN LWRs, temperature-compensated AlN/SiO$_2$ LWRs, and high-$Q$ AlN/3C–SiC LWRs in the following chapters.

2.1 Why AlN Thin Film

Although PZT shows strong piezoelectric coupling coefficients and has been used in MEMS devices for many years, its large acoustic losses and high dielectric constants limit its use in high-frequency applications [36]. III-V compounds such as AlN and GaN or II-VI compounds like ZnO are the most common piezoelectric thin films for high-frequency acoustic transducer applications. As illustrated in Fig. 2–1, AlN, GaN, and ZnO are all wurtzite-structured materials with $a$- and $c$-axes, belonging to hexagonal crystal system, with polarized direction along the $c$-axis (0001) which is usually normal to the substrate. The piezoelectric thin films can be synthesized and grown on substrates by using reactive sputtering, MOCVD, or molecular beam epitaxy (MBE). Since the
deposition temperatures of MOCVD and MBE are usually higher than 800°C, causing some issues with post-deposition processes, reactive sputtering is greatly preferred due to the low thermal budget with temperatures below 400°C.

Among common sputtered piezoelectric thin films, AlN is always considered a highly desirable thin film material for electroacoustic devices since it has high acoustic velocity, good thermal conductivity, large Young’s modulus, moderate piezoelectric coupling

![Hexagonal wurtzite crystal structure of AlN.](image)

Table 2-1. Physical properties of ZnO, AlN, and GaN [36], [76]–[80].

<table>
<thead>
<tr>
<th>Property</th>
<th>ZnO</th>
<th>AlN</th>
<th>GaN</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>5.680</td>
<td>3.260</td>
<td>6.150</td>
<td>(kg/m³)</td>
</tr>
<tr>
<td>Longitudinal acoustic wave velocity</td>
<td>~6,350</td>
<td>~11,300</td>
<td>~8,050</td>
<td>(m/s)</td>
</tr>
<tr>
<td>Shear acoustic wave velocity</td>
<td>~2,720</td>
<td>~6,000</td>
<td>~4,130</td>
<td>(m/s)</td>
</tr>
<tr>
<td>Lattice constant, $a$</td>
<td>3.249</td>
<td>3.112</td>
<td>3.189</td>
<td>(Å)</td>
</tr>
<tr>
<td>Lattice constant, $c$</td>
<td>5.207</td>
<td>4.982</td>
<td>5.186</td>
<td>(Å)</td>
</tr>
<tr>
<td>Thermal expansion (300 K), $\alpha_a$</td>
<td>4.75</td>
<td>5.27</td>
<td>5.59</td>
<td>($10^{-6}$/°C)</td>
</tr>
<tr>
<td>Thermal expansion (300 K), $\alpha_c$</td>
<td>2.92</td>
<td>4.15</td>
<td>3.17</td>
<td>($10^{-6}$/°C)</td>
</tr>
<tr>
<td>Piezoelectric coefficient, $e_{15}$</td>
<td>−0.48</td>
<td>−0.48</td>
<td>−0.33</td>
<td>(C/m²)</td>
</tr>
<tr>
<td>Piezoelectric coefficient, $e_{31}$</td>
<td>−0.57</td>
<td>−0.58</td>
<td>−0.33</td>
<td>(C/m²)</td>
</tr>
<tr>
<td>Piezoelectric coefficient, $e_{33}$</td>
<td>1.32</td>
<td>1.55</td>
<td>0.65</td>
<td>(C/m²)</td>
</tr>
<tr>
<td>Electromechanical coupling coefficient, $k^2$</td>
<td>−8.5</td>
<td>−6.5</td>
<td>−1.2</td>
<td>(%)</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>60</td>
<td>280</td>
<td>130</td>
<td>(W/mK)</td>
</tr>
<tr>
<td>TCF</td>
<td>−60</td>
<td>−25</td>
<td>–</td>
<td>(ppm/°C)</td>
</tr>
</tbody>
</table>
coefficient, low acoustic loss, and relatively small TCF [76]–[80]. Table 2–1 compares physical properties of ZnO, AlN, and GaN. Despite ZnO exhibits a slightly stronger electromechanical coupling coefficient ($k^2$) than AlN, its lower acoustic velocity, higher acoustic loss and larger TCF limits its applications on high-frequency electroacoustic devices. By contrast, GaN exhibits a smaller $k^2$ than AlN and ZnO. Therefore, the AlN thin film is selected for demonstrating the temperature-compensated and high-$Q$ LWR technologies herein. In the following sections, the acoustic propagation characteristics of the two fundamental Lamb wave modes in a piezoelectric AlN thin film, an AlN/SiO$_2$ composite plate, and an AlN/3C–SiC multi-layer will be theoretically studied.

2.2 Theoretical Analysis of Lamb Wave Modes Propagating in an AlN Membrane

The effective permittivity based on a transfer matrix is used to calculate the phase velocities of Lamb wave modes propagating in a piezoelectric thin plate [81], [82]. The electromechanical coupling coefficient $k^2$ of Lamb waves excited by an IDT can be analyzed using an approximation method, which is based on the velocity difference under the free-surface and metalized-surface electrical boundary conditions [81]. The other approach for exact analysis of the $k^2$ of Lamb waves is the Green’s function method [83]–[86]. In this subsection, the phase velocity and $k^2$ of the two fundamental Lamb wave modes propagating in a piezoelectric plate (i.e. AlN plate) will be theoretically analyzed. The $k^2$ of the two fundamental Lamb wave modes in a piezoelectric plate calculated using the two above methods will be compared as well.

2.2.1 Transfer Matrix

Figure 2–2 shows the geometry of the wave problem to be analyzed. Lamb wave modes propagate along the $x$-direction of a piezoelectric thin plate bounded by the planes $z = 0$ and $h$, respectively. The governing field equations of piezoelectricity can be expressed as

$$\sigma_{ij} = \rho \ddot{u}_i, \quad (2.1)$$

$$D_{i,j} = 0, \quad (2.2)$$

where $\sigma_{ij}$ and $u_i$ denote the Cauchy stress tensor and the mechanical displacement, respectively. $\rho$ is the mass density and $D_i$ is the electric displacement, respectively. The piezoelectric constitutive relations with the mechanical displacement $u_i$ and electric potential $\phi$ as variables are of the form

$$\sigma_{ij} = c_{ijkl} u_{k,l} + e_{ijl} \phi_l, \quad (2.3)$$
\[ D_i = e_{ijl}u_{k,l} - e_{ij}\phi_j, \]  

(2.4)

where \( c_{ijkl} \) is the elastic stiffness at the constant electric field of the piezoelectric medium, \( e_{ijl} \) is the piezoelectric constants, and \( \varepsilon_{il} \) is the dielectric constants at the constant strain of the piezoelectric medium.

For a plane harmonic wave propagating in the \( x \)-direction, the displacement vector \( \mathbf{u} \), the \( z \)-component of the electric displacement vector \( D_z \), the traction vector \( \mathbf{t} \), and the electric potential \( \phi \) are given by

\[
\mathbf{u}(x, y, z) = \mathbf{u}(z)\exp[i(\omega t - k_x x)],
\]

(2.5)

\[
D_z(x, y, z) = D_z(z)\exp[i(\omega t - k_x x)],
\]

(2.6)

\[
\mathbf{t}(x, y, z) = \mathbf{t}(z)\exp[i(\omega t - k_x x)],
\]

(2.7)

\[
\phi(x, y, z) = \phi(z)\exp[i(\omega t - k_x x)],
\]

(2.8)

where \( \omega \) is the angular frequency and \( k_x \) is the wave vector of the plane harmonic waves in the \( x \)-direction. According to the state vector formulation of the acoustic elastic waves in anisotropic solids, the governing equations (2.1)–(2.4) can be rearranged in a matrix form as [82], [84]

\[
\frac{d}{dz} \xi(z) = -iN(z)\cdot \overline{\xi}(z),
\]

(2.9)

\[
\overline{\xi}(z) = \begin{bmatrix} \mathbf{u}(z) \\ \phi(z) \\ \mathbf{t}(z) \\ iD_z(z) \end{bmatrix},
\]

(2.10)

---

Figure 2-2. Coordinate system used in the theoretical analysis of a single piezoelectric layer.
where $\vec{\xi}(z)$ is the state vector and $N(z)$ is the fundamental acoustic tensor [87]. When the propagation medium is considered homogeneous, the tensor $N$ is independent of $z$-component. Thus the solution of this differential equation system can be expressed as

$$\vec{\xi}(z) = \exp(-iNz) \cdot \vec{\xi}(0),$$  \hspace{1cm} (2.11)$$

where $\exp(-iNz)$ is called the transfer matrix and $\vec{\xi}(0)$ is the initial condition at $z=0$. It should be noted that this solution is appropriate for a layered system because the overall solution can be obtained by multiplication of the solutions of each layer. For multilayer media, the surface impedance approach can be adopted to avoid the numerical difficulties [87], [88]. Based on this approach, the generalized traction vector $T = \{i\vec{\Im}(z) \quad i\vec{\Re}(z)\}^T$ and the generalized displacement vector $U = \{\vec{u}(z) \quad \vec{\phi}(z)\}^T$ are defined at a plane normal to the $z$-axis. By using the eigenvalue-eigenvector decomposition of the transfer matrix, (2.11) can be rearranged in the following form

$$\begin{bmatrix} U \\ T \end{bmatrix} = \begin{bmatrix} A_1 & A_2 \\ L_1 & L_2 \end{bmatrix} \begin{bmatrix} \Phi_1 & 0 \\ 0 & \Phi_2 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \end{bmatrix},$$  \hspace{1cm} (2.12)$$

where $\begin{bmatrix} A_1 & A_2 \\ L_1 & L_2 \end{bmatrix}$ is the matrix of eigenvalues of $N$, which are arranged such that the first four eigenvalues of the tensor $N$ corresponded to waves decaying in the $z$-direction. $A_1$, $A_2$, $L_1$, and $L_2$ are $4 \times 4$ matrices. $C_1$ and $C_2$ are constant vectors which are related to the initial condition at $z = 0$. The diagonal matrices are

$$\Phi_1 = \text{diag}(e^{-ik_1z}, e^{-ik_2z}, e^{-ik_3z}, e^{-ik_4z}),$$  \hspace{1cm} (2.13)$$

$$\Phi_2 = \text{diag}(e^{-ik_5z}, e^{-ik_6z}, e^{-ik_7z}, e^{-ik_8z}),$$  \hspace{1cm} (2.14)$$

with $k_{ij}$ the eigenvalues of the tensor $N$. With the above arrangement of the transfer matrix, the surface impedance tensor of the layered piezoelectric medium can be defined as [84], [87]

$$T = i\omega G U,$$  \hspace{1cm} (2.15)$$

where the surface impedance tensor $G$ is a $4 \times 4$ matrix. The recursive formulas of $G$ for layered media are then given by

$$G_j = \left[ Z_{ij} W_{ij}(z) R_{j-1} W_{2j}^{-1} + Z_{2j} \right] \left[ W_{ij}(z) R_{j-1} W_{2j}^{-1} + I \right]^{-1},$$  \hspace{1cm} (2.16)$$
\[ Z_{aj} = -\frac{1}{\omega} L_{aj} A^{-1}_{aj}, \]  
\[ W_{aj} = A_{aj} \Phi_{aj} A^{-1}_{aj}, \]  
\[ R_{j-1} = \left[ Z_{ij} - G_{j-1} \right]^{-1} \left[ G_{j-1} - Z_{2j} \right], \]

where \( j = 1 \) represents the piezoelectric membrane. \( Z_{aj} \) are local impedances for the up-going wave and the down-going wave. \( \alpha = 1 \) represents decaying waves in the positive z-direction (up-going), and \( \alpha = 2 \) represents decaying waves in the negative z-direction (down-going).

### 2.2.2 Boundary Conditions

Generally two electrode configurations for a piezoelectric plate are considered and shown in Fig. 2–3. Type A device is a single piezoelectric membrane with IDTs on the top surface combined with a non-metallized (i.e. free or open-circuited) bottom surface and type B device has IDTs on the top surface combined with a metallized (i.e. short-circuited) bottom surface. For the type A device, to satisfy the boundary conditions of the bottom surface at \( z = 0 \), including traction free and continuity of the normal electric displacement, the surface impedance tensor \( G_0 \) of the bottom surface can be expressed as

\[ G_0 = \begin{bmatrix} 0 & 0 \\ 0 & -i\varepsilon_0 k_x \end{bmatrix}, \]  

Figure 2-3. Cross-sectional illustrations of two electrode arrangements of common piezoelectric LWRs: (a) non-metallized bottom surface and (b) metallized bottom surface.
where $\varepsilon_0$ is the vacuum permittivity and the Laplace equation of the electric potential in the vacuum has been satisfied. For the type B device, to satisfy the boundary conditions of the bottom surface at $z=0$, which include traction free and zero potential, the surface impedance tensor $G_0$ of the bottom surface can be expressed as

$$G_0 = 0 .$$  \hfill (2.21)

### 2.2.3 Effective Permittivity

In order to conveniently define the effective permittivity, the surface impedance tensor $G_j$ in (2.16) can be rearranged in the form

$$G_j = \begin{bmatrix} G_m & g_{T\phi} \\ g_{DU}^T & g_{D\phi} \end{bmatrix} , \hfill (2.22)$$

where $G_m$ is a $3 \times 3$ matrix representing the mechanical part of $G_j$. $g_{T\phi}$ and $g_{DU}^T$ are $3 \times 1$ vectors standing for the electromechanical coupling terms of $G_j$ where $g_{T\phi}$ is the coupling between the traction and the electric potential, and $g_{DU}^T$ is the coupling between electric displacement and particle displacement. The superscript “T” in $g_{DU}^T$ denotes the transpose. The scalar $g_{D\phi}$ relates the electric potential to the electric displacement. Equation (2.15) can be expanded as

$$i\bar{f} = i\omega \begin{bmatrix} G_m \bar{u} + g_{T\phi} \bar{\phi} \end{bmatrix} ,$$  \hfill (2.23)

$$i\bar{D}_z = i\omega \begin{bmatrix} g_{DU}^T \bar{u} + g_{D\phi} \bar{\phi} \end{bmatrix} .$$ \hfill (2.24)

Since the tractions on the top surface are vanishing, the electric displacement at $z = h$ in the solid side is denoted as $\bar{D}_z |_{z=h^-}$ and is given by

$$\bar{D}_z |_{z=h^-} = \omega (-g_{DU}^T G_m^{-1} g_{T\phi} + g_{D\phi}) \bar{\phi} |_{z=h^-} . \hfill (2.25)$$

In the vacuum side, $z > h$, the electric potential should satisfy the Laplace equation. The normal electric displacement $\bar{D}_z |_{z=h}$ at $z = h$ in the vacuum side is given by

$$\bar{D}_z |_{z=h} = \varepsilon_0 k_x \bar{\phi} |_{z=h} . \hfill (2.26)$$

The effective permittivity at the interface between the vacuum and the piezoelectric membrane can then be written as
\[
\varepsilon_s = \frac{\overline{D}_{z=z+h^-} - \overline{D} \bigg|_{z=z+h^-}}{k_x \phi} = \varepsilon_0 - \frac{\omega}{k_x} \left( -g_{DU}^T G_m^{-1} g_{T\phi} + g_{D\phi} \right),
\]

where the continuity of the electric potential at the interface has been employed.

Two sets of AlN stiffness constants are widely used in theoretical analysis as listed in Table 2–2 [66], [77], [89]. In this dissertation, the AlN stiffness constants reported in [77] are employed in the theoretical simulation. Figure 2–4 shows effective permittivity of Lamb wave modes propagating in an AlN thin membrane with the free bottom surface condition while the AlN thin film thickness \((h_{\text{AlN}})\) is 1 µm and the wavelength \((\lambda)\) corresponds to 12 µm within a phase velocity range of 12,000 m/s. As shown in Fig. 2–4, the solid line represents the real part of effective permittivity and the dashed line represents the imaginary part. The effective permittivity values of the Lamb wave modes are real in this case, indicating that the two Lamb wave modes would not attenuate since most surfaces of the AlN membrane are in contact with air. There are two poles and two zeros in Fig. 2–4 where the zeros are corresponding to Lamb wave mode solutions for a free top surface due to the zero charge density whereas the poles indicate Lamb wave solutions for a metallized top surface because it gives a finite charge density and a zero electric potential.

In general, the Lamb wave modes only have displacements in the \(x\)- and \(z\)-directions as depicted in Fig. 2–2 and they are usually sorted into antisymmetric and symmetric modes according to their unique displacement fields in the piezoelectric thin plate. It is well-known that the antisymmetric Lamb waves exhibit antisymmetric \(x\)-displacements and symmetric \(z\)-displacements and the symmetric Lamb wave modes show symmetric \(x\)-

<table>
<thead>
<tr>
<th>Symbol</th>
<th>AlN [77]</th>
<th>AlN [89]</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>(C_{11})</td>
<td>3.45</td>
<td>4.105</td>
<td></td>
</tr>
<tr>
<td>(C_{12})</td>
<td>1.25</td>
<td>1.485</td>
<td></td>
</tr>
<tr>
<td>(C_{13})</td>
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<td>0.989</td>
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<td>(C_{33})</td>
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</tr>
<tr>
<td>(C_{44})</td>
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<td></td>
</tr>
<tr>
<td>(C_{66})</td>
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<td>1.31</td>
<td></td>
</tr>
<tr>
<td>(\rho)</td>
<td>3,260</td>
<td>3,255</td>
<td>(kg/m³)</td>
</tr>
<tr>
<td>(e_{15})</td>
<td>-0.48</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(e_{31})</td>
<td>-0.58</td>
<td></td>
<td>(C/m²)</td>
</tr>
<tr>
<td>(e_{33})</td>
<td>1.55</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\varepsilon_{13})</td>
<td>8.0</td>
<td></td>
<td>((10^{11} \text{ F/m}))</td>
</tr>
<tr>
<td>(\varepsilon_{33})</td>
<td>9.5</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
displacements and antisymmetric z-displacements with respect to the neutral axis [60]. According to the displacement profiles illustrated in Fig. 2–5, the first Lamb wave mode observed in Fig. 2–4 is called the lowest-order antisymmetric (A₀) mode and the second mode is called the lowest-order symmetric (S₀) mode. While the thickness of the piezoelectric plate is comparable to the acoustic wavelength, the propagation properties of the acoustic waves are dispersive with respect to the thickness of the piezoelectric AlN thin plate [90].

Figure 2-4. The effective permittivity of Lamb waves propagating in an AlN plate with the electrically free bottom surface while the AlN thickness (h_{AlN}) is 1 µm and the wavelength (λ) corresponds to 12 µm.

Figure 2-5. Normalized displacement profiles to surface potentials of the (a) A₀ and (b) S₀ Lamb wave modes in a 1-µm-thick AlN plate.
2.2.4 Phase Velocity of the $A_0$ and $S_0$ Modes in an AlN Membrane

Figure 2–6 presents the simulated phase velocity dispersion of the first two Lamb wave modes propagating in a piezoelectric AlN membrane with free top and bottom surfaces, which were calculated using the transfer matrix. The $S_0$ Lamb wave mode shows a phase velocity in excess of 9,800 m/s which is close to the phase velocity of the BAW mode in the AlN membrane, and it exhibits much weaker phase velocity dispersion than the $A_0$ Lamb wave mode. The high phase velocity of the $S_0$ Lamb wave mode in an AlN membrane is highly suitable for high-frequency electroacoustic devices and the weak phase velocity dispersion is desirable since its resonance frequency is more insensitive to variations of AlN thickness during the sputtering deposition of the AlN thin films. While the normalized AlN thickness ($h_{\text{AlN}}/\lambda$) is within 0.2, the phase velocity of the $S_0$ mode is almost constant, indicating the AlN thickness should be designed in the region. In addition, both the phase velocities of the $A_0$ and $S_0$ Lamb wave modes are close to that of Rayleigh mode while the $h_{\text{AlN}}/\lambda$ approaches to 1.

2.2.5 Electromechanical Coupling of the $A_0$ and $S_0$ Modes in an AlN Membrane

After the extraction of the free velocity ($v_o$) and metallized velocity ($v_m$) from the zero and pole of the effective permittivity, the intrinsic $k^2$ of each Lamb wave mode can be easily evaluated by the velocity difference equation,

\[
k^2 \approx \frac{v_o^2 - v_m^2}{v_o^2} \approx \frac{2(v_o - v_m)}{v_o},
\]

(2.28)

![Figure 2-6. Simulated phase velocities of the first two Lamb wave modes propagating in an AlN plate.](image)
For more exact simulations, the Green’s function method can be adopted to calculate the 
$k^2$ in the piezoelectric membrane [84], [88],

$$k^2 = 2\Gamma_s \varepsilon_s^{(e)}.$$  \hfill (2.29)

where $\varepsilon_s^{(e)}$ is the effective permittivity at the infinite slowness and $\Gamma_s$ is the coupling 
parameter which is expressed as [88]

$$\frac{1}{\Gamma_s} = -\beta \left[ \frac{\partial \varepsilon_s(k_s)}{\partial k_s} \right]_{\beta},$$  \hfill (2.30)

where $\beta$ is the wave number at the open-circuited surface condition and defined as

$$\beta = \frac{2\pi f}{v_o(f)},$$  \hfill (2.31)

which is a function of frequency since the Lamb wave velocity is frequency dependent.

Figure 2–7 shows the intrinsic $k^2$ of the $A_0$ and $S_0$ Lamb wave modes based on the 
two backside configurations using the velocity difference equation and Green’s function.
The simulation results indicate the $S_0$ mode usually exhibits a larger $k^2$ than the $A_0$ mode 
for both configurations. Without the metallized backside surface, the $k^2$ of the $S_0$ mode is 
limited to about 1.5%. By adding the metallized bottom surface, the $k^2$ can be increased 
to approximately 3.5%. This can be understood by considering an electric field applied.

Figure 2-7. Comparison of $k^2$ computed from the Green’s function with the velocity difference method.
between two IDT electrodes with a pitch of $\lambda/2$ on an AlN plate and another electric field through the AlN plate is generated by the backside metallization, enhancing the intrinsic $k^2$. In addition, the $k^2$ of the unwanted $A_0$ mode which shows a lower phase velocity has a comparable coupling strength and will appear as a spurious mode in the frequency spectrum. Fortunately, the conductive layer on the backside of the AlN thin film not only boosts the intrinsic $k^2$ of the $S_0$ mode but also reduces the coupling strength of the unwanted $A_0$ mode. Moreover, it is interesting to compare the intrinsic $k^2$ of the $A_0$ and $S_0$ modes obtained from the two approaches and they show agreement with each other.

### 2.3 Quasi-Lamb Waves in an AlN/SiO$_2$ Composite Plate

Similar to the FBARs and SMRs using AlN thin films, the uncompensated AlN LWRs have a first-order TCF of $-20$ to $-30$ ppm/°C [66]–[68]. This level of the frequency-temperature stability is unacceptable for frequency reference applications. It is well-known that the temperature-dependent frequency variation mainly results from material softening of the mechanical structures when the environment temperature increases. A temperature compensation technique using additional SiO$_2$ layer has been widely applied to different kinds of piezoelectric resonators [65]–[69] and Si-based electrostatic MEMS resonators [62]. Therefore, it is important to analyze the wave propagation properties of Lamb waves in a multilayer plate including a piezoelectric layer and a non-piezoelectric layer. Fig. 2–8 shows the geometry of the wave problem for a composite layer to be analyzed. Lamb wave modes propagate along the $x$-direction of a non-piezoelectric plate bounded by the planes $z = 0$ and $H$, and another piezoelectric layer bounded by the planes $z = H$ and $H+h$, respectively. As mentioned above, the transfer matrix is appropriate for a multilayer system because the overall solution can be obtained by the multiplication of the solutions of each layer. It should be noticed that $j=1$ represents the non-piezoelectric membrane and $j=2$ means the piezoelectric membrane in the equations (2.16)–(2.19) respectively. Another difference between the single piezoelectric layer and the composite membrane is the boundary conditions.

![Figure 2-8. Coordinate system used in the analysis of a multilayer plate including a non-piezoelectric layer and a piezoelectric layer.](image_url)
2.3.1 Boundary Conditions and Effective Permittivity

In the piezoelectric composite membrane, four types of electrode arrangements can be considered as shown in Fig. 2–9. In the multilayer system, the IDTs are deposited on the top surface of the piezoelectric thin film and the interface can be either open-circuited or short-circuited. Moreover, the IDTs can be deposited at the interface and the top surface of the piezoelectric layer can be either open-circuited free or short-circuited. The metallization means zero potential and no mechanical loading in this dissertation. For the four configurations of electrode arrangements, to satisfy the boundary conditions of the bottom surface at $z=0$ which include traction free and continuity of normal electric displacement, the surface impedance tensor $G_0$ of the bottom surface is the same as the equation (2.20).

In the type C configuration in Fig. 2–9, the boundary conditions of the interface at $z=H$ are continuous, so the recursive formulas can be employed directly. However, for the type D device, to satisfy the boundary conditions of the interface at $z=H$ which include the continuity of the traction and displacement as well as the zero potential, the surface impedance tensor $G_1$ of the interface can be expressed as [85]

$$G_1 = \begin{bmatrix} G_m & 0 \\ 0 & 0 \end{bmatrix}.$$  \hspace{1cm} (2.32)

Since the tractions on the top surface are vanishing for the both cases, the normal electric

---

Figure 2-9. Cross-sectional illustrations of four configurations of LWRs on a composite membrane with a piezoelectric layer and a non-piezoelectric layer: (a) free interface, (b) metallized interface, (c) free top surface, and (d) metallized top surface.
displacement at \( z = H + h \) in the solid side is denoted as \( \vec{D}_t \big|_{z = (H + h)^+} \), and it can be given by

\[
\vec{D}_t \big|_{z = (H + h)^+} = \omega \left( -g_{DU}^{-1} g_{m \phi}^{-1} g_{m \phi}^T g_{D \phi} + g_{D \phi} \right) \vec{\phi} \big|_{z = (H + h)^+}.
\] (2.33)

In the vacuum side (i.e. \( z > H + h \)), the electric potential satisfies the Laplace equation. The normal electric displacement \( \vec{D}_t \big|_{z = (H + h)^+} \) at \( z = H + h \) in the vacuum side is given by

\[
\vec{D}_t \big|_{z = (H + h)^+} = \varepsilon_0 k_x \vec{\phi} \big|_{z = (H + h)^+}.
\] (2.34)

The effective permittivity at the top surface can then be written as

\[
\varepsilon_z = \frac{\vec{D}_t \big|_{z = (H + h)^+} - \vec{D}_t \big|_{z = (H + h)^+}}{k_x \vec{\phi} \big|_{z = (H + h)^+}} = \varepsilon_0 - \frac{\omega}{k_x} \left( -g_{DU} g_{m \phi}^{-1} g_{m \phi}^T + g_{D \phi} \right),
\] (2.35)

where the continuity of the electric potential on the top surface has been employed.

For the type E device in Fig. 2–9, to satisfy the boundary conditions of the top surface at \( z = H + h \), which include traction free and continuity of normal electric displacement, the surface impedance tensor \( G_2 \) of the top surface can be expressed as [85]

\[
G_2 = \begin{bmatrix} 0 & 0 \\ 0 & i\varepsilon_0 k_x \end{bmatrix}.
\] (2.36)

where the Laplace equation of the electric potential in the vacuum has been satisfied. However, in the layered structure of type F, to satisfy the boundary conditions of the top surface at \( z = H + h \), which include the traction free and zero potential, the surface impedance tensor \( G_2 \) of the top surface can be expressed as [85]

\[
G_2 = 0.
\] (2.37)

At the interface of the two plates, the relation between the generalized traction vector and the displacement vector at \( z = H^+ \) in the piezoelectric side can be expressed as

\[
\begin{bmatrix} \vec{iT} \\ i\vec{D}_c \end{bmatrix} \big|_{z = H^+} = i\omega G \begin{bmatrix} \vec{u} \\ \vec{\phi} \end{bmatrix} \big|_{z = H^+} = i\omega \begin{bmatrix} G_m^+ & g_{m \phi}^T \\ g_{DU}^T & g_{D \phi}^T \end{bmatrix} \begin{bmatrix} \vec{u} \\ \vec{\phi} \end{bmatrix} \big|_{z = H^+}.
\] (2.38)

and at \( z = H^- \) in the non-piezoelectric membrane side, the generalized traction vector and the displacement vector can be expressed as
\[
\left\{ \begin{array}{l}
\mathbf{t} \\
\mathbf{D}_z
\end{array} \right|_{z=H^-} = i \omega \mathbf{G}^r \left. \mathbf{u} / \phi \right|_{z=H^-} = i \omega \left[ \mathbf{G}_m^- - \mathbf{g}^{T \phi}_{T_\phi m} \mathbf{G}_m^- \right] \left. \mathbf{u} / \phi \right|_{z=H^-}.
\]

(2.39)

Since the tractions, mechanical displacement, and electric potential at the interface \( z = H \) are continuous, the \( z \)-component of the electric displacements on the both sides of the interface are therefore given by

\[
\left. \mathbf{D}_z \right|_{z=H^+} = \omega \left[ \mathbf{g}^{T \phi}_{T_\phi m} \left( \mathbf{G}_m^- - \mathbf{G}_m^+ \right)^{-1} \left( \mathbf{g}_T^+ - \mathbf{g}_T^\phi \right) + \mathbf{g}_D^+ \right] \left. \mathbf{\phi} \right|_{z=H^+},
\]

(2.40)

\[
\left. \mathbf{D}_z \right|_{z=H^-} = \omega \left[ \mathbf{g}^{T \phi}_{T_\phi m} \left( \mathbf{G}_m^- - \mathbf{G}_m^+ \right)^{-1} \left( \mathbf{g}_T^+ - \mathbf{g}_T^\phi \right) + \mathbf{g}_D^- \right] \left. \mathbf{\phi} \right|_{z=H^-}.
\]

(2.41)

Accordingly, the effective permittivity at the interface can be written as

\[
\varepsilon_s = \frac{\left. \mathbf{D}_z \right|_{z=H^+} - \left. \mathbf{D}_z \right|_{z=H^-}}{k_x \left. \mathbf{\phi} \right|_{z=H^-}} = \frac{\varepsilon}{k_x} \left[ \left( \mathbf{g}^{T \phi}_{T_\phi m} - \mathbf{g}^{T \phi}_{T_\phi D} \right) \left( \mathbf{G}_m^- - \mathbf{G}_m^+ \right)^{-1} \left( \mathbf{g}_T^+ - \mathbf{g}_T^\phi \right) + \mathbf{g}_D^+ - \mathbf{g}_D^- \right].
\]

(2.42)

The AlN material constants listed in Table 2–2 and the SiO\(_2\) material constants listed in Table 2–3 are employed in the theoretical computing [66]. Figure 2–10 shows the effective permittivity of Lamb waves propagating in an AlN/SiO\(_2\) composite membrane with the electrically free interface while the \( h_{\text{AlN}} \) is 1 \( \mu \text{m} \), the SiO\(_2\) layer thickness (\( h_{\text{SiO}2} \)) is 0.8 \( \mu \text{m} \), the wavelength \( \lambda \) corresponds to 12 \( \mu \text{m} \), and the phase velocity range is within 12,000 m/s. In Fig. 2–10, the solid line represents the real part of effective permittivity and the dashed line represents the imaginary part. There are two poles and two zeros in

---

Table 2-3. Material constants of Al, SiO\(_2\), and 3C–SiC used in the calculation.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Al</th>
<th>SiO(_2)</th>
<th>3C–SiC</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( C_{11} )</td>
<td>( 1.113 )</td>
<td>( 0.785 )</td>
<td>( 3.90 ) ( \times 10^{11} \text{ N/m}^2 )</td>
</tr>
<tr>
<td></td>
<td>( C_{12} )</td>
<td>( 0.591 )</td>
<td>( 0.161 )</td>
<td>( 1.42 )</td>
</tr>
<tr>
<td></td>
<td>( C_{13} )</td>
<td>( 0.591 )</td>
<td>( 0.161 )</td>
<td>( 1.42 )</td>
</tr>
<tr>
<td></td>
<td>( C_{33} )</td>
<td>( 1.113 )</td>
<td>( 0.785 )</td>
<td>( 3.90 )</td>
</tr>
<tr>
<td></td>
<td>( C_{44} )</td>
<td>( 0.261 )</td>
<td>( 0.312 )</td>
<td>( 2.56 )</td>
</tr>
<tr>
<td></td>
<td>( C_{66} )</td>
<td>( 0.261 )</td>
<td>( 0.312 )</td>
<td>( 2.56 )</td>
</tr>
<tr>
<td>Mass density</td>
<td>( \rho )</td>
<td>( 2,700 )</td>
<td>( 2,200 )</td>
<td>( 3,210 ) ( \text{kg/m}^3 )</td>
</tr>
<tr>
<td>Piezoelectric constants</td>
<td>( e_{14} )</td>
<td>–</td>
<td>–</td>
<td>( -0.349 ) ( \text{C/m}^2 )</td>
</tr>
<tr>
<td></td>
<td>( e_{13} )</td>
<td>( 1 )</td>
<td>( 3.32 )</td>
<td>( 5.77 ) ( \times 10^{-11} \text{ F/m} )</td>
</tr>
<tr>
<td></td>
<td>( e_{33} )</td>
<td>( 1 )</td>
<td>( 3.32 )</td>
<td>( 5.77 ) ( \times 10^{-11} \text{ F/m} )</td>
</tr>
</tbody>
</table>
Fig. 2–10 where the zeros are corresponding to the Lamb wave mode solutions for a free top surface due to the zero charge density whereas the poles indicate the Lamb wave mode solutions for a metallized top surface of the AlN thin film because it gives a finite charge density and a zero electric potential.

As discussed above, Lamb waves are sorted into antisymmetric and symmetric modes according to their unique displacement fields. However, the different material properties of the AlN and SiO$_2$ layers make the Lamb wave displacement profiles no longer simply

Figure 2-10. The effective permittivity of Lamb waves propagating in an AlN/SiO$_2$ membrane with the electrically free interface while $h_{\text{AIN}}$ is 1 $\mu$m, $h_{\text{SiO}_2}$ is 0.8 $\mu$m, and $\lambda$ corresponds to 12 $\mu$m.

Fig. 2–10 where the zeros are corresponding to the Lamb wave mode solutions for a free top surface due to the zero charge density whereas the poles indicate the Lamb wave mode solutions for a metallized top surface of the AlN thin film because it gives a finite charge density and a zero electric potential.

As discussed above, Lamb waves are sorted into antisymmetric and symmetric modes according to their unique displacement fields. However, the different material properties of the AlN and SiO$_2$ layers make the Lamb wave displacement profiles no longer simply

Figure 2-10. The effective permittivity of Lamb waves propagating in an AlN/SiO$_2$ membrane with the electrically free interface while $h_{\text{AIN}}$ is 1 $\mu$m, $h_{\text{SiO}_2}$ is 0.8 $\mu$m, and $\lambda$ corresponds to 12 $\mu$m.

Figure 2-11. Normalized displacement profiles to surface potentials of the (a) QA$_0$ and (b) QS$_0$ Lamb wave modes in an AlN/SiO$_2$ multilayer plate while $h_{\text{AIN}}$ is 1 $\mu$m and $h_{\text{SiO}_2}$ equals 0.8 $\mu$m.
antisymmetric or symmetric with respect to the neutral axis. As shown in Fig. 2–11, when the 0.8-µm-thick SiO$_2$ layer is attached to the 1-µm-thick AlN plate, the normalized displacement profiles to the surface potentials of the Lamb wave modes are distorted. It should be noted that the SiO$_2$ layer exhibits larger displacement profiles for both plate acoustic modes because SiO$_2$ has lower acoustic impedance than AlN [36], [91]. In this dissertation, as a result, the plate acoustic wave modes propagating in the composite plate are classified as quasi-Lamb wave modes. According to their displacement profiles in Fig. 2–11, the first mode in Fig. 2–10 is called the lowest-order quasi-antisymmetric (QA$_0$) mode and the second mode is classified as the lowest-order quasi-symmetric (QS$_0$) mode.

### 2.3.2 Phase Velocity of the QS$_0$ Mode in an AlN/SiO$_2$ Plate

Since the S$_0$ mode shows the higher phase velocity and larger $k^2$ than the A$_0$ mode in an AlN thin plate, only the QS$_0$ mode will be investigated in the AlN/SiO$_2$ composite layer. Similar to the Lamb wave modes propagating in the AlN layer, while the thicknesses of the piezoelectric thin film and non-piezoelectric layer are comparable to the wavelength, the acoustic wave propagation properties are dispersive with respect to the thicknesses of the two layers. That is to say, both of the AlN and SiO$_2$ thicknesses should be considered in achieving the high phase velocity and large $k^2$ of the QS$_0$ mode.

Figure 2–12 shows the phase velocity dispersions of the QS$_0$ mode in the AlN/SiO$_2$ membrane with the open-circuited top surface and interface while the normalized SiO$_2$ thickness ($h_{SiO_2}/\lambda$) varies from 0 to 0.15 with a step of 0.05. The QS$_0$ Lamb wave mode shows the phase velocity decreases with the increasing SiO$_2$ thickness because SiO$_2$ has

![Figure 2-12. Simulated phase velocity dispersion of the QS$_0$ Lamb wave mode for $h_{SiO_2}/\lambda$ equal to 0, 0.05, 0.1, and 0.15, respectively.](image)
smaller material stiffness constants and lower phase velocities than AlN. The QS₀ mode propagating in the AlN/SiO₂ composite layer exhibits a relatively large phase velocity in the \( h_{\text{AlN}} \) range from 0.2\( \lambda \) to 0.4\( \lambda \).

### 2.3.3 Electromechanical Coupling of the QS₀ Mode in an AlN/SiO₂ Plate

The intrinsic \( k^2 \) of the QS₀ mode in the AlN/SiO₂ composite membrane is evaluated using the velocity difference method in the subsection. Figure 2–13 shows the intrinsic \( k^2 \) of the AlN/SiO₂ LWRs using the QS₀ mode with the four configurations of Fig. 2–9 while the \( h_{\text{SiO₂}} \) is equal to 0.1\( \lambda \). Although the type F device shows a large \( k^2 \) among the four configurations when the \( h_{\text{AlN}}/\lambda \) equals 0.5, the thick AlN thin film is not preferred for manufacture. In contrast to the type F configuration, for the \( h_{\text{AlN}}/\lambda \) thinner than 0.4, the type D device using the QS₀ mode exhibits relatively large intrinsic \( k^2 \) than the other configurations so the type D configuration is desirable for the temperature-compensated AlN/SiO₂ LWRs. Moreover, from the standpoint of the AlN thin film deposition, type F device is not preferred since the edge discontinuities of the patterned IDT electrodes in the interface would result in poor step coverage of AlN thin films, which harms the AlN crystalline growth and causes cracks in AlN thin films [5].

Figure 2–14 illustrates the intrinsic \( k^2 \) dispersion of the type C device utilizing the QS₀ Lamb wave mode for the \( h_{\text{SiO₂}}/\lambda \) equal to 0, 0.05, 0.1, and 0.15, respectively. With various SiO₂ thicknesses, the type C configuration exhibits a maximum \( k^2 \) while the \( h_{\text{AlN}} \) is around 0.5\( \lambda \) which is not desirable for the low-cost AlN/SiO₂ LWRs. Moreover, the type D transducer also shows a larger \( k^2 \) in contrast to the type C configuration as shown in Fig. 2–13.

![Figure 2-13. Comparison of the \( k^2 \) of the QS₀ AlN/SiO₂ LWRs with various electrode configurations while the \( h_{\text{SiO₂}} \) is equal to 0.1\( \lambda \).](image-url)
Fig. 2–15 illustrates the intrinsic $k^2$ dispersion of the type D transducer configuration for the $h_{\text{SiO}_2}/\lambda$ equal to 0, 0.05, 0.1, and 0.15, respectively. The type D device utilizing the QS$_0$ Lamb wave mode exhibits a maximum $k^2$ while the $h_{\text{AlN}}$ is around 0.1$\lambda$ showing an excellent design region of the SiO$_2$ thickness for the AlN/SiO$_2$ LWRs. This feature is desirable for the cost-effective AlN/SiO$_2$ LWRs since only the thin AlN layer is required.

Figure 2-14. Simulated $k^2$ of the type C device utilizing the QS$_0$ mode for $h_{\text{SiO}_2}/\lambda$ equal to 0, 0.05, 0.1, and 0.15, respectively.

Figure 2-15. Simulated $k^2$ of the type D device utilizing the QS$_0$ mode for $h_{\text{SiO}_2}/\lambda$ equal to 0, 0.05, 0.1, and 0.15, respectively.
to achieve a larger $k^2$. The only concern is how to successfully deposit the highly $c$-axis oriented AlN thin films on the bottom metal substrates, which will be emphasized and characterized in Chapter 3.

### 2.4 Quasi-Lamb Waves in an AlN/3C–SiC Composite Plate

The AlN LWRs utilizing the $S_0$ mode have advantages of high phase velocity and weak velocity dispersion, but the LWRs based on a single piezoelectric AlN layer have some drawbacks, such as lower $Q$ and larger frequency-temperature drifts in comparison to the quartz-based resonators. Several significant research efforts are ongoing to enhance the performance of Lamb wave devices by attaching a substrate layer to the piezoelectric layer. The temperature-frequency stability issue of the AlN LWRs can be potentially addressed by adding additional $\text{SiO}_2$ layer to the resonator. The $Q$ of the AlN LWRs can be efficiently enhanced using a low acoustic loss layer of single crystal Si as the substrate layer [92]. However, the introduction of the single crystal Si layer degrades the series resonance frequency $f_s$ of the Lamb wave device.

It was reported that SiC has a larger $f_s$·$Q$ product and a higher acoustic velocity than Si [93], making SiC a potential substrate material for boosting the $Q$ of the AlN LWRs. Among over 200 known SiC polytypes, 3C–SiC is the only polytype which can be grown on Si substrates, providing various well-established bulk micromachining techniques to fabricate suspended membranes [94]. Therefore, the AlN/3C–SiC composite structure is a promising material combination for high-frequency and high-$Q$ LWRs.

In this subsection, the acoustic propagation characteristics of Lamb wave modes in a composite membrane consisting of an AlN thin film and an epitaxial 3C–SiC (100) layer are theoretically investigated. The influences of the 3C–SiC layer thicknesses and Lamb wave propagation directions on the phase velocities and electromechanical coupling coefficients are also discussed. Since 3C–SiC is a piezoelectric thin film as well, the propagation characteristics of Lamb waves in the composite membrane consisting of two piezoelectric layers should be considered. Figure 2–16 describes the geometry of the wave problem for a composite layer to be analyzed. Lamb wave modes propagate along

![Figure 2-16](image-url)
the $x$-direction of a first piezoelectric plate bounded by the planes $z = 0$ and $H$, and another second piezoelectric layer bounded by the planes $z = H$ and $H + h$, respectively.

### 2.4.1 Boundary Conditions and Effective Permittivity

In a multilayer membrane composed of two piezoelectric layers, four configurations can be considered as shown in Fig. 2–17. In the piezoelectric composite plate, the IDTs are placed on the top surface of the second piezoelectric layer and the interface can be either electrically free or metalized. The IDTs can be deposited at the interface and the top surface of the second piezoelectric layer can be either electrically free or metallized. The boundary conditions of the four electrode configurations on the multilayer membrane composed of two piezoelectric layers are the same as the case of the composite plate in section 2.3.1. The only difference between the two cases is the piezoelectric constants of the first piezoelectric layer are considered herein.

The AlN and 3C–SiC layers are treated as hexagonal and cubic crystals, respectively, in the calculation and The 3C–SiC material constants employed in the simulation are summarized and listed in Table 2–3 [79], [86], [95]. The $c$-axis of the AlN thin film and the crystalline X-axis of the epitaxial 3C–SiC (100) layer are oriented perpendicular to the interface. Figure 2–18 shows the effective permittivity of Lamb waves propagating along the [011] direction in an AlN/3C–SiC multilayer plate with the electrically free interface while the $h_{\text{AlN}}$ is 1 $\mu$m, the 3C–SiC layer thickness ($h_{\text{3C–SiC}}$) is 1 $\mu$m, the wavelength $\lambda$ corresponds to 12 $\mu$m, and the phase velocity range is within 12,000 m/s. The first two Lamb waves are separated into the QA$_0$ and QS$_0$ modes due to the different

Figure 2-17. Cross-sectional illustrations of four configurations of LWRs on a composite membrane with two piezoelectric layers: (a) free interface, (b) metallized interface, (c) free top surface, and (d) metallized top surface.
material properties of AlN and 3C–SiC, making the Lamb wave displacement profiles no longer simply antisymmetric or symmetric with respect to the neutral axis.

As shown in Fig. 2–19, when the 1-µm-thick 3C–SiC layer is attached to the 1-µm-thick AlN plate, the normalized displacement profiles to the surface potentials of the Lamb wave modes are distorted. It is noted that the AlN layer exhibits slightly larger

![Figure 2-18](image1)

**Figure 2-18.** The effective permittivity of Lamb wave modes propagating along the [011] direction in an AlN/3C–SiC composite membrane with the electrically free interface while $h_{\text{AlN}}$ is 1 µm, $h_{\text{3C-SiC}}$ is 1 µm, and $\lambda$ corresponds to 12 µm.

![Figure 2-19](image2)

**Figure 2-19.** Normalized displacement profiles to surface potentials of the (a) QA$_0$ and (b) QS$_0$ Lamb wave modes propagation along the [011] direction in an AlN/3C–SiC multilayer plate while $h_{\text{AlN}}$ is 1 µm and $h_{\text{3C-SiC}}$ equals 1 µm.
displacement profiles for both Lamb wave modes because AlN has similar an acoustic impedance to 3C–SiC. In comparison with the $A_0$ and $S_0$ modes propagating in the AlN plate, the $QA_0$ and $QS_0$ modes traveling in the AlN/3C–SiC composite membrane exhibit higher phase velocities because 3C–SiC has slightly larger stiffness constants than AlN.

### 2.4.2 Phase Velocity of the $QS_0$ Mode in an AlN/3C–SiC Plate

Since 3C–SiC is not an isotropic material, it is of interest to investigate the effects of the propagation directions on phase velocity and coupling strength of the $QS_0$ Lamb wave mode. Figure 2–20 (a) shows the phase velocity dispersion of the $QS_0$ Lamb wave mode propagating along the [010] direction for five normalized 3C–SiC thicknesses ($h_{3C-SiC}/\lambda$), namely, 0, 0.1, 0.2, 0.3, and 0.4. The computing results show that the phase velocities decrease with increasing $h_{AlN}/\lambda$. In addition, the phase velocity increases slightly in the $h_{AlN}/\lambda$ region smaller than 0.1 due to the introduction of the 3C–SiC layer, but it decreases with increasing 3C–SiC layer thicknesses even though 3C–SiC has a higher acoustic velocity than AlN. In general, the increase of the 3C–SiC layer thickness can enhance the $Q$ of the LWRs on the AlN/3C–SiC composite membrane. However, a thick 3C–SiC layer leads to the degradation of $k^2$ due to the weak piezoelectricity of 3C–SiC.

Considering the trade-off between $Q$ and $k^2$, the case of the $h_{3C-SiC}/\lambda$ equal to 0.2 was taken to study the influence of the $QS_0$ mode propagation direction on phase velocity dispersion. Because of the face-centered-cubic crystal (FCC) crystal structure of the 3C–SiC material, four propagation directions of $0^\circ$, $15^\circ$, $30^\circ$, and $45^\circ$ with respect to the [010] axis are considered in the following calculations. As shown in Fig. 2–20 (b), the $QS_0$ Lamb wave mode propagating along the [011] direction has the highest phase

![Figure 2-20](image_url)

*Figure 2-20. (a) Phase velocity dispersion of the $QS_0$ mode propagating along the [010] direction for $h_{3C-SiC}/\lambda$ equal to 0, 0.1, 0.2, 0.3, and 0.4. (b) Phase velocity dispersion of the $QS_0$ mode propagating along the $0^\circ$, $15^\circ$, $30^\circ$, and $45^\circ$ directions relative to the [010] axis when $h_{3C-SiC}/\lambda$ is equal to 0.2.*
velocity up to 12,000 m/s, which is beneficial for high-frequency Lamb wave devices.

2.4.3 Electromechanical Coupling of the QS<sub>0</sub> Mode in an AlN/3C–SiC Plate

The $k^2$ of the QS<sub>0</sub> mode in the AlN/SiO<sub>2</sub> composite plate is evaluated using the Green’s function method. Figure 2–21 shows the intrinsic $k^2$ dispersion of the four transducer configurations, respectively, for QS<sub>0</sub> mode propagating along the [010] direction and five normalized 3C–SiC thicknesses, namely, 0, 0.1, 0.2, 0.3, and 0.4. The four transducer configurations show different $k^2$ behaviors because the imposition of electrical boundary conditions at the interfaces influences the potential depth profile [86]. Due to the weak

![Figure 2-21. $k^2$ dispersion of four LWR configurations for the QS<sub>0</sub> Lamb wave mode propagating along the [010] direction and $h_{3C-SiC}/\lambda$ equal to 0, 0.1, 0.2, 0.3, and 0.4.](image-url)
piezoelectricity of the 3C–SiC layer, the $k^2$ decreases with increasing 3C–SiC thicknesses for each transducer configuration. However, the $k^2$ of types G and I dramatically increase when the normalized 3C–SiC thicknesses equal 0.1 and 0.2. In the $h_{\text{AlN}}/\lambda$ range smaller than 0.2, the type H and J configurations exhibit the higher $k^2$ than the type G and I transducers because a strong electric field can be induced between the IDT and grounded electrode. Except for the higher $k^2$, higher phase velocities can be obtained in the $h_{\text{AlN}}/\lambda$ range smaller than 0.2 as well.

Figure 2–22 shows the electromechanical coupling dispersion of the four transducer configurations, respectively, for the normalized 3C–SiC thickness equal to 0.2 and Lamb waves propagating along the 0°, 15°, 30°, and 45° directions relative to the [010] axis. As shown in simulation results, Lamb waves propagating along the 30° direction exhibit
smaller $k^2$, whereas Lamb waves propagating along the 45° direction show higher $k^2$. It is worth noting that Lamb waves in AlN/3C–SiC composite membranes with a thicker AlN layer show higher $k^2$; however, a thicker AlN layer results in a lower phase velocity. For instance, the type G transducer in the [011] propagation direction shows a $k^2$ of 2.4% but the phase velocity decreases to 8,800 m/s in the meantime. Fortunately, the type H transducer in the [011] propagation direction exhibits a $k^2$ of approximately 2% while $h_{\text{AlN}}/\lambda$ and $h_{3C-\text{SiC}}/\lambda$ are equal to 0.2 where the phase velocity is still higher than 10,000 m/s. The obtained results confirm the feasibility of the highly c-axis oriented AlN thin film deposited on the epitaxial 3C–SiC (100) layer to enable high-frequency and high-$Q$ Lamb wave resonators.

### 2.5 Conclusions

This chapter proposes the theoretical analysis of Lamb waves in the piezoelectric AlN membrane with two types of the electrode arrangements. The transfer matrix method was employed to calculate the effective permittivity and phase velocity of the Lamb waves in the AlN thin plate. The electromechanical coupling coefficients of the LWRs with two bottom electrode configurations were calculated by the Green’s function method. The simulation results show the electromechanical coupling strength depends on the bottom electrode arrangements. Fortunately, the bottom electrode not only boosts the intrinsic $k^2$ of the $S_0$ mode but also reduces the coupling strength of the unwanted $A_0$ mode. The $S_0$ Lamb wave mode propagating in the AlN thin membrane exhibits high phase velocity, moderate electromechanical coupling coefficient, small first-order TCF, weak phase velocity dispersion, and high $Q$, showing the potential applications for the future high-frequency and narrowband wireless transmission systems.

The acoustic characteristics of the QS$S_0$ Lamb wave modes propagation in multilayer plates with four types of electrode configurations were also theoretically investigated. The formulae of effective permittivity were derived based on the transfer matrix method and further was employed to calculate the phase velocity dispersion of the composite plate, such as the AlN/SiO$_2$ and AlN/3C–SiC multilayer structure. The electromechanical coupling coefficients under various electrical boundary conditions were calculated by the Green’s function method. The acoustic characteristics of the multilayered plate are the design guideline for the electroacoustic resonators on them since their electromechanical coupling coefficients depends on the electrode allocations and plate thickness. The type D resonator using the QS$S_0$ Lamb wave mode in the AlN/SiO$_2$ membrane exhibits the larger coupling strength while the $h_{\text{AlN}}/\lambda$ is around 0.1, indicating the best design region of the AlN thickness for the temperature-compensated AlN/SiO$_2$ LWRs. Moreover, the type H resonator utilizing the QS$S_0$ mode propagating along the [011] direction in the AlN/3C–SiC composite plate exhibits the phase velocity higher than 10,000 m/s and the intrinsic $k^2$ larger than 2% while the $h_{3C-\text{SiC}}/\lambda$ and $h_{\text{AlN}}/\lambda$ are both equal to 0.2 which are feasible design region to enable high-frequency and high-$Q$ AlN/3C–SiC LWRs.
Chapter 3

Microfabrication Technology of AlN Lamb Wave Resonators

Bulk piezoelectric materials have been found for over 100 years and play an important role in the timing and frequency control applications for over 50 years. Microfabrication techniques for piezoelectric thin films compatible with the CMOS standard fabrication process have advantages in reducing the device sizes, manufacturing costs, and enabling integration with electronics. Fundamental limitation in the miniaturization process of piezoelectric devices concerns issues with deposition of well-textured piezoelectric thin films in a repeatable manner. Sputtered AlN thin films have demonstrated the fabrication of the piezoelectric devices on Si substrates, the capability of mass production, and the integration of the AlN BAW resonators above integrated circuits [96], [97]. Duplexers and oscillators based on the AlN FBARs have been commercially available [13], [36]. The chapter presents an overview of the microfabrication process technology of the AlN MEMS devices. A baseline five-mask fabrication process is described to manufacture the AlN and AlN/SiO$_2$ LWRs. If the backside metallization of the AlN-based devices is not required, the fabrication process steps can be reduced to two masks. The deposition and characterization of highly $c$-axis oriented AlN thin films on various bottom electrodes such as aluminum (Al), molybdenum (Mo), and platinum (Pt) are also presented. Some issues with Al bottom surface metallization and oxide hard mask deposition on the Al top electrode are discussed and addressed. It should be pointed out that some fabrication limitations described here derive from the technological limits of the semiconductor tools used for the microfabrication process. Advanced semiconductor fabrication tools would allow better and optimized fabrication processes in the future.

3.1 Fabrication Challenges

In various MEMS devices, the piezoelectric AlN layer is typically sandwiched between two metal electrodes such as Al, Mo, or Pt. The backside metallization is required for the FBARs and SMRs and optional for the AlN LWRs. According to the theoretical results, as observed in Fig. 2–7, the backside metal usually can improve the $k^2$ of the AlN LWRs.
utilizing the S\textsubscript{0} mode since the metallized backside surface strongly enhances the vertical electric field in the AlN thin film. To ensure a strong piezoelectric response, growth of highly c-axis oriented AlN thin films on bottom electrodes is imperative [36]. Since the AlN thin film quality heavily depends on the bottom metal properties, the deposition of the smooth and well-textured bottom electrode layer is imperative for the highly c-axis oriented AlN thin films [98]–[101]. In this subsection, the fabrication challenges to deposit the well-textured bottom electrodes and AlN films using the reactive sputtering process are introduced and addressed. The optimization and characterization of the bottom electrode layers are investigated first and the characterization of the AlN thin films on metal layers is then studied using X-ray diffraction (XRD).

3.1.1 Bottom Electrode Metallization

The crystal orientation of piezoelectric AlN thin films has direct correlation with the film quality of the underlying metals, especially its surface roughness and crystal orientation. In our experimental results, due to the poor crystal orientation of the amorphous low-stress nitride (LSN) layer, the sputtered bottom layer has no preferred orientation on the surface of the LSN layer which is usually used for electrical isolation to the Si substrates. However, a well-textured AlN seed layer enables growth of highly (111) oriented Al and highly (110) oriented Mo thin films [98], [99]. Therefore, an AlN seed layer is beneficial to form highly textured bottom electrodes, enabling to obtain a highly c-axis AlN thin film subsequently. The orientation efficiency of the AlN seed layer was significantly improved when the surface of the bottom layer was treated with RF plasma etching prior to the AlN seed layer deposition.

In the works presented in this dissertation, the AlN seed layer and bottom electrode such as Al or Mo were deposited in the same process module equipped with AC (40 kHz) powered S-Gun for sputtering [98]–[100]. First, the main process flow to prepare highly textured Al (111) bottom electrodes is presented in the following steps:

1. Etch the surface of the substrate in argon (Ar) plasma using a capacitive-coupled RF (13.56 MHz) plasma source for 180 sec at least.
2. Deposit a 25-nm-thick AlN seed layer using reactive sputtering to enhance the crystallization of the subsequently deposited Al film.
3. Deposit the 150-nm-thick Al electrode by sputtering with Ar gas right after the AlN seed layer deposition without the Al target cleaning.

Using the above process flow, smooth Al electrodes with surface roughness as low as 2 nm and low residual tensile stress below 100 MPa can be successfully deposited on either a Si substrate, a LSN layer, or a SiO\textsubscript{2} layer.

XRD provides a non-destructive and efficient method to analyze the crystallized material structure. A normal coupled scan (i.e. \(0-2\theta\) scan) is utilized to know the number of the crystallized material structures and a rocking curve (i.e. \(\omega\) curve) scan is used to determine the film quality of the bottom electrode and piezoelectric AlN thin film. Figure 3–1 (a) shows a normal coupled scan of the Al(111)/AlN(0002)/LSN/Si layered structure, and the presence of the Al (111) and Al (222) reflection peaks centered at 38.6° and 82.6° indicate a crystallized Al layer has been deposited. The small reflection peak centered at 36.1° means a well-textured AlN seed layer was deposited on the LSN layer.
and enabled the growth of the highly crystallized Al bottom electrode layer. As shown in Fig. 3–2 (b), the 150-nm-thick Al bottom electrode shows a rocking curve of full width at half maximum (FWHM) value of 1.13°, indicating highly crystallized Al metal layer was successfully grown on the LSN layer. Most recently, the Al bottom electrode layer with excellent crystallinity exhibited the single (111) crystal orientation, showing a excellent rocking curve FWHM of 0.7° was demonstrated using a optimization of film nucleation conditions as well as sputtering with low deposition rate and low sputtering Ar gas pressure [99].

Based on a similar deposition process flow to the above process steps, a 100-nm-thick Mo electrode layer is also prepared for the growth of the AlN film on it. The modified process flow to prepare highly textured Mo (110) bottom electrodes is described in the following steps:

1. Etch the surface of the substrate in argon (Ar) plasma using a capacitive-coupled RF (13.56 MHz) plasma source for 180 sec at least.
2. Deposit a 25-nm-thick AlN seed layer using reactive sputtering to enhance the crystallization of the subsequently deposited Mo thin film.
3. Deposit the 100-nm-thick Al electrode by sputtering with Ar gas right after the AlN seed layer deposition with the Mo target cleaning.

Figure 3–1 (a) depicts a normal coupled scan of the Mo(110)/AlN(0002)/LSN/Si layered structure and the presence of the (110) Mo and (220) Mo reflection peaks centered at 40.75° and 87.35° reveals a high-textured Mo electrode layer was successfully grown on the LSN layer. As shown in Fig. 3–2 (b), the 100-nm-thick Mo bottom electrode shows a rocking curve FWHM value of 2.09°, indicating highly crystallized Mo metal layer was successfully grown on the LSN layer.

Platinum (Pt) is another common metallization material for AlN-based devices and one of the best films to have well-textured AlN thin films on it [36]. It is one of the few
metal materials which can withstand the high temperature environment [102]. It usually exhibits a FCC crystal structure and a preferred orientation of (111) plane. Usually a thin adhesion layer is required to glue Pt bottom electrodes on the LSN and SiO\(_2\) substrate. In this work, considering the process compatibility with the following device release step, Chromium (Cr) is chosen as the adhesion layer for Pt deposited on the LSN layer using sputtering. A 20-nm-thick Cr film was deposited on the LSN layer prior to the deposition of the 100-nm-thick Pt layer sputtered on it.

Figure 3–3 depicts a normal coupled scan of the Pt/Cr/LSN/Si layered structure. It was found that there was no preferred orientation for the 100-nm-thick Pt electrode layer.
on the LSN layer. Except for the degree of the substrate material crystallinity, obtaining highly $c$-axis oriented AlN thin films on different electrode materials is a function of the surface quality [103]. Although the 100-nm-thick Pt electrode layer is not crystallized, the sputtered Pt layer usually shows a smooth surface for AlN deposition, improving the film nucleation. Several research works have demonstrated high-textured AlN thin film can be grown on the Pt electrode layer with no preferred orientation [20], [45], [54].

3.1.2 Deposition and Characterization of AlN Thin Films on Metals

The grain orientation of the AlN exhibits a strong correlation with the electromechanical coupling strength and quality factor so the deposition of highly $c$-axis oriented AlN thin films is the most critical process for piezoelectric devices. The correlation between $k^2$ and AlN grain orientation has been found and suggests that maximum coupling can be achieved if the rocking curve FWHM value of the AlN film is below 2° [104]. Except for the crystalline orientation, a low residual stress is equally important since the released devices might break due to a high residual stress. In this work, the AlN thin film was deposited on various substrates by AC (40 kHz) powered S-Gun magnetron. Prior to the AlN film deposition, the surface of the substrate was pretreated by RF plasma etching to achieve smooth surface roughness. For different substrate materials, the required RF plasma etching time would be different since they have different atomic binding energy and lower sputtering yield [99], [100]. For example, a RF plasma etching duration of 180 sec is long enough to achieve highly $c$-axis oriented AlN thin films on a Si substrate but a plasma etching time of 300 sec is required to deposit highly textured AlN thin films on a 3C–SiC substrate [105], [106].

The AlN film sputtering process was performed at the ambient temperature of around 300–350°C and the common reactive sputtering conditions are summarized in Table 3–1. Figure 3–4 (a) shows a normal coupled scan of the AlN(0002)/Al(111)/LSN/Si layered structure. The presence of the (0002) and (0004) AlN reflection peaks centered at 36.2° and 76.65°, respectively, give the indication of a highly $c$-axis oriented AlN thin film grown on the well-textured Al electrode layer. As shown in Fig. 3–4 (b), the 1-µm-thick AlN layer shows a rocking curve FWHM value of 1.17°, implying highly $c$-axis oriented AlN thin film was successfully grown on the 150-nm-thick Al bottom electrode layer. In addition, it should be pointed out that the AlN thin film grown on the non-crystallized Al

| Table 3-1. Reactive sputtering conditions for AlN thin film deposition. |
|-------------------------------------------------|-----------------|
| Al target purity | 99.999 (%) |
| Base pressure | $< 2 \times 10^{-7}$ (torr) |
| AC power (40 kHz) | 4–6.5 (kW) |
| Ar flow rate | 0–10 (sccm) |
| $N_2$ flow rate | 18–30 (sccm) |
| Deposition rate | 50–60 (nm/min) |
electrode layer shows a rocking curve FWHM value higher than 3°. In this case, the worse rocking curve width of the AlN film is mainly caused by the rough surface of the Al bottom electrode [100], [103].

Based on the same sputtering process, a 1-µm-thick AlN layer was also deposited on the well-textured Mo electrode and non-crystallized Pt electrode. Figure 3–5 (a) shows a normal coupled scan of the AlN(0002)/Mo(110)/LSN/Si layered structure. As shown in Fig. 3–5 (b), the 1-µm-thick AlN thin film shows a rocking curve FWHM value of 1.24°.

Figure 3-4. (a) Normal coupled scan of the AlN(0002)/Al(111)/LSN/Si layered structure. (b) Rocking curve scan of the 1-µm-thick AlN (0002) film on the Al electrode layer.

Figure 3-5. (a) Normal coupled scan of the AlN(0002)/Mo(110)/LSN/Si layered structure. (b) Rocking curve scan of the 1-µm-thick AlN (0002) film on the Mo electrode layer.
showing highly c-axis oriented AlN layer was successfully grown on the 100-nm-thick Mo bottom electrode layers. Figures 3–6 (a) and (b) shows the normal coupled scan of the AlN(0002)/Pt/LSN/Si layered structure and the rocking curve FWHM value of 1.11° of the AlN thin films grown on the non-crystallized Pt electrode layer. The experimental results present that the surface roughness of the bottom electrode layer plays an important role on the AlN film quality, showing good agreement with the conclusion in [103].

Moreover, the residual stress of the AlN thin film can be measured by a laser interferometer, determining the curvature of the whole 4 inch wafer before and after the deposition of the AlN thin film. By adjusting the AC power or the Ar and nitrogen (N\textsubscript{2}) flow rates, the residual stress of the deposited AlN thin film can be controlled within tensile and compressive 100 MPa. It should be noted that the AC power and the gas flow rate also influence the deposition rate and the uniformity of the AlN thin film on the whole wafer.

3.1.3 Silicon Oxide Hard Mask

Another fabrication challenge is how to keep the bottom and top electrode undamaged at high temperature environment, especially for Al, during the deposition of the SiO\textsubscript{2} hard mask used for the following dry etch step. Since the melting point of Al is approximately 650°C, the high deposition temperature of the oxide layer would cause some damage on Al. Although the low-temperature oxide (LTO) layer can be deposited at around 400°C in the low pressure chemical vapor deposition (LPCVD) furnace, as shown in Fig. 3–7, the sputtered or evaporated Al top finger electrodes on the AlN thin films had some damages due to its stay in the elevated temperature environment for eight hours at least. Therefore, an additional protection layer is required for Al electrode layer to stay in the high-temperature furnace.
As niobium (Nb) has a melting point up to around 2,450°C, showing excellent high temperature stability, and it can be easily removed by chlorine (Cl\textsubscript{2})-based dry etching, it was selected as the protection layer for the Al top electrodes. First a 20-nm-thick Nb as sputtered on the surface of the Al layer right after the 150-nm-thick Al deposition. The Nb/Al top electrode was patterned using a lift-off process and then a 2-\(\mu\)m-thick LTO layer was deposited on the surface of the Nb/Al top electrodes. For the 2-\(\mu\)m-thick LTO layer deposition, it usually takes six hours at least for temperature stabilization and deposition in the LPCVD furnace. Figure 3–8 (a) shows the microscope image of the Nb/Al top finger electrodes after the LTO layer deposition. The Nb/Al top electrodes still had serious damages after long-time stay in the high-temperature furnace.

An alternative approach is to deposit thin plasma enhanced chemical vapor deposition (PECVD) oxide layer at a low temperature (i.e. 300°C) first and then 2-\(\mu\)m-thick LPCVD LTO layer. There is no obvious damage on the Al top electrodes under the microscope.

![Figure 3-7. Microscope image of the Al electrode after LTO layer deposition.](image)

![Figure 3-8. Microscope images of the Al finger electrodes with (a) 20-nm-thick Nb layer and (b) 400-nm-thick PECVD oxide layer after LPCVD LTO deposition.](image)
after 400-nm-thick PECVD oxide layer deposition which usually takes 30 minutes to deposit in total. However, as shown in Fig. 3–8 (b), the Al top finger electrodes exhibited notable damages after the LPCVD oxide deposition.

Finally, the issue with the Al damages can be addressed using the 20-nm-thick Nb layer combined with the 400-nm-thick PECVD oxide layer. As shown in Fig. 3–9 (a), there is no damage hole in the Nb/Al top finger electrodes under the microscope after the deposition of the 400-nm-thick PECVD oxide layer. The Nb/Al top electrodes still have no defects after the deposition of the 2-µm-thick LPCVD LTO layer as shown in Fig. 3–9 (b). As a result, the Al top finger electrodes can sustain the high temperature of the LPCVD furnace and the 2-µm-thick LPCVD LTO layer can be used as the hard mask for the subsequent AlN etching step. It should be noted that the different color of Figs. 3–9 (a) and (b) is caused by the different thicknesses of the silicon oxide layer.

### 3.2 Fabrication Process Flow of AlN Lamb Wave Resonators

The fabrication process employed for manufacturing the AlN LWRs is based on surface micromachining techniques, which are compatible with the CMOS processes. A baseline five-mask fabrication process is described to manufacture the AlN LWRs with grounded Al bottom electrodes. The fabrication process could be easily modified for other bottom electrode metals, such as Mo, Pt, or tungsten (W). If other metal materials withstanding attack from the AlN etchant were used for bottom metallization, the fabrication process could be reduced to a four-mask process. Given that the bottom electrode is unnecessary to be grounded, the fabrication process steps would be further reduced to a three-mask process for the AlN LWRs with floating bottom electrodes. In order to completely describe the baseline microfabrication process for the AlN LWRs, the five-mask process is introduced as followings.

First, as shown in Figs. 3–10 (a) and (b), a 300-nm-thick LSN layer was deposited on Si (100) wafers in a LPCVD furnace under 835°C. The LSN stress depends on the film
thickness and the film stress is around 300 MPa while the LSN thickness is 300–500 nm. The LSN layer is used for the electrical isolation with the Si substrates and eliminates unwanted current feedthrough and substrate losses.

A 25-nm-thick AlN seed layer was grown on the LSN layer first and 150-nm-thick Al bottom electrode layer with strong crystalline orientation at (111) was then deposited by sputtering. The top finger electrodes were patterned by a wet etching process using commercial Al etchant solution. It should be pointed out that a Shipley Microposit CD30 developer is used in the photoresist development process step since the existing OCG 934 2:1 and OPD 4262 developer containing tetramethylammonium hydroxide (TMAH),
which attacks Al and AlN during the development process step. Mo or Nb that can be used for etching stop layer was deposited and patterned by a lift-off process on the Al bottom electrodes as shown in Fig. 3–10 (d).

A highly c-axis oriented AlN thin film was deposited by AC reactive sputtering using an Endeavor-AT sputtering tool from the Tegal Corporation [97]. The preparation of highly textured AlN thin films on the Al bottom electrodes and the AlN characterization has been discussed in details in previous sections. As shown in Fig. 3–10 (f), electrical contact via holds through the AlN layer were opened by wet etching using the developer OCG 4262 at 40–50°C. Since the developer is utilized as the AlN etchant, the photoresist should be hot baked using ultraviolet light at 240°C for 4 minutes before the wet etching process. If other metal materials which can stand the attack from the developer, such as Mo, Pt, or W, were used as the bottom electrode, the process step of forming the etching stop layer in Fig. 3–10 (d) can be neglected.

Consequently dual photoresist layers were coated and patterned for the lift-off process of the 150-nm-thick Al top finger electrodes on the AlN thin film as shown in Fig. 3–10 (g). Prior to the dry etching of the AlN thin film, as shown in Figs. 3–10 (h) and (i), a LTO layer was deposited using LPCVD at around 400°C, patterned using C₄F₈-based inductively coupled plasma (ICP) etching, and used as the hard mask for the following AlN etching process. Since the deposition temperature of the LTO layer is about 400°C, causing damages on Al bottom electrodes, the 20-nm-thick Nb and 400-nm-thick PECVD oxide layers were deposited in sequence and used as the protection layers for Al to stay in the LPCVD LTO furnace.

The photoresist used to define the patterns of the LTO hard mask has to be removed after the LTO dry etching step as the photoresist would generate some organic byproducts on the sidewalls in the dry etching chamber. The AlN film was patterned by Cl₂-based transformer coupled plasma (TCP) etching as depicted in Fig. 3–10 (j). The optimized conditions for AlN etching are summarized in Table 3–2. Based on the above etching recipes, the Cl₂-based TCP etching selectivity of AlN to LTO is around 2.5. In addition to the etching rate, the sidewall of the AlN layer is critical for the performance of the LWRs, especially for the spurious mode issue. In order to achieve vertical the sidewalls of the AlN layer, the LTO hard mask should have sidewalls as vertical as possible since

<table>
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<tr>
<th>Units</th>
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<tr>
<td>Cl₂ flow rate</td>
<td>90 (sccm)</td>
<td></td>
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<tr>
<td>BCl₃ flow rate</td>
<td>10 (sccm)</td>
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<td>Ar flow rate</td>
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<td>Bias RF power</td>
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<tr>
<td>AlN etching rate</td>
<td>~250 (nm/min)</td>
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<td>LTO etching rate</td>
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the sidewall angle of the LTO layer would be transferred to the AlN sidewalls. As illustrated in Figs. 3–11 (a) and (b), the C₄F₈-based ICP etching yields a sidewall angle of around 85° for the LTO layer and the Cl₂-based TCP etching yields a sidewall angle of roughly 82° for the AlN thin film [107].

As depicted in Fig. 3–10 (k), a CF₄-based reactive ion etching (RIE) process was used to remove the remaining oxide hard mask. Finally, as shown in Fig. 3–10 (l), the AlN plate structure was released by using xenon difluoride (XeF₂)-based isotropic dry etching of the Si substrate, and the LSN layer beneath the AlN layer can be also removed by XeF₂ during the device release process.

### 3.3 Fabrication Process Flow of AlN/SiO₂ Lamb Wave Resonators

Al is selected as the metal material of the bottom electrode metallization for temperature-compensated AlN/SiO₂ LWRs at room temperature since it shows small lattice mismatch with AlN, low resistivity, and light mass density. As shown in the Fig. 3–12, a five-mask fabrication process, compatible with CMOS chips, was utilized to fabricate the temperature-compensated AlN/SiO₂ LWRs. The process flow of the AlN/SiO₂ LWRs is similar to that of the LWRs fabricated on an AlN thin plate. Therefore, the details of the process flow are not discussed herein. It should be noticed that the CF₄-based RIE process can be used to simultaneously remove the remaining oxide hard mask and pattern the thermal compensation oxide layer after the AlN layer was patterned by the Cl₂-based TCP etching as shown in Fig. 3–12 (k).

As shown in Fig. Fig. 3–12 (b), the well-textured Al (111) layer is grown on the oxide layer using the same deposition process as described in section 3.1.1. Before the 25-nm-thick AlN seed layer was grown on the oxide layer using reactive sputtering, the oxide surface was treated with RF plasma for 180 sec. Then the 150-nm-thick Al electrode layer was deposited on the oxide layer by sputtering right after the deposition of the AlN seed layer. As presented in Fig. 3–13 (a), the 150-nm-thick Al bottom electrode shows a
rocking curve FWHM value of 2.4°, which is worse than the value of the Al electrode on the LSN. The worse crystalline degree of the Al electrode was caused by the rougher top surface of the LTO layer.

As depicted in Fig. 3–13 (b), due to the worse microcrystalline texture and rougher surface of the LTO layer, the 1-µm-thick AlN thin film shows a rocking curve FWHM value of 1.77° on the Al bottom electrode layer. This level of AlN grain orientation is still good to obtain decent electromechanical coupling for piezoelectric AlN resonators as
suggested in [104]. Longer duration of the RF plasma treatment or chemo-mechanical planarization (CMP) can be performed to smooth the top surface of the LTO layer to improve the crystallinity of the Al and AlN layers [99], [103].

Al is not preferred for the AlN/SiO$_2$ LWRs operating at high temperatures due to its low melting point of 660°C. Pt with a melting point at 1,768°C can be formed as the metallization of the bottom electrode for temperature compensation of AlN/SiO$_2$ LWRs at high temperatures. Although Pt did not show good crystallinity on the LTO layer, as depicted in Fig. 3–14, the 1-µm-thick AlN thin film shows a rocking curve FWHM value

Figure 3-13. Rocking curve scans of (a) 150-nm-thick Al (111) on the LTO/LSN/Si layered structure with a 1.3-µm-thick LTO layer and (b) 1-µm-thick AlN (0002) thin film on the Al/LTO/LSN/Si layered structure.

![Figure 3-13](image1.png)

Figure 3-14. Rocking curve scan of 1-µm-thick AlN (0002) film on the Pt/LTO/LSN/Si layered structure.

![Figure 3-14](image2.png)
of 1.45° on the Pt bottom electrode layer. The results imply that obtaining high quality AlN thin films on different electrode materials is a function of the surface roughness and to a much lesser extent on the crystallinity of the substrate material [103].

3.4 Fabrication Process Flow of AlN/3C–SiC Lamb Wave Resonators

The use of the low acoustic loss materials such as single crystal silicon (SCS), sapphire, quartz, and SiC as substrates can decrease the mechanical loss and increase the $Q$ of the piezoelectric resonant devices. Although Si has been reported to efficiently enhance the $Q$ of piezoelectric resonators, the low acoustic velocity of Si is disadvantage for high-frequency devices [92], [108]. In contrast, SiC has a high acoustic velocity up to 13,000 m/s. Therefore, SiC warrants the investigation of enhancing the $Q$ of the AlN-based resonant devices without compromising the resonance frequency [86], [109]. It is well reported that, although SiC has over 200 different crystal symmetries, the cubic (3C–SiC) and hexagonal (4H–SiC and 6H–SiC) polytypes are most commonly synthesized [94]. Recently, several research groups have investigated and demonstrated the deposition of AlN thin films onto 4H–SiC [110] and 6H–SiC [111] substrates. However, AlN thin films grown on hexagonal SiC polytypes are unsuitable for fabrication of piezoelectric resonant devices because the growth of epitaxial 4H–SiC and 6H–SiC thin films is currently limited to SiC substrates of the same polytypes [94]. To date, only the growth of epitaxial 3C–SiC thin films on Si substrates have been demonstrated. The use of the 3C–SiC layer on the Si substrate is attractive because Si shows cost-effective and well-established micromachining techniques, enabling piezoelectric AIN devices based on Si substrates to be compatible with various micromechanical structures.

In this subsection, highly $c$-axis oriented AlN thin films grown on epitaxial 3C–SiC layers on Si (100) substrates using alternating current reactive magnetron sputtering are developed and experimentally characterized. Although AIN (0002) and 3C–SiC (100) have a lattice mismatch of 28.6%, this challenge was addressed by a two-step deposition process. AIN films deposited on epitaxial 3C-SiC layers were characterized using the XRD, SEM, and transmission electron microscopy (TEM). The 3C–SiC layers were epitaxially grown on Si substrates using hot-wall chemical vapor deposition (CVD) and chemo-mechanically polished by NOVASiC SA [112]. Prior to AIN film deposition, the surface of the epitaxial 3C–SiC layer was treated by low energy (150–200 eV) Ar ions from capacitively coupled RF (13.56 MHz) plasma. To mitigate the effect of the lattice mismatch between AIN (0002) and 3C–SiC (100), a 50-nm-thick AIN seed layer was deposited with high N$_2$ concentration in Ar and N$_2$ gas mixture. These initial grains served as the seeds for the growth of higher quality columnar grains as the AIN film thickness increased. The seed layer also served to reduce the negative effect of lattice mismatch between AIN (0002) and 3C–SiC (100).

The deposition processes were performed at the ambient temperature (300–350°C) for the majority of the AIN film thickness but at an elevated temperature (approximately 450°C), using an external infrared heater, for the 50-nm-thick AIN seed layer. The S-Gun magnetron was powered with an AC power of 3 kW during the seed layer deposition
and 5.5 kW during the deposition of the remaining AlN film, providing a deposition rate of approximately 66 nm/min. The detailed process recipes are listed as following steps:

1. RF plasma etching at RF power = 200 W and Ar flow = 5 sccm for 600 s.
2. Wafer preheated for 50 s (maximum temperature is about 350°C).
3. 50-nm-thick AlN seed layer deposition at elevated temperatures (approximately 450°C), AC power = 3 kW, Ar flow = 4 sccm, and N2 flow = 25 sccm.
4. AlN layer deposition at the ambient temperature (300–350°C), AC power = 5.5 kW, Ar flow = 6 sccm, and N2 flow = 17 sccm.

The crystalline structure was determined by XRD as shown in Fig. 3–15 (a) where the diffraction peaks correspond to a hexagonal wurtzite-type AlN (0002) film, a cubic zinc-blende-type SiC (100) film, and a Si (100) substrate, respectively. As shown in Fig. 3–15 (b), the rocking curve of the 1-µm-thick AlN film shows a FWHM value of 1.73° which implies the AlN film has good crystallinity on the 3C–SiC layer.

In addition to the sputtering temperatures, the degree of c-axis texturing of the reactively sputtered AlN thin film is closely related to the substrate texture and surface roughness. The surface pretreatment of the 3C–SiC layer can significantly influence the AlN film orientation. The RF plasma etching can decrease the surface roughness of the 3C–SiC layer and hence can improve the AlN crystal alignment. As depicted in Fig. 3–16, 1-µm-thick AlN films with different RF plasma etching duration of 180 s, 360 s, and 600 s exhibit the FWHM values of 2.29°, 1.89°, and 1.73°, respectively. As a result, the longer RF plasma etching duration of 600 s is required to achieve the best crystallinity of AlN films on the epitaxial 3C–SiC (100) layer. For comparison, the RF plasma etching duration of 180 s is enough to achieve highly c-axis oriented AlN films on Si substrates under the same sputter conditions. This phenomenon might be due to the higher atomic binding energy and the lower sputtering yield of SiC [105], [106]. The sputtering yield ratio for SiC to Si is approximately 0.5 [79].

![Figure 3-15. (a) Normal coupled scan of the AlN(0002)/SiC(100)/Si layered structure. (b) Rocking curve scan of 1-µm-thick AlN (0002) thin film on the 3C–SiC layer on the Si substrate.](image-url)
The cross-sectional SEM image of the AlN/3C–SiC/Si composite structure is shown in Fig. 3–17 (a) where the AlN and 3C–SiC film thicknesses are 1 μm and 2.3 μm, respectively. The void defects with trapezoid shape at the 3C–SiC/Si interface are due to silicon outdiffusion [106]. As shown in Fig. 3–17 (b), the AlN seed layer and textured AlN layer can be identified in the bright field (BF) TEM image. It is clear that the AlN thin film exhibits numerous columnar grains which are perpendicular to the surface of the epitaxial 3C–SiC layer. Figure 3–17 (c) shows a typical high resolution (HR) TEM image of the interface between the AlN and 3C–SiC layers. The HRTEM image reveals an amorphous AlN starting layer between AlN and 3C–SiC layers which has been previously reported to appear at the beginning of AlN sputtering processes [113]. The electron diffraction (ED) patterns of 1-μm-thick AlN (0002) film and 2.3-μm-thick epitaxial 3C–SiC (100) film along the [110] zone axis are shown in Figs. 3–17 (d) and (e), respectively. This result supports the conclusion that the AlN grains on the epitaxial 3C–SiC layer are well-textured and approximately along the same direction.

Once high c-axis oriented AlN thin films can be successfully on the 3C–SiC layer, the fabrication process flow of the AlN/3C–SiC LWRs would be very similar to the process flow of the AlN LWRs. Although the metallized interface electrode between the AlN and 3C–SiC layers usually can improve the intrinsic $k^2$ since a metallized interface strongly enhances the vertical electric field in the AlN layer, the electrode-to-resonator interface stress generally causes the degradation in $Q$ [36]. In order to eliminate the undesired effects caused by the interface electrode layer, the AlN/3C–SiC LWRs are intentionally designed with a non-metallized interface to achieve a high $Q$.

Figure 3–18 describes a simple two-mask fabrication process flow for manufacturing the AlN/3C–SiC LWRs with no bottom electrode layer. As presented in Fig. 3–18 (a), a 150-nm-thick Al layer was deposited on the prepared AlN/3C–SiC/Si layered structure.
using electron beam evaporation, followed by the conventional lithography and lift-off process to pattern the IDT fingers. Prior to dry etching of the AlN thin film and epitaxial 3C–SiC layer, a LTO layer was deposited using LPCVD at approximately 400°C, and patterned using C₄F₈-based ICP etching as described in Figs. 3–18 (b) and (c).

As shown in Figs. 3–18 (d) and (e), the AlN thin film and epitaxial 3C–SiC layer can
be then simultaneously patterned using Cl$_2$-based TCP etching to define the AlN/3C–SiC composite plate. Based on the same recipes, the etching rate of 3C–SiC is approximately 200 nm/min, showing selectivity of 2 to the LTO hard mask. Subsequently the remaining LTO hard mask above the AlN thin film was removed using CF$_4$-based dry etching. Finally, the AlN/3C–SiC LWRs were baked at 120°C for 10 minutes to dehydrate the resonators as much as possible and afterward released using isotropic XeF$_2$-based dry etching as shown in Fig. 3–18 (f).

3.5 Conclusions

In this chapter, the baseline five-mask microfabrication processes for the AlN, AlN/SiO$_2$, and AlN/3C–SiC LWRs are briefly presented. Depending on the bottom electrode materials and configurations, the process steps can optionally reduced to four masks or even three masks. If the backside metallization of the AlN devices is not required, the fabrication process steps can be simply reduced to two masks. The deposition of the c-axis oriented AlN thin films were also characterized on various substrates such as Al, Mo, Pt, SiO$_2$, and 3C–SiC. A two-step deposition process can be used to overcome the lattice mismatch between the substrates and the AlN thin film. The crystalline degree and roughness of the substrate play the important roles on the growth of the highly c-axis oriented AlN thin films. Some fabrication issues with the Al bottom metallization and
oxide hard mask deposition on the Al top electrode are addressed. The fabrication processes are employed to manufacture the piezoelectric AlN resonators presented in Chapter 4, 5, and 6.
Chapter 4

Piezoelectric AlN Lamb Wave Resonators

The increasing demand for high-$Q$, temperature-stable, low-impedance, low-power, and miniaturized resonators employed for the reference oscillators and bandpass filters in the communication systems has led our research efforts towards the single-chip RF front-end solutions. Among various MEMS resonator technologies, the AlN LWRs utilizing the $S_0$ mode have showed the most promising technology for ultimately realizing this vision. However, the $Q$’s of the AlN LWRs with a bottom electrode are rarely higher than 2,000, and the improvement in $Q$ is a key to achieving better performance of low-loss filters and low-phase-noise oscillators. Though research studies have shown novel approaches to boosting the $Q$ of the micromechanical resonator, some other drawbacks such as larger impedance accompany the enhanced $Q$. In this chapter, the characteristics of the AlN LWRs will be studied and the energy loss mechanisms in the resonators will be also discussed. Suspended convex edges which can efficiently reflect the propagating Lamb waves back towards the transducer and confine the mechanical energy in the resonant body will be presented. Accordingly, the energy dissipation through the support tethers can be significantly minimized to boost the $Q$ [57], [58]. Moreover, the finite element method is performed to take an insight into static capacitance characteristics of the AlN plates with various bottom surface conditions. The IDT with a floating bottom electrode shows the same transduction efficiency with that with a grounded bottom electrode but the floating bottom electrode can efficiently reduce the static capacitance in the AlN thin plate, enhancing the effective coupling coefficient of the AlN LWR [59].

4.1 Metallization Material Selection for AlN Lamb Wave Resonators

The bottom electrode beneath the AlN thin film can effectively enlarge the $k^2$ of the $S_0$ mode since the metallized bottom surface strongly enhances the vertical electric field in the AlN thin film as observed in Fig. 2–7. Figure 4–1 illustrates the one-port LWR consisting of one IDT, a grounded bottom electrode, and two suspended free edges at both sides of the AlN thin plate. As discussed in Chapter 3, since the AlN thin films are
grown onto the substrates using AC reactive sputtering, the AlN quality heavily depends on the property of the bottom metal layer [97]. Highly c-axis oriented AlN thin films have been successfully deposited on various metals for a lot of applications [36], [98]–[102]. Generally speaking, the surface roughness, the crystallinity degree of the substrate, the substrate temperature, and the lattice mismatch between AlN and substrates are the most important factors which affect the quality and residual stress of the AlN thin films. The substrate temperature can be increased by using external heating during the initial stage of AlN nucleation on the surface of the bottom metal electrode [100] and the surface roughness can be significantly reduced by treating the bottom electrode metals with RF plasma etching [99]. As a result, selection of bottom electrode metals is essential for achieving high-quality AlN thin films. Ideally, if the metal surface has a low degree of lattice mismatch with AlN, a high degree of crystallinity, and an extremely smooth surface, it would be easy to obtain high-quality AlN thin films [101].

### 4.1.1 Lattice Mismatch between AlN and Metals

As it is pointed out that except for the texture and surface roughness of the underlying electrode metals, the degree of c-axis orientation of AlN thin films is strongly dependent on their crystal structures and lattice mismatch with AlN [101]. The most suitable metal for the growth of highly c-axis oriented AlN thin films appears to have hexagonal (0001) crystal structure, such as titanium (Ti). However, Ti shows a high bulk resistivity up to 55 $\mu\Omega\cdot\text{cm}$ which is not preferred for low-impedance acoustic wave devices. Since most metals have a cubic crystal structure, it is interesting to investigate the suitable crystalline orientation planes for the AlN (0002) thin film grown on the cubic crystal structures. Experimental studies have demonstrated that a suitable texture for the FCC crystal structure, such as Al and Pt, appears to be (111) and a suitable texture for the body-centered-cubic (BCC) crystal structure, such as Mo and W, appears to be (100) [101].
That is, for the same crystal structure, the lattice mismatch between the AlN thin film and the substrate metal layer becomes more important if the degree of the metal crystallinity and the surface roughness are assumed to be the same.

Table 4–1 summarizes and compares the physical properties of several common metal materials used for the bottom surface metallization of AlN-based devices [36]. Since the lattice mismatch between AlN and Pt is as large as 12.18% and Pt has higher resistance and larger mass density than the other selected metals, Pt is less used for AlN-based devices. However, Pt is an excellent metal material for the metallization of AlN-based devices used for high-temperature applications [102]. Although Mo and W show less lattice mismatch than Al, W usually tends to have a high level of residual film stress and large surface roughness and Mo would be attacked by xenon difluoride (XeF₂) during the structure release process of the AlN LWRs. The lattice mismatch issue can be addressed by using an AlN seed layer, and as presented in Chapter 3, AlN films showed excellent crystalline orientation on Al and Pt. Moreover, the electrode resistance is a secondary but important factor for the bottom metallization. Given Al shows lower resistivity than Mo and W, Al and Pt are employed for bottom metallization of the AlN LWRs herein.

### 4.1.2 Effects on Phase Velocity and Electromechanical Coupling

Except for the effects on the quality of the AlN thin films grown on the metallized bottom surface, there are two main concerns of the bottom metallization which strongly affect the performance of the AlN LWR: phase velocity and electromechanical coupling strength. As shown in Table 4–1, most of metal materials usually have a low acoustic velocity so the phase velocity of the S₀ Lamb wave mode is decreased by the bottom metallization. Figure 4–2 illustrates the mass loading effect of various metals on the phase velocity of the S₀ Lamb wave mode for a normalized metal thickness \((h_{metal}/\lambda)\) fixed to 0.015 and Pt decreases the phase velocity most since Pt has the highest mass density among the selected metal materials. Contrary to Pt, Al slightly decreases the phase velocity because of its relatively low mass density.
As presented in Fig. 4–3, the electromechanical coupling coefficient would also be decreased by the bottom metallization and Al decreases the $k^2$ less than the other selected metals. It is also interesting to point out that Pt reduces the $k^2$ less than Mo and W while the $h_{\text{AIN}}$ is within 0.2$\lambda$. Considering the quality of the AlN thin films grown on the metal layer, the fabrication complexity, and the effects on phase velocity and electromechanical

Figure 4-2. Simulated phase velocity of the $S_0$ mode in the AlN films with various bottom metals while the metal thicknesses normalized to the wavelength are fixed to 0.015.

Figure 4-3. Simulated $k^2$ of the $S_0$ mode in the AlN thin films with various bottom metals while the metal thicknesses normalized to the wavelength are fixed to 0.015.
coupling strength of the $S_0$ Lamb wave mode, Al and Pt are the better metal choices for the bottom surface metallization.

### 4.2 TCF of AlN Lamb Wave Resonators

Most materials have negative TCEs, implying that they become soft and their resonance frequencies would decrease as temperature increases. However, SiO$_2$ exhibits positive TCEs which can be used to compensate the elasticity decrease of the other materials caused by the temperature increase. Table 4–2 lists the temperature coefficients of Al, AlN, and SiO$_2$ which are used to predict the frequency-temperature behavior of the AlN LWR shown in Fig. 4–1. The frequency drift of the AlN LWR relates to the changes in the stiffness constants with temperature and the thermal expansion coefficients, which affect not only the dimensions of the resonator but also the density of the material. The temperature dependence of the stiffness coefficients $C_{ij}(T)$ and the mass density $\rho(T)$ can be defined as [114]

$$
C_{ij}(T) = C_{ij}(T_0)(1 + TC_{ij}\Delta T), \quad (4.1)
$$

$$
\rho(T) = \rho(T_0)\left[1 - (\alpha_x + \alpha_y + \alpha_z)\Delta T\right], \quad (4.2)
$$

where $T_0$ refers to the reference temperature of the material constants; $\Delta T$ is a relative temperature change; $TC_{ij}$ refers to the relative temperature dependence of the stiffness constants $C_{ij}$; $\alpha_x$ (i.e. $\alpha_{11}$) and $\alpha_y$ (i.e. $\alpha_{22}$) are the thermal expansion coefficients along the $x$- and $y$-directions, respectively, which are assumed to be identical herein; $\alpha_z$ (i.e. $\alpha_{33}$) is the thermal expansion coefficient along the $z$-direction. Under linear approximation of the temperature dependence of the stiffness constants in (4.1), the mass density in (4.2), and the thermal expansion coefficients, the TCF of the AlN LWR can be written as [114]

| Table 4-2. Temperature coefficients of Al, AlN, and SiO$_2$ used in simulation. |
|-----------------|---|---|---|---|
| Symbol          | Al | AlN| SiO$_2$ | Units |
| $TC_{11}$       | -590 | -37 | 239 | $(10^{-6} \text{ } \text{1/K})$ |
| $TC_{12}$       | -80 | -1.8 | 584 |
| $TC_{13}$       | -80 | -1.8 | 584 |
| $TC_{33}$       | -590 | -65 | 239 |
| $TC_{44}$       | -520 | -50 | 151 |
| $TC_{66}$       | -520 | -57 | 151 |
| $\alpha_{11}$  | 18 | 5.27 | 0.55 | $(10^{-6} \text{ } \text{1/K})$ |
| $\alpha_{33}$  | 18 | 4.15 | 0.55 |
where the first term refers to the temperature dependence of Lamb wave velocity which is computed using all the temperature dependent parameters, \( C_{ij}(T) \) and \( \rho(T) \), for \( \Delta T \) equal to 10°C, \( v_{LW} \) is the phase velocity of the \( S_0 \) mode propagating in the piezoelectric plate, and \( \alpha_x \) corresponds to the thermal expansion coefficient along the propagation direction (i.e. \( x \)-direction in this case).

Neglecting the mass loading effects of the electrode layer, the TCF of the AlN LWR can be theoretically predicted using the above formulas and the temperature dependence of material coefficients listed in Table 4–2. Since there are only first-order temperature coefficients of stiffness constants available in the literature [66], all theoretical simulation only considers the first-order effect on the TCF in this study. The simulated TCFs of the AlN LWRs with and without metalized bottom surface are shown in Fig. 4–4. The AlN LWR using the \( S_0 \) mode shows a theoretical TCF of around –22 ppm/°C which is close to the experimental results [58]. Moreover, it is interesting to note that a thicker AlN plate shows a worse first-order TCF, especially for an AlN membrane thicker than 0.4λ.

4.3 Resonator Basics and Equivalent Circuits

As mentioned in Chapter 1, an IDT usually consists of two sets of electrodes connected alternatively to two bus bars placed on a piezoelectric substrate. The space \( \Lambda \) between two adjacent electrode fingers and their overlap length \( W \) are called pitch and aperture,
respectively. As shown in Fig. 1–10 (b), the electrode finger width (w) and the distance between them are equal so the metallization ratio (\(\eta\)) is 0.5 and the IDT finger width is equal to quarter wavelength (\(\lambda/4\)) in this case. Once the phase velocity of the Lamb wave mode of interest is obtained, the resonance frequency can be intuitively estimated by assigning the acoustic wavelength as

\[
f_0 = \frac{v_{LW}}{\lambda} = \frac{v_{LW}}{2\Lambda} = \frac{v_{LW}}{4w}.
\] (4.4)

The resonance frequency of the LWR is determined by the width of the IDT so a thinner electrode finger width in the transducer can achieve higher operation frequencies and it is limited by the lithographic resolution. In addition, by employing high-order Lamb wave modes with higher phase velocities in the piezoelectric plate, one can obtain higher operation frequencies using the same electrode finger width w.

A piezoelectric resonator can be described using the Butterworth-Van Dyke (BVD) equivalent circuit which consists of a mechanical resonance branch including a motional resistor (\(R_m\)), a motional capacitor (\(C_m\)), and a motional inductor (\(L_m\)) and a clamped capacitor (\(C_0\)) in shunt [115], [116]. The acoustic wave contribution is represented by the \(R_m-L_m-C_m\) circuit which is usually referred to as the motional branch. The clamped capacitor \(C_0\), simply formed by the capacitance between the IDT electrodes and the plate capacitance sandwiched between the top and bottom electrodes is parallel to the motional branch. Figure 4–5 illustrates the modified Butterworth-Van Dyke (MBVD) lumped-parameter circuit, proposed by Larson et al. to improve match to the experimental results of the AlN BAW resonators [117]. The MBVD lumped circuit is representative for the one-port resonator, including two loss resistors, \(R_s\) and \(R_0\). Nominally, the series resistor \(R_s\) describes the resistance of the routing pads and electrodes, and the parallel resistor \(R_0\) represents the dielectric losses of the piezoelectric layer and the parasitic resistance in the Si substrate [56], [117].

The series and parallel resonance frequencies, \(f_s\) and \(f_p\), are the frequencies of the maximum conductance (the real part of the admittance) and the maximum resistance (the real part of the impedance). Based on the six parameters of the MBVD equivalent circuit, the series and parallel resonance frequencies, \(f_s\) and \(f_p\), the impedance \(Z(\omega)\), and the admittance \(Y(\omega)\) can be expressed as [117]

\[
f_s = \frac{\omega_s}{2\pi} = \frac{1}{2\pi} \sqrt{\frac{1}{L_m C_m}},
\] (4.5)
A typical admittance spectrum including the magnitude and phase of a micromechanical resonator is depicted in Fig. 4–6.

The electromechanical coupling coefficient is a measure of energy transduction efficiency between the electrical and mechanical domains. In the literature, several different definitions are used for evaluating the effective electromechanical coupling coefficient \( k_{\text{eff}}^2 \) of piezoelectric resonators from the measured results. One of the most often used definitions is IEEE standard definition which is fully consistent with analytical derivation for a BAW resonator [113], [115]

\[
k_{\text{eff}}^2 = \frac{\pi f_s}{2 f_p} \left[ \tan \left( \frac{\pi f_s}{2 f_p} \right) \right]^{-1}.
\]  

\( f_p = \frac{\omega_p}{2\pi} = f_s \sqrt{\frac{1+C_m}{C_0}} = \frac{1}{2\pi} \sqrt{\frac{1}{L_mC_m} \left( 1+\frac{C_m}{C_0} \right)}, \)  

\( Z(\omega) = R_s + \frac{1}{j\omega C_0} \left( R_m + \frac{1}{j\omega L_m} \right), \)  

\( Y(\omega) = \frac{1}{Z(\omega)}. \)
The most used approximation for the effective coupling coefficient is defined as

\[ k_{\text{eff}}^2 = \frac{\pi^2}{4} \left( \frac{f_p - f_s}{f_p} \right) \],

which is simply estimated by the relative difference of the series and parallel resonance frequencies. The \( k_{\text{eff}}^2 \) can be also expressed as the parameters of the MBVD equivalent circuit, \( C_m \) and \( C_0 \),

\[ k_{\text{eff}}^2 = \frac{\pi^2}{8} \left( \frac{C_m}{C_0} \right) \],

which provides the direct connection of the effective coupling coefficient \( k_{\text{eff}}^2 \) to the ratio between the motional capacitance and the clamped capacitance. In this dissertation, the IEEE standard definition in (4.9) is used to evaluate the \( k_{\text{eff}}^2 \) of the AlN LWRs.

The qualify factor, \( Q \), is a measure of the energy losses in the micromechanical resonators. A very basic definition of the \( Q \) represents the ratio of the energy stored in a system to the energy dissipated per cycle:

\[ Q = \frac{2\pi \cdot E_{\text{stored}}}{\Delta E} \].

where \( E_{\text{stored}} \) is the total energy stored in the system and \( \Delta E \) is the energy dissipated per radian of vibration cycle [36], [119]. Assuming there are a variety of energy loss mechanisms occurring in micromechanical resonators, each of those loss mechanisms individually contributes the \( Q \) according to the following equation:

\[ \frac{1}{Q_{\text{total}}} = \sum_i \frac{1}{Q_i} \].

where \( Q_{\text{total}} \) is the total quality factor in a resonator, and \( Q_i \) is the quality factor associated with each loss mechanism in a resonator.

The quality factors of the resonance peaks at the series and parallel frequencies, \( Q_s \) and \( Q_p \), can be expressed using the MBVD equivalent circuit parameters [36],

\[ Q_s = \frac{1}{\omega_s (R_m + R_s) C_m} \],

\[ Q_p = \frac{1}{\omega_p (R_m + R_0) C_m} \].

For an simple RLC circuit, the quality factor \( Q \) is defined as the ratio of the resonance
frequency $f_0$ to the two-sided 3dB BW, $\Delta f_{3dB}$ [118],

$$Q = \frac{f_0}{\Delta f_{3dB}}.$$  

(4.16)

The quality factor $Q$ can also be determined by using the phase slope of the admittance and defined as [118]

$$Q = \frac{\omega_0}{2} \left| \frac{d\Phi}{d\omega} \right|,$$  

(4.17)

where $\omega_0$ is the angular frequency at the resonance frequency $f_0$ and $d\Phi/d\omega$ denotes the phase slope of the admittance with respect to angular frequency.

### 4.4 Energy Loss Mechanisms in AlN Lamb Wave Resonators

Although a variety of loss mechanisms may yield the decrease in the $Q$’s of the AlN LWRs, according to the equation (4.13), the total quality factor $Q_{\text{total}}$ is usually dominated by one or two of the loss mechanisms, which results in most energy loss [119]–[122]. Here, possible energy loss mechanisms in piezoelectric Lamb wave resonators, such as tether loss, electrical losses, mode conversion loss, material loss, and air damping loss are discussed in this section [36], [119]–[145].

#### 4.4.1 Tether Loss

Tether loss, also referred to as anchor loss or support loss, is attributed to the radiation of the acoustic wave energy from the resonant body through the support tethers, keeping the AlN thin plate suspended in air as shown in Fig. 4–1. While the resonator structure is vibrating, elastic waves are excited and propagate in the support tethers which anchor the resonator structure to its surroundings. The acoustic wave energy is not well confined in the resonant body and part of the vibration energy would radiate through the support tethers and leak into the supporting media [123]–[125]. The support tethers could be designed in many forms but they contribute to the energy loss in the resonator $Q$ in the same way. A perfectly matched layer (PML) approach based finite element analysis (FEA) allows one to efficiently model the energy loss into the surrounding media and predict the resonator $Q$ values [124]. In order to reduce the tether loss in the support anchors, some experiments have shown that anchor loss can be minimized by placing anchors at nodal points of the resonant structure [126]. Most recently, in-plane arc acoustic reflectors were proposed to enhance the mechanical $Q$’s in the laterally vibrating micromachined resonators [127]. Lossless tether strips based on the phononic band-gap structures which are able to eliminate the vibrations in the anchors were designed for
micromechanical resonators to reduce the tether loss as well [128]–[130].

4.4.2 Electrical Loss

The second energy loss mechanism discussed herein is electrical losses, associated with finite resistance of the electrodes, leads, and probing pads. While the electrical resistivity of the electrodes is considered, two main effects should be concerned in the $Q$. As it has been discussed, the finite electrode resistivity can be modeled as the $R_s$ in the MBVD equivalent circuit, which lowers the mechanical $Q$ to a certain extent. The second effect of the electrode layer is the possible non-uniform stress distribution [36] and electrode-to-resonator interfacial strain [131], [132] which might cause the degradation in $Q$. In order to overcome the low $Q$ induced by the metal layer, a capacitive piezoelectric transducer that separates a piezoelectric resonant body from its electrodes via tiny air gaps to eliminate the resonator-to-electrode strain loss has been applied to the quartz resonators [133], contour-mode resonators [134], [135] and Lamb wave resonators [136]. Although the separation of the electrodes from the piezoelectric thin film is able to increase the $Q$’s of the piezoelectric resonators, the tiny air gaps sacrifice the transduction efficiency and then increase the motion impedance to a large extent.

4.4.3 Mode Conversion Loss

In general, SAWs and Lamb waves cannot satisfy the stress free boundary conditions at the free edges because of the complicated structure. To satisfy the stress free boundary conditions, the SAWs and Lamb waves are converted to other modes in such a way that all the acoustic modes together can satisfy the boundary conditions. SAWs convert to the bulk acoustic wave modes, diffract their energy into bulk substrate and lose Lamb wave energy. However, since SH waves can be completely reflected at the free edge of the substrate without mode conversion, SH waves have been employed in tiny acoustic wave resonators without grating fingers [137].

For Lamb wave modes propagation in a thin plate, the conversion to from one Lamb wave mode to other propagating Lamb modes is only possible to those with their cut-off frequencies bellow the operating frequency. Thus the $S_0$ mode can only convert to the $A_0$ mode eventually. Fortunately since the $S_0$ and $A_0$ modes have a great difference in their mode symmetry, the $S_0$ Lamb wave mode propagating in an acoustically thin plate does not exhibit greatly energy loss upon the reflection at the suspended free edges due to the mode conversion [138]. Moreover, the mode conversion loss significantly depends on the wavelength, plate thickness, and Lamb wave mode. With an appropriate selection of wavelength and plate thickness, the mode conversion loss can be minimized and the reflection coefficient at the suspended free edges can be maximized [60].

4.4.4 Material Loss

The next loss mechanism is material loss, referring to the energy loss mechanisms via an
irreversible transformation of the acoustic energy to the thermal energy, which is intrinsic to the resonant structure. There are two mechanisms for the attenuation of the acoustic wave by thermal phonons: thermoelastic damping (TED) and phonon-phonon attenuation. The TED is a loss mechanism of the structural damping in which the acoustic energy is dissipated due to irreversible heat conduction in a vibrating thermoelastic structure. This phenomenon was first studied by Zener in the 1930s [139]. For example, the TED loss occurs when a microcantilever beam executing flexural vibrations, different portions of the beam are forced periodically into compression and tension. As a consequence of thermoelastic coupling, an oscillating temperature field would be generated within the vibrating beam structure, and the finite temperature gradient will lead to the irreversible heat conduction, entropy generation, and energy dissipation [140]. The material damping loss is dominant in the close vicinity of the frequency, corresponding to the thermal relaxation time constant of the micromechanical resonator, which is usually considered at a low frequency [141].

Another thermally induced loss mechanism is phonon-phonon dissipation [93], [142]. If the acoustic wavelength is considerably larger than the mean free path of the phonons, the acoustic wave can be assumed to be interacted with the thermal phonons, resulting in attenuation of acoustic waves. This phenomenon is well-known as Akhiezer effect (AKE), which usually limits the absolute maximum $Q$ of a micromechanical resonator made of a certain material [93]. The contribution of this loss mechanism is usually quantified by a coefficient called acoustic attenuation ($\alpha$). Since we have very little knowledge about the actual values of the attenuation coefficient $\alpha$ at a relevant frequency, it is difficult to judge if this loss mechanism should be considerable in practical devices [36]. However, interestingly, the TED and phonon-phonon dissipation have reciprocal dependences on temperature so the maximum $Q$ of the micromechanical resonator was demonstrated at cryogenic temperatures when operating in AKE regime [93], [142] and Landau-Rumer regime [143].

### 4.4.5 Air Damping Loss

The final loss mechanism considered here is air damping which is a well-known loss mechanism for micromechanical devices. The air damping losses are usually separated into two categories: slide film damping and squeeze film damping. The slide film damping occurs when two parallel plates move in tangential directions [144] and the squeeze film damping happens while two parallel plates move in normal directions [145]. The viscous energy dissipation in the fluid between the two parallel plates becomes the dominant loss mechanism in electrostatic resonators. A narrow gap in hundreds or tens of nanometer is required for the capacitively transduced resonators to enable efficient transduction so it becomes the source of the air damping mechanism. For capacitively transduced disk resonators, the squeeze film damping loss can considerably reduce the $Q$ of the electrostatic disk resonators [3]. Operation of the electrostatic resonators in low pressure vacuum can significantly decrease the air damping losses.

Since the required narrow gap for operating electrostatic resonators is not present in piezoelectric resonators, the piezoelectric resonators are less susceptible to squeeze film damping in comparison with the electrostatic resonators. Given that piezoelectric Lamb
wave resonators exhibit relatively small in-plane displacements, the slide film damping is not the primary loss mechanism either. In general the support tether loss and electrical loss are regarded as the dominant loss mechanisms in the LWRs using the S\textsubscript{0} mode. The Akhiezer effect is considered when the AlN LWRs are operating at elevated or cryogenic temperatures due to the reciprocal dependences on temperature.

4.5 High-\textit{Q} AlN Lamb Wave Resonators with Convex Edges

As mentioned above, a variety of energy loss mechanisms occur in the AlN LWRs, but only one or two mechanisms would dominate the final \textit{Q} values of the resonators. So far, for the AlN LWRs utilizing the S\textsubscript{0} mode, the tether and electrical losses are generally considered the primary loss sources. Therefore, plenty of research works keep seeking for efficient methods to enhance the \textit{Q}'s of the piezoelectric AlN resonators. The in-plane arc acoustic reflectors placed in the end of the support tethers were used to reflect acoustic waves to enhance the \textit{Q} \cite{127}. The phononic band-gap structures were designed as the lossless support tethers to eliminate vibrations in the tethers to reduce the anchor loss and improve the \textit{Q} \cite{128}–\cite{130}. A capacitive-piezoelectric transducer with tiny gaps between the AlN layer and metal electrodes was introduced to boost the \textit{Q}'s of the piezoelectric AlN resonators \cite{134}–\cite{136}. The experimental results demonstrate that the separation of the electrode layer from the piezoelectric thin film increased the \textit{Q} value twice, but the tiny air gap sacrificed the \textit{k}\textsuperscript{2} and then increase the \textit{R}\textsubscript{m} to a large extent.

4.5.1 Energy Confinement using Convex Edge Reflectors

This present work introduces a novel convex shape employed for the suspended free edges to confine the energy in the resonance body of the AlN LWR and eliminate the tether loss. The convex free edges can efficiently reflect the acoustic waves back towards the AlN LWR as well as confine the displacement and mechanical energy in the resonant body. Accordingly, the energy dissipation through support tethers can be considerably minimized to enhance the mechanical \textit{Q} \cite{57}, \cite{58}.

Figure 4–7 (a) illustrates a conventional LWR which consists of one IDT and one grounded bottom electrode on the opposite sides of an AlN thin plate with suspended flat edges. Three dimensional (3D) COMSOL FEA simulation result depicts the resonance mode shape (displacement profile) of the AlN LWR with the flat edge reflectors as presented in Fig. 4–8 (a). Obviously, the displacement occurring in the support tethers implies that part of acoustic energy is leaky through the tethers even though the tether lengths have been designed as an odd multiple of a quarter-wavelength. Moreover, because most surfaces of the AlN thin plate are in contact with air and there is a large acoustic mismatch between AlN and air, a very small amount of acoustic energy is transmitted into air. Therefore, except for energy loss caused by the electrode layer, the mechanical energy loss via the support tethers dominates the decrease in \textit{Q}, especially for the AlN LWRs operating at high frequencies.
It is known that the convex shape placed in the BAW propagation direction has been applied to quartz resonators to trap mechanical energy in the center and reduce the energy dissipation at the edges [146]. In this work, based on the same concept, the biconvex free edges are implemented into the lateral direction of the AlN thin plate to trap the mechanical energy in the AlN resonator to enhance the $Q$. As illustrated in Fig. 4–7 (b), an AlN LWR is composed of the same IDT electrode configuration as Fig. 4–7 (a) but with the convex free edges in the lateral direction. Figure 4–8 (b) pictures the resonance mode shape of the AlN LWR with the convex free edge reflectors. Due to the biconvex shape, the mechanical displacement is mostly confined in the resonant body of the AlN LWR and only little displacement occurs in the support tethers, which indicates that very little energy loss through the tethers and accordingly a higher $Q$ can be attained.

In contrast to the convex free edges, the biconcave free edges are also implemented into the lateral direction of the AlN thin plate as illustrated in Fig. 4–7 (c) where an AlN LWR is constructed of the same IDT electrode configuration as Fig. 4–7 (a) but with the concave free shape in the lateral free edges. Figure 4–8 (c) depicts the resonance mode shape of the AlN LWR with the concave free edge reflectors. Apparently the biconcave
free edges disperse the acoustic waves into the surroundings, causing most displacement occurred in the support tethers rather than the resonant body. It can be expected that only little mechanical energy is confined in the resonant body and accordingly the AlN LWR with the biconcave free edges would exhibit a lower $Q$ than those with flat and biconvex shape reflectors.

4.5.2 Experimental Results and Discussions

In order to study the effect of edge shape on the mechanical $Q$, three AlN LWRs utilizing the suspended flat edges, as well as the convex and concave edge reflectors with various radii of curvature are designed and manufactured using the microfabrication process flow described in section 3.2. The design parameters are summarized and listed in Table 4–3.
To minimize the experimental errors resulting from the microfabrication processes, all the resonators were fabricated on the same wafer and placed in the vicinity. Figure 4–9 presents the SEM image of one fabricated AlN LWR with the convex edge reflectors. In this work, the AlN LWRs were all tested in air at room temperature and $S_{11}$ parameters were extracted using an Agilent E5071B network analyzer. The measured mechanical $Q$ was extracted from the admittance plot by dividing the series resonance frequency $f_s$ by the 3dB BW and the effective coupling coefficient $k^2_{eff}$ of the measured devices is defined by the IEEE standard definition.

Figure 4–10 presents the measured frequency characteristics for the LWRs using the flat edges and the biconvex edges with a curvature radius of 209.2 µm, showing their loaded $Q$’s of 1,255 and 3,280, respectively, on a 1.5-µm-thick AlN plate. The loaded $Q$

| Table 4-3. Geometric dimensions of AlN Lamb wave resonators with various edge-type reflectors. |
|-----------------------------------------------|-----------------|-----------------|-----------------|-----------------|
| Flat edge | Convex edge | Concave edge | Units |
| IDT electrode number | 6 | 6 | 6 | – |
| IDT electrode width | 4.44 | 4.44 | 4.44 | (µm) |
| IDT electrode thickness | 100 | 100 | 100 | (nm) |
| IDT aperture | 100 | 100 | 100 | (µm) |
| Pt electrode thickness | 100 | 100 | 100 | (nm) |
| Radius of curvature $R$ | $\infty$ | 200–500 | 200–500 | (µm) |
| AlN plate length | 150 | 150 | 150 | (µm) |
| AlN plate width | 97.68 | 97.68 | 97.68 | (µm) |
| AlN plate thickness | 1.5 | 1.5 | 1.5 | (µm) |

Figure 4-9. SEM image of one fabricated AlN LWR with the convex edge-type reflector.
of the resonator with the convex edges represents a 2.6× increase in $Q$ over that with the flat edges. Moreover, the resonator with the convex edge reflectors shows an $R_m$ of 364 Ω for and that with the flat free edges exhibits an $R_m$ of 395 Ω. Figure 4–11 compares the measured mechanical $Q$’s for the AlN LWRs using the convex free edges with various radii of curvature equal to 209.2 µm, 302.3 µm, and 493.8 µm, exhibiting their loaded $Q$’s of 3,280, 2,932, and 3,196, respectively. Obviously, unlike the capacitive-piezoelectric transducer utilizing the small air gaps to reduce electrical loss, the convex edge reflectors can considerably eliminate the tether loss and boost the $Q$ of the AlN LWR without increasing its $R_m$. The experimental results also confirm the FEA results that the convex edge reflectors can efficiently confine the mechanical energy in the resonator body and reduce the energy loss leaky through the support tethers so that the mechanical $Q$ can be significantly boosted.

However, as depicted in Fig. 4–11, the resonator with the flat edges shows a $k_{\text{eff}}^2$ of 0.35% and the resonators utilizing the biconvex edges with various radii of curvature equal to 209.2 µm, 302.3 µm, and 493.8 µm, exhibiting the $k_{\text{eff}}^2$ of 0.18%, 0.2%, and 0.24%, respectively. Clearly, the energy confinement using convex edges reduces the $k_{\text{eff}}^2$ because the side parts of the IDT do not excite the resonance mode and receive the acoustic energy as depicted in Fig. 4–8 (b).

The resonators studied herein with the convex edges nominally have the loaded $Q$’s of approximately 3,000. As a result, the $Q-k_{\text{eff}}^2$ product can be increased from 4.4 to 7.7 simply through the use of the convex edge reflectors with a larger curvature radius of 493.8 µm. However, it should be noticed that the loaded mechanical $Q$ may decrease as the radius of curvature increases significantly. The $Q$ and $k_{\text{eff}}^2$ reported herein are not optimal by far. The radius of curvature and the ratio of the AlN thickness normalized to the wavelength could be further optimized to increase the $Q-k_{\text{eff}}^2$ product. Furthermore, a
floating bottom electrode configuration which will be discussed in next section can be employed in the resonator design to improve the $Q \cdot k_{\text{eff}}^2$ product \[59\].

In contrast to those with the convex edge reflectors, as shown in Fig. 4–12, the AlN LWRs using the concave edge reflectors with various radii of curvature do not show any large resonance peak in the measured frequency responses. Apparently the suspended
concave edges disperse the acoustic waves to the support surroundings and then the degradation of the resonance peak is caused by the leakage of the mechanical energy through the support tethers.

In addition to the mechanical $Q$, the frequency-temperature characteristics of the AlN LWRs with different free edge shapes are of interest. Here, the room temperature ($25^\circ C$) is used as the reference temperature to study the frequency-temperature behavior of the resonators. As illustrated in Fig. 4–13, the AlN LWRs utilizing the flat free edges and the convex free edges with the curvature radius of 209.2 $\mu m$ exhibit their first-order TCFs of $–22.5$ ppm$/^\circ C$ and $–22.4$ ppm$/^\circ C$, respectively. These resonators show almost the same first-order TCF because they are composed of the same Pt/AlN/Pt stack and employ the $S_0$ mode. Moreover, the measured first-order TCFs are very close to the predicted values shown in Fig. 4–4, showing the theoretical model presented in section 4.2 is valid to predict the TCF of the AlN LWRs. The overall performance of the AlN LWRs with the

![Figure 4-13. Measured fractional frequency variation versus temperature of the AlN LWRs using the flat edge and the convex edge with a curvature radius of 209.2 $\mu m$.](image)

<table>
<thead>
<tr>
<th>Table 4-4. Performance of the AlN LWRs with flat and convex free edges.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Radius of curvature $R$</strong></td>
</tr>
<tr>
<td><strong>Series resonance frequency $f_s$</strong></td>
</tr>
<tr>
<td><strong>Motional resistance $R_m$</strong></td>
</tr>
<tr>
<td><strong>Effective coupling coefficient $k_{eff}^2$</strong></td>
</tr>
<tr>
<td><strong>Loaded quality factor $Q_{load}$</strong></td>
</tr>
<tr>
<td><strong>First-order TCF at $25^\circ C$</strong></td>
</tr>
</tbody>
</table>
flat and convex edge-type reflectors is summarized in Table 4–4.

4.6 High-Coupling AlN Lamb Wave Resonators

In recent years, there are a large number of long-term evolution (LTE) frequency bands that are being designated as the possibilities for the third generation (3G) and the fourth generation (4G) wireless mobile systems. For the frequency division duplex (FDD) and time division duplex (TDD) technologies, the LTE frequency bands are mostly allocated within the ultra-high-frequency (UHF) region (i.e. 0.3–3 GHz) and some LTE frequency bands have been designated with narrow bandwidths between 0.75% and 2% [59]. As illustrated in Fig. 2–7, in comparison with the Rayleigh mode showing a small \( k^2 \) of around 0.28%, the \( A_0 \) and \( S_0 \) Lamb wave modes exhibit relatively large \( k^2 \) in an AlN thin plate. Especially, for the metallized bottom surface configurations, the \( S_0 \) mode offers a large \( k^2 \) up to 3% in the AlN membrane while the AlN thickness \( h_{AlN} \) is around 0.1\( \lambda \). The desirable features of the \( S_0 \) Lamb wave mode in an AlN thin plate simultaneously enable high phase velocity, weak dispersion, and moderate \( k^2 \) for the bandpass filter design using the high-coupling LWRs at high frequencies.

However, as observed in Fig. 4–11, the AlN LWR with the Pt bottom electrode and flat edges only shows a \( k^2_{\text{eff}} \) of 0.35%, which is less than the theoretical value. Although the intrinsic \( k^2 \) is originally given for an idealized simple structure composed of uniform thin film materials, in fact the real devices are more complex: the influence of electrode thickness, electrode arrangement, and AlN thin film quality are not considered in the theoretical calculation. Except for the above possible extrinsic factors, the six IDT electrodes are not enough to offer good transduction efficiency. In addition, the parasitic capacitances might also cause the degeneration in \( k^2_{\text{eff}} \). In this section, the flat edge-type AlN LWRs utilizing the \( S_0 \) mode with various bottom surface configurations are theoretically and experimentally studied. Apparently the different bottom surface configurations of the LWRs result in distinct static capacitance \( C_0 \) characteristics in the AlN thin membrane, and their different electric field distributions would considerably affect the effective coupling coefficient \( k^2_{\text{eff}} \) of the LWRs. Moreover, in contrast to the AlN LWR without the bottom electrode, the electrode-to-resonator interface strain (i.e. electrical loss) is found to cause the degradation in the \( Q \) of the resonator with the Pt bottom electrode.

4.6.1 Static Capacitance in an AlN Membrane

Figure 4–14 shows the cross-sectional illustrations of the LWRs with open, grounded, and floating bottom surface configurations and their schematic electric field distributions in the AlN membrane. As predicted in Fig. 4–11, the theoretical electromechanical coupling coefficients \( k^2 \) of the AlN LWRs with the free and metallized bottom surface conditions can be obtained using the velocity difference approach or Green’s function, but the electromechanical coupling coefficients \( k^2 \) are identical for the grounded and
floating bottom surface conditions because the short-circuited boundary condition is considered in both configurations. Obviously this is not true for practical AlN LWRs since the parallel resonance frequency $f_p$ and effective coupling coefficient $k^2_{\text{eff}}$ are significantly influenced by the electric fields and static capacitances in the AlN thin plate. Therefore, the actual $k^2_{\text{eff}}$ for the grounded and floating bottom electrodes are different because of the distinct electric fields and static capacitances in these two configurations.

As shown in Fig. 4–5, the AlN LWR can be described using the MBVD equivalent circuit which consists of a motional $R_mL_mC_m$ branch and a static capacitance $C_0$ in shunt, which is simply formed by the capacitance between the IDT electrodes and the plate capacitance sandwiched between the top and bottom electrodes. Figure 4–15 illustrates a simple physical model which can be used to describe the capacitive feedthrough to ground in the one-port AlN LWRs and the corresponding static capacitances in their MBVD circuits for those resonators with the open, grounded, and floating bottom surface conditions [59]. As depicted in Fig. 4–15 (a), the electric potentials in the IDT finger electrodes are presumed to be $U$ and $0$, and then the static capacitance $C_{01}$ is simply equal to the in-line capacitance $C_1$ in the open bottom surface topology. For the grounded bottom surface topology shown in Fig. 4–15 (b), the lateral and vertical electric fields induce the in-line capacitance $C_1$ and the cross-field capacitance $C_2$ so the static capacitance $C_{02}$ is simply assumed to be the summation of $C_1$ and $C_2$. As for the floating bottom surface topology presented in Fig. 4–15 (c), the electric potentials in the IDT finger electrodes are equivalent to be $U$ and $0$, and the electric potential in the bottom electrode can be presumed to be $U/2$ because of the symmetric electric fields in this case. As a result, the $C_{03}$ is simply assumed to be the summation of $C_1$ and $C_2/2$ for the floating bottom surface topology.

Figure 4-14. Cross-sectional illustrations of the AlN LWRs with the open, grounded, and floating bottom surface configurations and the corresponding electric fields.
The excitation efficiency would be the same for the grounded and floating bottom surface topologies but the open bottom surface topology would have weaker excitation efficiency because the backside metallization strongly enhances the vertical electric field in the AlN thin plate. In addition, the open bottom surface topology has the smallest static capacitance $C_0$ among the three one-port resonator configurations since there is only the in-line capacitance $C_1$ existing in the AlN thin plate. The static capacitance $C_{03}$ in the floating bottom surface topology is smaller than the $C_{02}$ in the grounded bottom surface, resulting in a larger $k^2_{\text{eff}}$ for the LWR with the floating bottom electrode.

In order to verify the above physical model, as shown in Fig. 4–16, a two-dimensional (2D) FEA model in COMSOL software is used to simulate the electric potentials and electric fields in the AlN membrane for the one-port AlN LWRs with open, grounded, and floating bottom surface configurations. As shown in Fig. 4–16 (c), the electric potential in the bottom electrode is close to 0.5 V because of the symmetric electric fields in the AlN thin plate, confirming the proper assumption of the above model for the floating bottom surface configuration. Figure 4–17 illustrates the normalized static capacitances $C_n$ per IDT pair which are calculated for three bottom surface configurations using the 2D FFM COMSOL model. The $C_n$ per IDT pair over the grounded bottom electrode is relatively large among the three resonator topologies because the cross-field capacitance $C_2$ is much larger than the in-line capacitance $C_1$. While the normalized AlN thickness is close to 1, the static capacitance of the grounded bottom surface topology is close to that of the floating bottom configuration. In addition, for the AlN thickness larger than 0.42, the static capacitance of the open bottom surface topology is very close to that of the floating one since the cross-field capacitance $C_2$ is much smaller than the in-line capacitance $C_1$ [147].
The frequency spectra of the one-port AlN LWRs with the open, grounded, and floating bottom surface configurations are also computed using the COMSOL FEA software. As shown in Fig. 4–18, when the same IDT finger electrodes but different electric conditions in the bottom surfaces are employed, the 2D FEA model predicts that the resonator with the floating bottom electrode provides a 1.8 times larger \( k_{\text{eff}}^2 \) than that with the grounded bottom electrode for 11 IDT finger electrodes with 2.77 \( \mu \)m width on a 1.5-\( \mu \)m-thick AlN thin plate. The simulation results also confirm that the resonator with

![Figure 4-16](image)

Figure 4-16. Cross-sectional illustrations of the electric potentials and electric fields in the AlN thin plates for the LWRs with open, grounded, and floating bottom surface configurations.

![Figure 4-17](image)

Figure 4-17. Normalized static capacitances \( C_n \) per IDT pair in conjunction with the open, grounded, and floating bottom surface configurations.
the open bottom surface topology shows smaller transduction efficiency among the three configurations while the same IDT finger electrodes are employed. The transduction efficiency of the IDTs over the grounded and floating bottom electrodes would be identical when the same even IDT finger electrodes and acoustic loss mechanisms are considered in the simulation. The transduction efficiency ratio of the IDTs over the floating and grounded bottom electrodes is decreased to around 0.91 when the odd IDT finger electrodes are employed in the resonators. The different transduction efficiency of the odd IDT finger electrodes over the floating and grounded bottom electrodes is caused by the unsymmetrical electric fields in the AlN thin plate.

4.6.2 Experimental Results and Discussions

In order to experimentally study the effect of the electric bottom surface condition on the

Figure 4-18. Simulated admittance spectra of one-port AlN LWRs with the open, grounded, and floating bottom surface configurations using the 2D FEA model in COMSOL.

<table>
<thead>
<tr>
<th>Open</th>
<th>Grounded</th>
<th>Floating</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>IDT finger electrodes</td>
<td>11</td>
<td>11</td>
<td>11</td>
</tr>
<tr>
<td>IDT aperture</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>IDT electrode width</td>
<td>2.77</td>
<td>2.77</td>
<td>2.77</td>
</tr>
<tr>
<td>Pt top electrode thickness</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>Pt bottom electrode thickness</td>
<td>N/A</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>AlN membrane thickness</td>
<td>1.5</td>
<td>1.5</td>
<td>1.5</td>
</tr>
</tbody>
</table>
resonator performance, three AlN LWRs with the open, grounded, and floating bottom surface configurations were fabricated using the microfabrication process flow described in section 3.2. Their design parameters are summarized in Table 4–5. To diminish the experimental errors resulted from the fabrication process, the resonators were fabricated on the same wafer and placed in the vicinity. Figure 4–19 shows the SEM image of one fabricated AlN LWR with the grounded bottom electrode.

Figure 4–20 (a) compares the measured frequency spectra of one-port AlN LWRs with the open, grounded, and floating bottom surface conditions. While the same 11 IDT finger electrodes but different electric bottom configurations are employed, the AlN LWR with the open bottom surface topology exhibits the weakest transduction efficiency and the smallest $k_{\text{eff}}^2$ of 0.18% as it is predicted in the FEA simulation. The transduction efficiency and effective coupling strength of the resonator with the open bottom surface configuration can be enhanced by increasing the number of the IDT finger electrodes or the AlN membrane thickness [5]. On the other hand, the AlN LWR with the floating bottom electrode shows the highest $k_{\text{eff}}^2$ of 1.05%, presenting a 1.35× enhancement in $k_{\text{eff}}^2$ over that with the grounded bottom electrode. In addition, Figs. 4–20 (b)–(d) show the measured spectra of the AlN LWRs with the open, grounded, and floating bottom surface topologies and their six equivalent circuit parameters in the MBVD model, respectively. Clearly the resonator with the Pt bottom electrode show a lower series resonance frequency $f_s$ of around 850 MHz caused by the mass loading effect of the Pt bottom electrode. The extracted static capacitance $C_0$ in the resonators with the floating and grounded bottom electrodes are 195 fF and 355 fF, respectively. In the 2D FEA model, the simulated static capacitance ratio of the grounded bottom electrode to the floating one is approximately equal to 2 for the design parameters listed in Table 4–5. However, the measured $C_0$ ratio is equal to 1.82 because some additional parasitic capacitances occurred in the AlN thin plate and influenced the experimental $C_0$ ratio. In fact, these additional parasitic capacitances do not take the responsibility for the Lamb
wave excitation, but only decrease the parallel resonance frequency $f_p$ and consequently reduce the $k^2_{\text{eff}}$ for a given AlN plate thickness. The experimental results confirm that the floating bottom electrode efficiently reduces the static capacitance $C_0$ and enhances the effective coupling coefficient $k^2_{\text{eff}}$ in the one-port AlN LWR. Moreover, the employment of the floating bottom electrode also offers a simpler microfabrication process because the process step for opening the electrical contact via holes can be neglected.

In addition to the $k^2_{\text{eff}}$ and $C_0$, the experimental transduction efficiency of the LWRs with the grounded and floating bottom electrodes is of great interest. For this purpose, the coupling-of-modes (COM) transduction coefficient, $\alpha(\omega_0)$, which is responsible for
the excitation efficiency of the IDTs, can be introduced to compare the excitation efficiency of the IDTs over the grounded and floating bottom electrodes. The COM transduction coefficient \( \alpha(\omega_0) \) is derived as [148]

\[
\alpha(\omega_0) = \frac{Q_F(\beta)}{\Lambda_T} \sqrt{\frac{\omega_0 WT_s}{2}}, \tag{4.18}
\]

where \( \Lambda_T \) is the wavelength of transduction, \( Q_F(\beta) \) is the elemental charge density function, \( k_s=2\pi/\Lambda_T \) is the acoustic wave number, \( \omega_0 \) is the resonance angular frequency, \( W \) is the IDT aperture, and \( \Gamma_s \) is a coupling parameter which is expressed as [147], [148]

\[
\Gamma_s = \frac{k^2}{2\varepsilon_s^{(\infty)}}, \tag{4.19}
\]

where \( \varepsilon_s^{(\infty)} \) is the effective permittivity at the infinite slowness (i.e. the effective static permittivity). Moreover, the acoustic conductance \( G_a(\omega_0) \) at the resonance angular frequency \( \omega_0 \) of a reflector-less IDT with an aperture \( W \) and \( N_P \) pairs of electrodes is defined as [88], [148]

\[
G_a(\omega_0) = \omega_0 WT_s \left| Q_F(\beta) \right|^2 N_P^2. \tag{4.20}
\]

\( G_a(\omega_0) \) can also be presented as a function of the COM transduction coefficient as

\[
G_a(\omega_0) = 2\left[ \Lambda_T \alpha(\omega_0) N_P \right]^2, \tag{4.21}
\]

which further reveals the physical meaning of the COM transduction coefficient. The latter is directly related to the IDT conductance which in turn is proportional to the radiated acoustic power.

When the performance of the AlN LWRs with distinct electrically bottom surface conditions is compared, one should bear in mind that the equation (4.21) becomes more general. The acoustic conductance at the resonance frequency depends not only on the COM transduction \( \alpha(\omega_0) \) and the IDT length \( W \) but also on the acoustic energy losses since the latter determines the \( Q \)'s. Accordingly, only the comparison for the resonators with the same acoustic loss mechanisms could reveal the information about the transduction efficiency. Here the transduction efficiency of the AlN LWRs with the grounded and floating bottom surface topologies can be compared since ideally their acoustic loss mechanisms are identical. As shown in Fig. 4–21 (a), the AlN LWRs with the grounded and floating bottom electrodes show quite similar acoustic conductance characteristics and their conductance ratio is equal to 0.88, resulting in a transduction efficiency ratio of 0.94, which is very close to the theoretical efficiency ratio of 0.91, obtained from the 2D FEA model in COMSOL. As mentioned above, when computing
the transduction efficiency of the IDTs over various bottom electrodes, all remaining contributions to the conductance should be kept the same in the simulation. The different transduction efficiency for the 11 IDT finger electrodes over the grounded and floating bottom electrodes is caused by the unsymmetrical electric field in the AlN thin plate. The experimental transduction efficiency ratio is 1.01 while 12 IDT finger electrodes were employed in the resonators. The results further confirm our preliminary observation that the excitation efficiency is the same for the even IDT electrodes over the grounded and floating bottom surface topologies, whereas as shown in Fig. 4–21 (b), the larger static capacitance of the LWR with the grounded bottom electrode results in a smaller $k^2_{\text{eff}}$.

Although the bottom electrodes beneath the AlN thin film significantly improve the strength of the $k^2_{\text{eff}}$, the electrical losses deteriorate the $Q$’s of the LWRs. The resonators with the grounded and floating bottom electrodes exhibit the loaded $Q_s$ of 800 and 850, respectively, since the presence of the bottom electrodes arise uniform strain contribution over the electrode-to-resonator interface area [36],[131], [132]. On the contrary, the LWR without the bottom electrode shows a loaded $Q_s$ as high as 3,033. However, as mentioned above, the finite resistance of the electrodes and different motional resistances of the resonators would have different loading effect on the mechanical $Q_s$. In order to make further precise comparison on the mechanical $Q_s$, the electrical loading effect should be eliminated and the unloaded $Q_s$ can be calculated by the following expression

$$Q_{s,\text{unload}} = \left( \frac{R_m + R_s}{R_m} \right) Q_s. \quad (4.22)$$

The AlN LWRs with the open, grounded, and floating bottom surface conditions exhibit the unloaded $Q_s$ of 3,209, 1,107, and 1,133, respectively. The LWRs with the grounded
and floating bottom electrode exhibit the similar mechanical $Q_s$ and that with the open bottom topology shows the highest mechanical $Q_s$ among the three LWR configurations. Clearly the high stress levels in the interface area decrease the mechanical $Q_s$ of the resonator with the bottom electrode. If the electrode-to-resonator stress is minimized with optimized deposition conditions, the AlN LWR with the floating bottom electrode was demonstrated to have a loaded $Q_s$ as high as 2140 at 970 MHz [149].

Figure 4-22 shows the plot of measured fractional frequency variation for the AlN LWRs from room temperature to 100°C. As it is expected, the resonator without the

![Figure 4-22. Measured fractional frequency variation versus temperature of the AlN LWRs with the open, grounded, and floating bottom surface configurations.](image)

Table 4-6. Performance of the AlN Lamb wave resonators with various bottom surfaces.

<table>
<thead>
<tr>
<th></th>
<th>Open</th>
<th>Grounded</th>
<th>Floating</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Series resonance frequency $f_s$</td>
<td>948.1</td>
<td>850.5</td>
<td>850.3</td>
<td>(MHz)</td>
</tr>
<tr>
<td>Motional resistance $R_m$</td>
<td>516</td>
<td>78</td>
<td>90</td>
<td>(Ω)</td>
</tr>
<tr>
<td>Motional capacitance $C_m$</td>
<td>0.148</td>
<td>2.247</td>
<td>1.666</td>
<td>(fF)</td>
</tr>
<tr>
<td>Static capacitance $C_0$</td>
<td>102</td>
<td>355</td>
<td>195</td>
<td>(fF)</td>
</tr>
<tr>
<td>Effective coupling coefficient $k_{eff}^2$</td>
<td>0.18</td>
<td>0.78</td>
<td>1.05</td>
<td>(%)</td>
</tr>
<tr>
<td>Loaded series quality factor $Q_s$</td>
<td>3,033</td>
<td>800</td>
<td>850</td>
<td>–</td>
</tr>
<tr>
<td>Unloaded series quality factor $Q_s$</td>
<td>3,209</td>
<td>1,107</td>
<td>1,133</td>
<td>–</td>
</tr>
<tr>
<td>Loaded parallel quality factor $Q_p$</td>
<td>1.686</td>
<td>803</td>
<td>1,242</td>
<td>–</td>
</tr>
<tr>
<td>Figure of merit $k_{eff}^2 Q_s$</td>
<td>4.6</td>
<td>6.2</td>
<td>8.9</td>
<td>–</td>
</tr>
<tr>
<td>First-order TCF</td>
<td>–25.9</td>
<td>–27.0</td>
<td>–26.6</td>
<td>(ppm/°C)</td>
</tr>
</tbody>
</table>
bottom electrode shows a smaller first-order TCF of $-25.9$ ppm/°C because the Pt bottom electrode exhibits a more negative TCF than AlN and decreases the overall TCF accordingly. The resonators with the grounded and floating bottom electrodes show the first-order TCF of $-27.0$ ppm/°C and $-26.6$ ppm/°C, respectively. Table 4–6 compares the overall performance of the AlN LWRs with the open, grounded, and floating bottom surface configurations. All in all, the experimental results are in qualitative agreement with the simulated predictions from the 2D FEA model. The AlN LWR with the floating bottom electrode exhibits the highest figure of merit ($k_{eff}^2 Q_s$) among the three resonator topologies. It should be noted that the $Q_s$ and $k_{eff}^2$ reported in this work are not optimal by far. Better resonator design, optimized microfabrication process, and well-controlled thin film stress can improve the figure of merit to a large extent.

### 4.7 Conclusions

In this chapter, the effects of the bottom electrode layer on the acoustic characteristics of the $S_0$ Lamb wave mode propagating in an AlN thin plate is theoretically investigated. The energy losses caused by the tether loss, electrical loss, and mode conversion loss are considered the dominant loss mechanisms in the AlN LWRs. For the fundamental Lamb wave modes, the mode conversion loss induced by reflection upon the suspended free edges can be significantly suppressed in the acoustically thin plate due to their great difference in mode symmetry, and the $S_0$ Lamb wave mode does not exhibit energy loss markedly. For the first time, the convex edge reflector was employed in the lateral Lamb wave propagation directions and demonstrated to successfully confine the acoustic energy in the resonant body. The 491.8-MHz LWR on the 1.5-µm-thick AlN thin plate utilizing the suspended convex edges yields a loaded $Q$ as high as 3,280, representing a 2.6x enhancement in $Q$ over a 517.9-MHz LWR with flat free edges. The experimental results confirm the FEA simulations that the suspended convex edges can efficiently reduce the tether loss, and accordingly the $Q$ of the AlN LWR can be remarkably boosted by using the convex edge reflectors.

Moreover, the one-port AlN LWRs with the electrically open, grounded, and floating bottom surface configurations are theoretically analyzed and experimentally investigated. The employment of the floating bottom electrode results in a lower static capacitance $C_0$ than the grounded bottom electrode in the AlN membrane and accordingly enhances the effective coupling coefficient $k_{eff}^2$. Based on the identical IDT design over the 1.5-µm-thick AlN thin plate, one-port AlN LWRs with the open, grounded, and floating bottom surface conditions are fabricated and their performance are compared herein. Clearly, without sacrificing the transducer transduction efficiency, the floating bottom electrode simultaneously offers a larger $k_{eff}^2$, an easier microfabrication process, and a higher figure of merit than the grounded bottom electrode. Based on the reported results herein, the AlN LWR with the floating bottom electrode showing a low motional resistance and a high figure of merit is suitable for synthesizing narrowband filters [150], [151] and that with the open bottom surface configuration providing a high loaded $Q_s$ is well suited for the oscillator and sensor applications.
Chapter 5

Temperature-Compensated AlN/SiO$_2$ Lamb Wave Resonators at Room Temperature and High Temperatures

Given that AlN becomes mechanically soft with an increasing temperature due to its negative TCEs, micromechanical AlN resonators usually show a first-order TCF of approximately $-25\ \text{ppm/}^\circ\text{C}$. Amorphous SiO$_2$ is well-known for its positive temperature dependence of elastic constants [64] and a passive thermal compensation technique using SiO$_2$ has been widely applied to different types of piezoelectric resonators [61], [65]–[69]. In this chapter, the TCF characteristics of the QS$_0$ mode in an AlN/SiO$_2$ composite plate are theoretical analyzed. A zero first-order TCF can be achieved in the AlN/SiO$_2$ composite plate using an appropriate thickness ratio of AlN to SiO$_2$ at room temperature. In addition, from the simulated results, near zero first-order TCFs over a wide frequency range from 100 MHz to 1000 MHz can be achieved simultaneously based on the same AlN/SiO$_2$ stack while the AlN layer is as thin as 250 nm. A temperature-compensated LWR utilizing the QS$_0$ Lamb wave mode was successfully fabricated on the AlN/SiO$_2$ plate composed of the 1-µm-thick AlN film and 0.83-µm-thick SiO$_2$ layer. An AlN LWR operating at 711 MHz is completely compensated at its turnover temperature, 18.05°C, and exhibits a zero first-order TCF, a small second-order TCF of $-21.5\ \text{ppb/}^\circ\text{C}^2$, a low motional resistance of 150 Ω, an effective coupling coefficient $k^2_{\text{eff}}$ of 0.56%, and a quality factor $Q$ of 980. Moreover, a novel temperature compensation approach for the AlN LWR operating at high temperature is also investigated herein. Based on different thickness ratios of the AlN thin film to the SiO$_2$ layer, complete thermal compensation of the AlN/SiO$_2$ LWRs was achieved at 214°C, 430°C, and 542°C, respectively.

5.1 Temperature-Compensated Lamb Wave Resonators at Room Temperature

In this dissertation, for the first time, a novel edge-type AlN/SiO$_2$ LWR with a zero first-order TCF is proposed. Fig. 5–1 illustrates the zero first-order TCF LWR consisting of
one IDT, a metallized interface between the AlN and SiO$_2$ layers and two flat free edges at both sides of the AlN/SiO$_2$ composite plate. The metallized interface can improve the $k^2$ of the QS$_0$ mode in the AlN/SiO$_2$ composite plate as depicted in Fig. 2–13.

5.1.1 TCF of AlN/SiO$_2$ Lamb Wave Resonators

The TCF of the AlN/SiO$_2$ composite membrane can be analyzed utilizing the same computation method as previously used for determining the TCF of the AlN thin plate. The only difference is the temperature dependent implementation of all the material parameters involved in the simulation. The temperature dependence of the phase velocity was first calculated for the QS$_0$ Lamb wave mode in an AlN/SiO$_2$ composite plate and then the effective thermal expansion in propagation direction of the stack is subtracted from the velocity dependence. As illustrated in Fig. 5–2, an effective thermal expansion

Figure 5-1. Illustration of an AlN/SiO$_2$ LWR utilizing the flat edge-type reflector.

Figure 5-2. The effective thermal expansion experienced at the neutral plane.
coefficient for estimating the elongation along the Lamb wave propagation direction is required for computing the TCF of the composite structures. The effective thermal expansion coefficient of an arbitrary stack of multiple layers is computed from the thermal expansion of the neutral plane in the stack [114]. The effective thermal expansion coefficient $\alpha_{\text{eff}}$ for a stack of $i$ layers is then given as

$$\alpha_{\text{eff}} = \frac{\sum_{i=1}^{n} E_i t_i \alpha_i}{\sum_{i=1}^{n} E_i t_i},$$

(5.1)

where $E_i$ is the Young’s modulus of $i$th layer, $t_i$ is the thickness of $i$th layer, and $\alpha_i$ is the thermal expansion coefficient of $i$th layer, respectively. The temperature dependence of mass density $\rho(T)$ can be defined as

$$\rho(T) = \rho(T_0) \left[ 1 - (\alpha_{\text{eff}} + \alpha_{\text{eff}} + \alpha_z) \Delta T \right],$$

(5.2)

where $\alpha_{\text{eff}}$ and $\alpha_{\text{eff}}$ are the effective thermal expansion coefficients of the composite layers along the $x$- and $y$-directions, respectively, which are assumed to be identical in this work. Neglecting electrode mass loading effect, the TCF of the LWR on a composite plate is written as [114]

$$\text{TCF}_{\text{LWR}} = \frac{1}{\nu_{\text{LW}}} \frac{\partial \nu_{\text{LW}}}{\partial T} = \alpha_{\text{eff}},$$

(5.3)

Figure 5-3. Simulated TCF dispersion of the AlN/SiO$_2$ LWRs utilizing the QS$_0$ mode.
where $v_{LW}$ is the phase velocity of the Lamb wave mode propagating in the composite plate and $\alpha_{\text{eff}}$ corresponds to the effective thermal expansion coefficient along the propagation direction (i.e. $x$-direction herein).

On the AlN/SiO$_2$ composite structures, the first-order TCF of the Q$S_0$ Lamb wave mode with various $h_{\text{AlN}}/\lambda$ of 0.05, 0.1, 0.15, and 0.2 are theoretically analyzed as shown in Fig. 5–3. The analysis shows that the first-order TCF of the Q$S_0$ Lamb wave mode in the AlN/SiO$_2$ composite membrane has a dispersive characteristic. In other words, the first-order TCF is a function of the relative SiO$_2$ thicknesses for different AlN thicknesses [114], [152], [153]. In order to achieve a zero first-order TCF, an appropriate thickness ratio of the SiO$_2$ layer to the AlN film is required and the ratio varies with the wavelength $\lambda$ and the operating frequency as shown in Fig. 5–4. Considering the electromechanical coupling strength, as predicted in Fig. 2–14, the type D device utilizing the Q$S_0$ Lamb wave mode exhibits a maximum intrinsic $k^2$ while the $h_{\text{AlN}}$ is around 0.1$\lambda$. Therefore, based on the simulated prediction, the AlN and SiO$_2$ thicknesses are selected as $0.1\lambda$ and $0.06\lambda$, respectively, to obtain a zero first-order TCF and a large $k^2$ simultaneously at room temperature.

The first-order TCF of the composite AlN/SiO$_2$ LWRs with the AlN thicknesses of 0.125 $\mu$m, 0.25 $\mu$m, 0.5 $\mu$m, and 1 $\mu$m are shown in Fig. 5–5. The lower dispersion for a very thin AlN plate makes it possible to achieve a very small first-order TCF over the entire frequency range from 100 MHz to 1000 MHz. A composite plate composed of a 1-$\mu$m-thick AlN thin film and a 0.72-$\mu$m-thick SiO$_2$ layer shows first-order TCFs varying from −2.45 to −13.86 ppm/°C over the entire frequency range. On the contrary, a Lamb wave device based on a 0.25-$\mu$m-thick AlN thin film and a 0.2-$\mu$m-thick SiO$_2$ layer leads to nearly zero first-order TCFs over the entire frequency range. The spurting deposition of such an ultrathin AlN film with strong piezoelectric response is practical. A 200-nm-thick AlN thin film has been successfully deposited on highly textured Mo (110) bottom

![Figure 5-4. Required thickness ratios for the zero-TCF AlN/SiO$_2$ LWRs operating at different frequencies.](image-url)
101

electrodes and shows a rocking curve FWHM value of 1.8°, showing the possibility to achieve the complete temperature compensation over a wide frequency range by using ultrathin AlN films [100].

5.1.2 Experimental Results and Discussions

For the temperature-compensated AlN/SiO₂ LWRs, Al was selected as the interfacial metallization material since Al only has slight loading effect on the phase velocity and intrinsic coupling coefficient as illustrated in Figs. 4–2 and 4–3. Micromechanical LWRs

<table>
<thead>
<tr>
<th>SiO₂ thickness, $h_{\text{SiO}_2}$ (µm)</th>
<th>First-order TCF (ppm/°C)</th>
</tr>
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<tbody>
<tr>
<td>0.125 µm</td>
<td>125 MHz</td>
</tr>
<tr>
<td>0.25 µm</td>
<td>250 MHz</td>
</tr>
<tr>
<td>0.5 µm</td>
<td>500 MHz</td>
</tr>
<tr>
<td>1.0 µm</td>
<td>750 MHz</td>
</tr>
<tr>
<td></td>
<td>1000 MHz</td>
</tr>
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Table 5-1. Dimensions of the thermally stable AlN/SiO₂ LWRs at room temperature.

<table>
<thead>
<tr>
<th></th>
<th>Design 1</th>
<th>Design 2</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top electrode finger number</td>
<td>13</td>
<td>13</td>
<td>–</td>
</tr>
<tr>
<td>Aperture W</td>
<td>125</td>
<td>125</td>
<td>(µm)</td>
</tr>
<tr>
<td>Electrode finger width $w$</td>
<td>4.44</td>
<td>2.76</td>
<td>(µm)</td>
</tr>
<tr>
<td>Wavelength $\lambda$</td>
<td>17.76</td>
<td>11.04</td>
<td>(µm)</td>
</tr>
<tr>
<td>Metallization ratio $\eta$</td>
<td>0.5</td>
<td>0.5</td>
<td>–</td>
</tr>
<tr>
<td>Top Al electrode thickness</td>
<td>150</td>
<td>150</td>
<td>(nm)</td>
</tr>
<tr>
<td>Bottom Al electrode thickness</td>
<td>150</td>
<td>150</td>
<td>(nm)</td>
</tr>
<tr>
<td>Normalized AlN thickness $h_{\text{AlN}}/\lambda$</td>
<td>0.056</td>
<td>0.091</td>
<td>–</td>
</tr>
<tr>
<td>Normalized SiO₂ thickness $h_{\text{SiO}_2}/\lambda$</td>
<td>0.047</td>
<td>0.075</td>
<td>–</td>
</tr>
</tbody>
</table>

Figure 5-5. SiO₂ thickness and frequency dependence of the first-order TCFs for four AlN thicknesses.
were fabricated on an AlN/SiO$_2$ multilayer plate composed of 1-µm-thick AlN and 0.83-µm-thick SiO$_2$ using the microfabrication process flow described in section 3.3. Their design parameters are summarized in Table 5–1. Figure 5–6 shows the SEM image of the fabricated AlN/SiO$_2$ LWR (design 2 device in Table 5–1). Figure 5–7 shows a cross-sectional SEM image of the AlN/SiO$_2$ composite plate with 1-µm-thick AlN and 0.83-µm-thick SiO$_2$ which was used for the temperature-compensated LWRs in this study.

The fabricated temperature-compensated AlN/SiO$_2$ LWRs were tested in a vacuum probe system (Suss MicroTec® PMC150) that allows probing of chuck-mounted wafers.

Figure 5-6. SEM image of the temperature-compensated AlN/SiO$_2$ LWR at room temperature (design 2 device in Table 5-1).

Figure 5-7. Cross-sectional SEM image of the AlN/SiO$_2$ composite membrane.
while they are cooled via liquid helium and heated by electric heating elements (on the chuck). A feedback controlled heating unit can provide a precise control of the chuck temperature during measurement. $S_{11}$ parameters for the resonators were extracted using an Agilent E5071B network analyzer. In order to determine the frequency-temperature characteristic of the AlN/SiO$_2$ LWRs, resonators were measured in the temperature range from –55°C to 125°C (military grade). The chuck temperature was varied in a 5°C step with a temperature stabilization time of 10 minutes before the measurement at each temperature, and the $S_{11}$ parameters of the resonator were measured five times at each 5°C step. Before the measurements were taken, the devices were temperature cycled over the full temperature range five times to eliminate observed hysteresis [153]. The quality factor of the series resonance frequency $Q_s$ was extracted using the $f_s$ divided by the 3dB BW from the admittance plot, and the six equivalent circuit parameters were determined by fitting to the measured results with the MBVD equivalent circuit.

In order to better understand the effect of the normalized thickness of each layer on the frequency-temperature behavior, two resonator designs with different wavelengths were compared, and their detailed dimensions are given in Table 5–1. As shown in Fig. 5–8, the design 1 resonator has an $f_s$ of 460 MHz, an $R_m$ of 107 Ω, a $k^2_{\text{eff}}$ of 0.33%, and a $Q_s$ of 1,532, and the design 2 resonator shows an $f_s$ of 711 MHz, an $R_m$ of 150 Ω, a $k^2_{\text{eff}}$ of 0.56%, and a $Q_s$ of 980. Some spurious modes at around 900 MHz for the design 1 resonator might be the high-order Lamb wave modes propagating in the AlN/SiO$_2$ thin plate. For the design 2 resonator, there is no spurious mode over a 1 GHz frequency range which is excellent for oscillator and filter applications.

As shown in Table 5–1, the wavelength of the design 2 resonator was 11.04 µm, and the measured resonance frequency is 711 MHz, so the measured Lamb wave velocity is roughly equal to 7,850 m/s. This measured value is close to the theoretical phase velocity of the $S_0$ mode, 8,435 m/s, for the $h_{\text{AlN}}$ and $h_{\text{SiO}_2}$ equal to 0.091$\lambda$ and 0.075$\lambda$, respectively.

![Figure 5-8. Measured broadband frequency spectrums of the two AlN/SiO$_2$ LWRs.](image-url)
If the 150-nm-thick Al bottom electrode \((h_{\text{Al}}/\lambda = 0.0136)\) were taken into account in the simulation, the theoretical phase velocity would be reduced to 8,142 m/s. The mismatch between theoretical and the experimental velocities of the \(S_0\) mode might be caused from the neglect of IDT and the inaccuracy of the AlN material constants in the simulation.

Figure 5–9 shows the close-up view of the frequency spectrums of the two LWRs and their MBVD equivalent circuit model fitting which is used for extracting the 6 equivalent circuit parameters. From the experimental results, we observe that the design 1 and 2 resonators show low effective coupling coefficients of 0.33% and 0.56%, respectively, which are less than the expected values. The electromechanical coupling coefficient is
originally given for an idealized simple structure composed of uniform thin film materials. In fact, the real devices are more complex: the influence of the electrode metallization, the electrode thickness, and the AlN thin film quality are not considered in the theoretical calculation. The intrinsic electromechanical coupling $k^2$ calculated using the equation (2.28) overestimates the effective electromechanical coupling $k^2_{eff}$ excited by the interdigital transducer [154]. In addition, as shown in Fig. 5–9 (b), a large electrical capacitance $C_0$ of 488.9 fF is observed from the MBVD equivalent circuit. The electrical capacitance, resulted from a static capacitance of 372.8 fF and an external parasitic capacitance of 116.1 fF, also reduces the effective coupling coefficient $k^2_{eff}$. The large capacitance can be reduced using the floating bottom electrode to increase the $k^2_{eff}$.

Furthermore, the AlN thin film has an FWHM value of 1.77° which indicates less than the perfect thin film quality. The combination of these phenomena is suspected to cause the low effective electromechanical coupling coefficients in the fabricated devices.

Figure 5–10 shows the plot of measured fractional frequency variation for the two design resonators in Table 3–3 over a wide temperature range from –55°C to 125°C. It should be noted that the total fractional frequency variation of the design 2 resonator is less than 250 ppm over the temperature range of 180°C and completely compensated at around room temperature. In addition, the temperature-dependent fractional frequency variation of the two LWRs shows a quadratic function of temperature since their linear TCF part was significantly reduced by the SiO$_2$ layer. As pointed out in Fig. 5–3, the first-order TCF is dispersive with the relative AlN and SiO$_2$ thicknesses. That is to say, the thickness ratio of AlN to SiO$_2$ determines the first-order TCF of the whole stacked structure. As a result, the first-order TCF of the design 2 resonator is almost cancelled out with an appropriate thickness ratio of SiO$_2$ to AlN.

As shown in Fig. 5–11, a quadratic polynomial is adopted to fit the experimental results for the design 1 resonator, which shows a first-order TCF of –7.61 ppm/°C and a

![Figure 5-10. Measured fractional frequency variation versus temperature of the two AlN/SiO$_2$ LWRs.](image-url)
second-order TCF of $-15.7$ ppb/°C$^2$ at room temperature, 25°C. The first-order TCF of the design 1 resonator is only reduced to $-7.61$ ppm/°C because the thickness ratio of AlN to SiO$_2$ is not correct for achieving the zero first-order TCF compensation at room temperature. Although the TCF of the design 1 resonator includes a sum of the first-, second-, and even higher-order terms, clearly the residual first-order TCF dominates its temperature-dependent fractional frequency variation.

In contrast, with a proper combination of AlN thin film and SiO$_2$ layer, the first-order TCF of the design 2 resonator is almost zero at room temperature so that the second-order
term dominates its characteristic of temperature-dependent fractional frequency variation. The experimental result shows a first-order TCF of –0.31 ppm/°C and a second-order TCF of –21.5 ppb/°C² at room temperature as depicted in Fig. 5–12. The fractional frequency variation of the resonator exhibits a temperature-dependent quadratic function with a turnover temperature \( T_o \) at 18.05°C. If room temperature is used as the reference temperature, the fractional frequency variation can be expressed as

\[
\frac{f(T) - f(25)}{f(25)} = -0.31 \times 10^{-6} \times (T - 25) - 21.5 \times 10^{-9} \times (T - 25)^2
\]

(5.4)

The turnover temperature \( T_o \) can be used as the reference temperature and the first-order TCF becomes zero at its turnover temperature so the fractional frequency variation can be expressed as

\[
\frac{f(T) - f(T_o)}{f(T_o)} = -21.5 \times 10^{-9} \times (T - T_o)^2
\]

(5.5)

The overall performance of the two AlN/SiO₂ LWRs is summarized in Table 5–2. The frequency-temperature stability of the design 2 resonator is also compared with that of the AT-cut and BT-cut quartz resonators as well as the watch-grade quartz tuning fork in a temperature range from –40°C to 85°C (industrial grade). As shown in Fig. 5–13, the performance of the design 2 resonator is only worse than the AT-cut quartz since it has both of zero first- and second- order TCFs. The second-order TCF of the AlN/SiO₂ LWR can be further reduced by using a metal with positive second-order TCEs as the bottom electrode metal, such as Mo [67].

In the case of the design 2 resonator, the excellent temperature compensation was achieved using 0.83-µm-thick SiO₂ and 1-µm-thick AlN layers, and the first-order TCF is successfully reduced to –0.31 ppm/°C at room temperature. However, the experimental results do not show good agreement with the theoretical predictions in Fig. 5–3. The slight difference between the experimental and theoretical results is likely due to the assumption of infinitely thin bottom electrodes and the neglect of IDT thickness in the simulation. As shown in Fig. 5–14, the dashed line represents the theoretical first-order

<table>
<thead>
<tr>
<th>Design 1</th>
<th>Design 2</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Series resonance frequency ( f_s )</td>
<td>460</td>
<td>711</td>
</tr>
<tr>
<td>Motional resistance ( R_m )</td>
<td>107</td>
<td>150</td>
</tr>
<tr>
<td>Effective coupling coefficient ( k^2_{\text{eff}} )</td>
<td>0.33</td>
<td>0.56</td>
</tr>
<tr>
<td>Series quality factor ( Q_s )</td>
<td>1,532</td>
<td>980</td>
</tr>
<tr>
<td>First-order TCF at 25°C</td>
<td>–7.61</td>
<td>–0.31</td>
</tr>
<tr>
<td>Second-order TCF at 25°C</td>
<td>–15.7</td>
<td>–21.5</td>
</tr>
</tbody>
</table>
TCF of the design 2 resonator when the Al bottom electrode is assumed to be infinitely thin in the metallized interface; in contrast, the solid line represents the theoretical first-order TCF while the 150-nm-thick Al bottom electrode is considered in the metallized interface, and the red dot represents the experimental result. As is shown in Table 4–2, Al has larger temperature coefficients than AlN and thermal expansion coefficients than AlN and SiO$_2$, and its thickness is comparable to the thicknesses of the AlN and SiO$_2$ layers used in this work. As a result, the theoretical first-order TCF of the design 2 resonator decreases from 9.62 to –11.2 ppm/°C when the 150-nm-thick Al bottom electrode is taken into account in the simulation. As depicted in Fig. 5–14, the experimental result lies between these two extremes.

There are several sources of uncertainty in the simulation. First, the accuracy of the first-order TCF prediction heavily relies on the accuracy of the material property data, in particular the TCEs of the materials used in the simulation. At least three different sets of the temperature coefficients of stiffness for the AlN thin film have been published and compared [155]. The low-temperature oxide layer is used as the thermal compensating material in this experiment but the material properties of bulk fused silica are used in the simulation due to the lack of reliable temperature coefficient data for the SiO$_2$ thin film. Furthermore, all of the thin films have residual stresses of several hundred MPa after deposition, which can affect the first-order TCF variation to a great extent [155]. Finally, although the two resonators were fabricated on the same wafer, the thin film depositions (AlN, Al, and SiO$_2$) were not ideally uniform across the wafer and the uncertainties in film thicknesses influence the accuracy of the predicted TCFs. In this study, the non-uniformity of the Al film thickness was about 3%, the non-uniformity of the AlN film was about 1%, and the non-uniformity of SiO$_2$ film was about 6%. The worst cases for the uncertainties in the simulated first-order TCF (–11.2 ppm/°C) caused by the film non-
uniformity are –15.8% and +14.2%, respectively. Despite all the sources of uncertainty, we are encouraged that the experimental results fall within the range of performance predicted by the model and it presents a useful tool for designing zero TCF LWRs. In the future, more accurate temperature coefficients of elasticity and residual stresses in thin films are needed to be introduced to the theoretical simulation for a better theoretical prediction of the TCF of the AlN/SiO\textsubscript{2} LWR.

5.2 Thermally Stable Lamb Wave Resonators at High Temperatures

Piezoelectric micromechanical resonators operating at high temperatures have gained great interest in various industries, including automotive, aerospace, aircraft, gas and petroleum exploration, and power electronics. It is well known that quartz is the most widely used piezoelectric material for resonators and sensors due to its chemical inertness and excellent thermal stability at room temperature, but quartz for frequency control, timing, or sensing applications at high temperatures is limited due to the phase transition from trigonal \(\alpha\)-quartz to hexagonal \(\beta\)-quartz at nearly 573°C. This transition causes discontinuities in the material properties and restricts the use of quartz to the temperatures below 350°C [156]. Therefore, other piezoelectric materials for the high-temperature resonators are of great interest, such as gallium orthophosphate (GaPO\textsubscript{4}), langatate (LGT), LGS, and AlN [156]–[159].

In addition to operation at high temperatures, maintaining the frequency-temperature stability of the piezoelectric MEMS resonators in the harsh environment is essential for high temperature applications. For piezoelectric single-crystal materials, different crystal
cuts and wave propagation directions can make acoustic devices thermally compensated at different temperatures [159], [160]. Recently, SAW devices based on LGT have been demonstrated to be temperature compensated at different temperatures by varying the SAW propagation directions [159]. For piezoelectric thin films, AlN is an interesting material for the high temperature applications because it can maintain its piezoelectric properties up to 1,150°C. In addition, AlN thin films do not exhibit phase transitions on heating from room temperature up to the melting point which exceeds 2,000°C in a nitrogen atmosphere [156]. Multiple research efforts are ongoing to demonstrate AlN-based piezoelectric sensors and resonators for high temperature applications [161], [162]. A challenge to achieving the good frequency-temperature stability at high temperatures requires a reliable temperature compensation technique for the piezoelectric devices.

5.2.1 Temperature Compensation of Lamb Wave Resonators at High Temperatures

The temperature compensation of the piezoelectric resonators at high temperatures means their turnover temperatures (TCF = 0) are designed at high temperatures, enabling them to be temperature-insensitive at high temperatures [163], [164]. Figure 5–15 illustrates the frequency-temperature characteristics of the SAW delay-line device based on the LGT substrate with a cut orientation (90°, 23°, 0°). The SAW device shows its turnover temperature $T_o$ at around 280°C and intriguingly it exhibits a positive first-order TCF at room temperature. In general, most materials exhibit negative second-order TCE and TCF [163]. If one resonator shows a positive first-order TCF at room temperature, the positive temperature-induced frequency variations would be decreased due to its negative second-order TCF when the temperature is higher than room temperature. While the operation temperature is increased over a certain value, the second-order TCF dominates

Figure 5-15. Frequency-temperature characteristics of one SAW device on LGT with an orientation (90°, 23°, 0°) [159].
the temperature-induced frequency variations, becoming negative at high temperatures. In other words, as shown in Fig. 5–15, the positive first-order and negative second-order TCFs at room temperature would locate the turnover temperature at high temperatures.

The temperature compensation technique utilizing the SiO$_2$ layer for the AlN LWRs has been theoretically analyzed and experimentally demonstrated at room temperature as discussed in section 5.1. The thermally stable AlN/SiO$_2$ LWR at high temperatures has the same physical structure as the resonator illustrated in Fig. 5–1. In the temperature-compensated AlN/SiO$_2$ LWRs at room temperature, as presented in the previous section, Al is used as the metal material for the bottom electrode and IDTs. However, the resonators have to withstand the high temperature operation up to 600°C so Al is not preferred in this case because of its low melting point at 660°C. In order to enable the AlN/SiO$_2$ resonators operating at high temperatures, Pt was selected as the metallization material for the bottom electrode and IDT fingers since Pt has a melting point at high temperature of 1,768°C.

As illustrated in Fig. 5–3, the first-order TCFs of the AlN/SiO$_2$ LWRs can be intentionally designed to be positive at room temperature using a larger SiO$_2$/AlN ratio to make the turnover temperature located at high temperatures. This design concept is very similar to the SAW devices on the LGT substrate for the high temperature compensation [159]. In order to investigate the intrinsic characteristics of the AlN LWRs operating at high temperatures, four different designs of the resonators were compared in this section with their geometric dimensions given in Table 5–3. Design 3 resonator has no SiO$_2$ layer beneath the AlN thin film so it would not be thermally stable. According to the first-order TCF simulation results in Fig. 5–3, a thicker SiO$_2$ layer can result in a more positive first-order TCF for a given wavelength and a given normalized AlN thickness $h_{AlN}/\lambda$. As a result, design 4 and 5 resonators have the same 1-μm-thick AlN thin film and a wavelength of 11.08 μm but 1-μm-thick and 1.26-μm-thick SiO$_2$ layer thicknesses, respectively, for comparison. The design 6 resonator also has 1-μm-thick AlN thin film and 1.26-μm-thick SiO$_2$ layer but the narrower IDT finger width and pitch (i.e. wavelength) among all the designed resonators for achieving larger $h_{AlN}/\lambda$ and $h_{SiO_2}/\lambda$.

Table 5-3. Dimensions of the thermally stable AlN/SiO$_2$ LWRs at high temperatures.

<table>
<thead>
<tr>
<th></th>
<th>Design 3</th>
<th>Design 4</th>
<th>Design 5</th>
<th>Design 6</th>
<th>Units</th>
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<td>13</td>
<td>13</td>
<td>7</td>
<td>13</td>
<td>–</td>
</tr>
<tr>
<td>Aperture W</td>
<td>125</td>
<td>125</td>
<td>100</td>
<td>125</td>
<td>(μm)</td>
</tr>
<tr>
<td>Electrode finger width w</td>
<td>2.77</td>
<td>2.77</td>
<td>2.77</td>
<td>2.21</td>
<td>(μm)</td>
</tr>
<tr>
<td>Wavelength λ</td>
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<td>11.08</td>
<td>11.08</td>
<td>8.84</td>
<td>(μm)</td>
</tr>
<tr>
<td>Metallization ratio η</td>
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<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>–</td>
</tr>
<tr>
<td>Top Pt electrode thickness</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>(nm)</td>
</tr>
<tr>
<td>Bottom Pt electrode thickness</td>
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<td>100</td>
<td>100</td>
<td>100</td>
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<tr>
<td>AlN thickness $h_{AlN}$</td>
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<tr>
<td>SiO$<em>2$ thickness $h</em>{SiO_2}$</td>
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<td>1</td>
<td>1.26</td>
<td>1.26</td>
<td>(μm)</td>
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</table>
5.2.2 Experimental Results and Discussions

The thermally compensated LWRs at high temperatures were fabricated on the AlN/SiO$_2$ multilayer plate using the fabrication process flow described in section 3.3. Figure 5–16 presents the SEM image of the fabricated AlN/SiO$_2$ LWR (design 5 device in Table 5–3). Figure 5–17 shows the cross-sectional SEM image of the AlN/SiO$_2$ membrane composed of 1-µm-thick AlN and 1.26-µm-thick SiO$_2$, used for the high temperature compensation of the LWRs.

Figure 5-16. SEM image of the thermally stable AlN/SiO$_2$ LWR at high temperatures (design 5 device).

Figure 5-17. Cross-sectional SEM image of the AlN/SiO$_2$ composite layer used for the high temperature compensation of the LWRs.
Figure 5–18 illustrates a high temperature measurement setup which was constructed to locally heat the resonators in an ambient condition. The chip was attached to a thermal insulating Fiberfrax substrate by using a ceramic adhesive (Contronics 940LE), which can withstand the high temperatures up to 1,370°C. A hole, allowing access to the backside of the MEMS chip, was machined into the Fiberfrax substrate. The test resonators were wire-bonded to a printed circuit board (PCB) for connection to the SMA (SubMiniature version A) connectors as well as the calibrated coaxial cable. Gold (Au) wires were used as the bonding wire material for high temperature testing purposes. A local heating temperature up to 982°C can be achieved using an infrared lamp (Research Inc. SpotIR M4150). The testing chip needs to be placed at the focal point of the infrared lamp for maximum heat intensity. Two thermocouples were attached directly to the chip for real-time monitoring the temperature on the resonators and to the PCB for avoiding overheating the board which withstands the temperatures around 200°C.

To determine the TCF of the AlN/SiO$_2$ LWRs at high temperature, the resonators were measured in the temperature range from 25°C to 600°C. The temperature was varied in 20°C steps with the 5 minutes of temperature stabilization time before each measurement. $S_{11}$ parameters for the resonators were extracted with a network analyzer (Agilent E5071B). To reduce the undesired influence on the TCFs due to measurement error, $S_{11}$ parameters were measured five times at each 20°C step. Before measurement characterization, the resonators were temperature cycled over the full temperature range several times to eliminate observed hysteresis [163], [164].

Figure 5–19 shows the plot of the measured fractional frequency variation versus temperature for the four designed resonators. As expected, the design 3 device exhibits a large fractional frequency variation which shows an approximate linear function of temperature and a first-order TCF of $-28.14$ ppm/$^\circ$C. In contrast to the design 3 device, the other three LWRs exhibit their turnover temperatures at 214°C, 430°C, and 542°C, respectively, at which their series resonance frequencies are insensitive to the temperature.
changes. The fractional frequency variations in these three temperature-compensated AlN/SiO$_2$ LWRs show a strong quadratic function of temperature. Figure 5–20 details the quadratic polynomial adopted to fit the experimental results of the four resonators.

Table 5–4 compares the simulated and measured first-order TCF values of the four designed resonators. All the experimental first-order TCF are smaller than the predicted values. The mismatch between the theoretical and measured TCF values is likely caused by the neglect of the bottom electrode and the IDTs in the theoretical calculation [153], [165]. The residual stresses of the thin films also result in remarkable changes in their TCFs [155]. In addition, the accuracy of the first-order TCF prediction heavily relies on the accuracy of the thermal property data of each material. However, the thermal data of the material properties at high temperatures might differ considerably from those at room temperature.

**Table 5-4. Performance of the temperature-compensated AlN/SiO$_2$ LWRs at high temperatures.**

<table>
<thead>
<tr>
<th></th>
<th>Design 3</th>
<th>Design 4</th>
<th>Design 5</th>
<th>Design 6</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normalized AlN thickness $h_{_{\text{AlN}}}/\lambda$</td>
<td>0.135</td>
<td>0.09</td>
<td>0.09</td>
<td>0.113</td>
<td>–</td>
</tr>
<tr>
<td>Normalized SiO$<em>2$ thickness $h</em>{_{\text{SiO}_2}}/\lambda$</td>
<td>–</td>
<td>0.09</td>
<td>0.114</td>
<td>0.143</td>
<td>–</td>
</tr>
<tr>
<td>$f_s$ at room temperature</td>
<td>861.6</td>
<td>710.3</td>
<td>677.7</td>
<td>835</td>
<td>(MHz)</td>
</tr>
<tr>
<td>Simulated first-order TCF</td>
<td>–21.1</td>
<td>18.95</td>
<td>31.7</td>
<td>43.38</td>
<td>(ppm/°C)</td>
</tr>
<tr>
<td>Measured first-order TCF</td>
<td>–28.14</td>
<td>9.63</td>
<td>22.19</td>
<td>35.73</td>
<td>(ppm/°C)</td>
</tr>
<tr>
<td>Measured second-order TCF</td>
<td>–9.62</td>
<td>–22.58</td>
<td>–25.81</td>
<td>–32.98</td>
<td>(ppb/°C$^2$)</td>
</tr>
<tr>
<td>Turnover temperature $T_o$</td>
<td>–</td>
<td>214</td>
<td>430</td>
<td>542</td>
<td>(°C)</td>
</tr>
</tbody>
</table>
Moreover, it should be noted that the second-order TCF becomes more pronounced for a thicker SiO$_2$ layer. The experimental data and other reported results [166] suggest that the second-order TCE of SiO$_2$ is negative even though the first-order TCE is positive. In addition, it is clear that the turnover temperature depends heavily on the first-order and second-order TCE data of the materials used in the composite plates. Therefore, it is difficult to predict the precise position of the turnover temperature because reliable TCE constants for AlN, Pt, and SiO$_2$ are not available in literature. Once reliable TCE data are available, the location of the turnover temperature of the LWRs based on the AlN/SiO$_2$ composite membranes can be accurately predicted.

As shown in Fig. 5–21, the design 3 resonator on the AlN/SiO$_2$ composite structure was tested for four testing cycles in the full temperature range from room temperature to 600°C. From the experimental results, the temperature-dependent fractional frequency variation shows a repeatable characteristic for the four testing cycles. However, the resonance frequency at room temperature decreases by about 500 kHz after each high...
temperature testing cycle. The reason for the phenomenon might be the residual stresses caused by the wide range of testing temperature. Another possible reason is that the AlN thin film might be oxidized at high temperature [167] because the high temperature measurement was taken in an ambient environment.

On the other hand, because the AlN/SiO$_2$ LWRs were wire-bonded to the PCB for the high temperature measurement as illustrated in Fig. 5–18, the parasitic bonding wire

Figure 5-21. Measured temperature dependence of fractional frequency variation of the AlN/SiO$_2$ LWR (design 5) in four testing cycles.

Figure 5-22. Measured frequency spectra of the AlN/SiO$_2$ LWR (design 5) before and after wire-bonding.
inductance and board pad capacitance affected the resonator performance. The behaviors of their $Q$, $k^2_{\text{eff}}$, and $R_m$ were much different from the intrinsic values due to the gold wire bonding. As shown in Fig. 5–22, the parasitic bonding wire inductance and board pad capacitance affected the resonator performance significantly. In order to extract the intrinsic value of the $Q$ and $R_m$, as depicted in Fig. 5–23, an MBVD equivalent circuit is used to simulate the effects of the parasitic inductance and capacitance upon the resonator performance [168]. In the equivalent circuits, $L_t$ represents the trace inductance, $L_w$ depicts the bonding wire inductance, and $C_p$ is the board pad capacitance.

Figure 5–24 compares the measured admittance and phase plots of design 5 resonator
before wire-bonding with the de-embedded admittance and phase plots by subtracting the parasitics ($L_t = 7\ \text{nH}$, $L_{w1} = L_{w2} = 10\ \text{nH}$, and $C_{p1} = C_{p2} = 1.25\ \text{pF}$) from the measured frequency response after Au wire-bonding. Since the chip was locally heated using an infrared lamp, the thermocouple shows that the PCB and bonding wires are only heated to around $120\degree\text{C}$ while the chip is heated up to $600\degree\text{C}$. As a result, the parasitic inductance and capacitance at high temperatures are presumed to be identical to the estimated values at room temperature which are utilized to extract the intrinsic $Q$ and $R_m$ of the LWRs at high temperatures.

By subtracting the unwanted parasitics from the measured admittance response after wire-bonding, the de-embedded admittance response at each temperature can be obtained. Accordingly, the $R_m$ can be extracted in the de-embedded admittance plots and the intrinsic $Q$’s were attained by using the phase slope method as shown in (4.17). Figure 5–25 presents the temperature dependence of the extracted $Q$ of the four AlN/SiO$_2$ LWRs. A clear decrease in $Q$ with the increasing temperature is observed for all resonators. As mention in section 4.4, although various mechanisms may yield the decrease in $Q$, the energy loss is usually dominated by certain loss mechanisms. The tether loss $Q_{\text{tether}}$ and electrical loss $Q_{\text{electrical}}$ are regarded as the dominant loss mechanisms in the LWRs using the $S_0$ mode. In addition, as the resonance frequencies of the resonators are within the Akhiezer regime, the minor loss mechanism, Akhiezer effect $Q_{\text{AKE}}$, shows reciprocal dependence on temperature as following [93]

$$Q_{\text{AKE}} \cdot T = \frac{2\pi\rho V_D^2 \left[ 1 + \left( \frac{\omega\tau_{\text{th}}}{V_D} \right)^2 \right]}{C_v \gamma^2 \omega \tau_{\text{th}}} \tag{5.6}$$

where $V_D$ is the Debye velocity, $C_v$ is the volumetric heat capacity, and $\tau_{\text{th}}$ is expressed as

![Figure 5-25. Temperature dependence of the extracted $Q$ in the four resonators.](image-url)
where $\kappa$ is the thermal conductivity and $n$ is a correction factor.

As it is discussed in section 4.4, the tether and electrical losses are assumed the main loss mechanisms in the $S_0$ mode LWRs, and the Akhiezer effect is taken into account while the LWRs operate at elevated temperatures. As a result, the total $Q$ can be obtained

$$\tau_{th} = \frac{3n\kappa}{C_v V_D^2},$$

(5.7)
using the relationship

\[
\frac{1}{Q_{\text{total}}} = \frac{1}{Q_{\text{tether}}} + \frac{1}{Q_{\text{electrical}}} + \frac{1}{Q_{\text{AKE}}}. \tag{5.8}
\]

As depicted in Fig. 5–26, even if the tether loss and electrical loss are assumed to be independent on temperature, the \(Q_{\text{total}}\) is still degraded with the increasing temperature since the \(Q_{\text{AKE}}\) decreases at high temperatures [168]. Fortunately the \(Q_s\) shows a linear decrease with the increasing temperature and the degeneration in \(Q_s\) is about 1,000 from room temperature to 600°C. For example, if a high \(Q\) of 4,000 was achieved at room temperature, the resonator could still exhibit its \(Q_s\) of round 3,000 at high temperatures.

Figure 5–27 shows the temperature dependence of the extracted motional resistance \(R_m\) of the four resonators. The increase in \(R_m\) with increasing temperature is caused by the higher metal resistance and lower \(Q\) at high temperatures. As shown in Fig. 5–24, the spurious mode occurring at the parallel resonance frequency \(f_p\), resulting in difficulty in extracting the effective coupling \(k^2_{\text{eff}}\). From the experimental results, larger effective coupling coefficients \(k^2_{\text{eff}}\) were observed at high temperatures due to the temperature-dependent AlN piezoelectric coefficients which have been found to be proportional to the absolute temperature [163], [168].

### 5.3 Power Handling and Nonlinearity

Despite the above advantages of the micromechanical resonators, unavoidably its small physical size usually results in small allowable stored energy, referring to its power handling capacity. Power handling, a measure of the amount of power applied to the resonator, is limited by the nonlinearity mechanisms existing in the resonator. The power handling plays an important role in setting the phase noise in the reference oscillators and limiting the applicable range for the bandpass filters since the nonlinear vibration of the resonator introduces noise and distortion into the output signal. As a result, keeping the applied power to the micromechanical resonator less than the nonlinear limits is essential to the performance of the oscillators and filters.

#### 5.3.1 Power Handling in AlN Lamb Wave Resonators

Although the nonlinearities might originate from different sources in the piezoelectric resonators, such as the nonlinear piezoelectric constants or permittivity, the nonlinearity of the Young’s modulus is usually considered the main reason. The nonlinear Young’s modulus can be defined as [169]

\[
Y = \frac{T}{S} = Y_0 \left(1 + Y_1 S + Y_2 S^2 \right), \tag{5.9}
\]
where $T$ is the stress, $S$ is the strain, and $Y_1$ and $Y_2$ are the first- and second-order corrections to the linear Young’s modulus $Y_0$, respectively.

In order to understand the nonlinear behavior of the resonator, as shown in Fig. 5–28, a second-order mass-spring-damper system is introduced and expressed as

$$m\ddot{x} + d\dot{x} + kx = F(t) = F_0(\omega t + \phi), \quad (5.10)$$

where $F(t)$ is the force with a frequency $\omega$ applied to the system, $x$ is the displacement, $m$, $d$, and $k$ are the equivalent mass, damping and stiffness coefficients of the resonator, respectively. In a linear system the spring coefficient $k$ is a constant $k_0$, but in a nonlinear system the nonlinear Young’s modulus cause the nonlinearity in the spring coefficient $k$ which can be written as [169]

$$k = k_0\left(1 + k_1x + k_2x^2 + \cdots\right), \quad (5.11)$$

where $k_1$ and $k_2$ are the first- and second-order corrections to the linear spring constant $k_0$, respectively. Since the displacement of the AlN LWR using the $S_0$ mode is symmetry, the quadratic nonlinear stiffness term can be neglected. The cubic nonlinear term is usually considered in the AlN LWR so the mechanical system can be rewritten as [170]

$$m\ddot{x} + d\dot{x} + k_0x + k_1k_2x^3 = F_0(\omega t + \phi). \quad (5.12)$$

The introduction of the nonlinear spring coefficient $k$ would cause higher harmonics of its natural resonance frequency [169]:

$$x(t) = A_0 + A_1 \cos \omega t + A_2 \cos 2\omega t + \cdots. \quad (5.13)$$

The peak of the natural resonance frequency $\omega_0$ either shifts toward the lower frequencies (material softening) or the higher frequencies (material hardening) and is related to the vibration amplitude $A_1$ by [169]

![Figure 5-28. Mass-spring-damper model of a resonator.](image-url)
\[ \omega_0 = \omega_0 \left(1 + \frac{3k_2}{8} A_i^2\right). \]  

(5.14)

Due to the symmetric deformation of the S\(_0\) Lamb wave mode, the first-order nonlinear spring coefficient \(k_1\) is excluded from the above expression. The second-order nonlinear coefficient \(k_2\) will shift the frequency peak either up or down depending on the second-order coefficient of the Young’s modulus \(Y_2\), which is negative in the AlN thin film.

In fact, the equation (5.12) can be easily converted from the mechanical domain to the electrical domain by means of the electromechanical coupling transduction (\(\eta\)) of the piezoelectric transducers. The transduction coefficient \(\eta\) is related to the displacement and charge, force, and voltage; therefore, an equivalent equation in the electrical domain can be expressed as [170]

\[ L_m \ddot{q} + R_m \dot{q} + \frac{1}{C_m} q + \frac{\alpha}{C_m} q^3 = V(t) = V_0 (\omega t + \phi), \]  

(5.15)

where \(V(t)\) is the voltage, \(q\) is the charge, and \(L_m, R_m,\) and \(C_m\) are the motional elements as depicted in the MBVD circuit. Here, the nonlinear term, \(\alpha\), is introduced to describe the third-order nonlinearity in the electrical domain and is usually caused by the Young’s modulus nonlinearity and self-heating. The third-order nonlinear \(\alpha_{\text{mechanical}}\) caused by the Young’s modulus is defined as [170]

\[ \alpha_{\text{mechanical}} = \frac{3\pi^2 Y_2}{16 (nw\eta)^2}, \]  

(5.16)

where \(n\) and \(w\) are the number and width of the IDT electrode fingers, respectively. When considering device heating via Joule’s law, an expression for the nonlinear \(\alpha_{\text{thermal}}\) can be derived as [170]

\[ \alpha_{\text{thermal}} = TCF \times R_{th} \times \left(R_s + R_m\right) \frac{\pi^2 Y_2}{W \rho}, \]  

(5.17)

where \(R_{th}\) is the thermal resistance of the material, \(R_s\) is the series resistance in the MBVD model.

Recently, the thermally induced nonlinearity has been experimentally proven to dominate the power handling characteristics of the AlN LWRs [171]. The amplitude-frequency (\(A-f\)) nonlinearity of the AlN LWRs is attributed to the material softening due to self-heating at resonance, implying the material with good thermal conductivity shows a better power handling capability, such as AlN.

Three AlN LWRs with the grounded, floating, and open bottom surface conditions are designed and fabricated here to study the nonlinear characteristics of the resonators. The resonators have eight finger electrodes and the electrode width and aperture are 2.77 and 100 \(\mu m\), respectively. They were fabricated on the 1.5-\(\mu m\)-thick AlN thin film based
on the fabrication process discussed above. The $S_{11}$ parameters of the one-port resonators are measured using an Agilent E5071B network analyzer with different RF input power levels from $-10$ to $10$ dBm.

Figure 5–29 shows the excerpt of the evolution of $A$–$f$ curves of the three resonators. When the input RF power is increased, the resonators exhibit a downward shift of the series resonance frequency as it is expected. The two AlN LWRs with the grounded and floating bottom electrode exhibited the similar $A$–$f$ responses as shown in Figs. 5–29 (a) and (b). For the resonator with the bottom electrode, their nonlinear behaviors occur at around $0$ dBm, and their $A$–$f$ bifurcations occur at an input power larger than $5$ dBm. In contrast, the resonator with no bottom electrode shows a better power handling capability. The onset of its nonlinear behavior occurs at around $2$ dBm and the $A$–$f$ bifurcation
occurs at an input power larger than 7 dBm. It is believed that the raised temperature due to self-heating in the resonator without the bottom electrode is lower than those with the bottom electrode since the electric field and the transduction efficiency are smaller [171].

5.3.2 Power Handling Improvement of AlN/SiO$_2$ Lamb Wave Resonators

In order to reduce the thermally induced nonlinearity in the AlN LWRs, the width of the tether can be extended to be equal to the width of the AlN thin plate. In this way the heat can dissipate through the complete device to eliminate the thermally induced nonlinearity [172]. Another approach is to reduce the TCF in the AlN LWR utilizing the SiO$_2$ layer since the thermally induced nonlinear term $\alpha_{\text{thermal}}$ correlates to its TCF. Three AlN/SiO$_2$

![Figure 5-30](image.png)

Figure 5-30. $A$–$f$ curves of the AlN/SiO$_2$ LWRs with the (a) grounded, (b) floating, and (c) open bottom surface conditions.
LWRs with the grounded, floating, and open bottom surface conditions are designed and fabricated on the multilayer membrane composed of a 1-µm-thick AlN film and a 1-µm-thick SiO₂ layer. These resonators have the same design parameters as those for the resonators studied in section 5.3.1. Their $A$–$f$ responses were measured by varying the input RF power levels from –10 to 10 dBm.

Figure 5–30 shows the evolution of the $A$–$f$ responses of the three AlN/SiO₂ LWRs. Interestingly while the RF input power is increased, the resonators with the grounded and floating bottom electrodes exhibit the upward shift of the series resonance frequency as illustrated in Figs. 5–30 (a) and (b). Their nonlinear behaviors occur at around 2 dBm, and their $A$–$f$ bifurcations occur at an input power larger than 6 dBm. As we discussed above, the AlN and AlN/SiO₂ LWRs both are expected to exhibit second-order TCEs so their resonance peaks would be shifted to a lower frequency if only the third-order nonlinearity of the Young’s modulus $\alpha_{\text{mechanical}}$ occurs in the resonator. However, the resonance peak of the AlN/SiO₂ LWRs with the bottom electrode shifted to a higher frequency, implying the $A$–$f$ nonlinearity in the AlN/SiO₂ LWRs is attributed to material hardening at resonance. Actually the composite membrane with the $h_{\text{AlN}/\lambda}$ and $h_{\text{SiO}_2}/\lambda$ both equal to 0.09 shows a positive first-order TCF of 9.63 ppm/°C at room temperature, explaining the thermally induced nonlinearity $\alpha_{\text{thermal}}$ is prior to the stiffness nonlinearity $\alpha_{\text{mechanical}}$ in the piezoelectric AlN LWRs, agreeing with the experimental observation in other works [170]–[173].

In contrast, the AlN/SiO₂ resonator with no bottom electrode shows an excellent power handling capability. As illustrated in Fig. 5–30 (c), the nonlinear behavior occurs at around 8 dBm and no $A$–$f$ bifurcation is observed even though the RF input power is as large as 10 dBm, suggesting the resonators with no bottom electrode suffer from less self-heating effect at resonance. In addition, the shift in the resonance peak caused by the thermally induced nonlinearity can be changed from downturn to upturn utilizing the SiO₂ layer, implying a possible solution for the power handling improvement of the piezoelectric resonators.

### 5.4 Conclusions

In this chapter, temperature-compensated AlN/SiO₂ LWRs using flat edge-type reflectors have been designed and fabricated. We have experimentally demonstrated that the LWRs could be thermally stable at room temperature and high temperatures using the SiO₂ layer beneath the AlN thin plate. In addition, in comparison with the LWR using grating-type reflectors, the edge-type reflector can efficiently reduce the resonator size without sacrificing the quality factor. The temperature-compensated LWR operating at 711 MHz exhibits a first-order TCF of –0.31 ppm/°C, a second-order TCF of –21.5 ppb/°C², a motional resistance $R_m$ of 150 Ω, an effective coupling coefficient $k^2_{\text{eff}}$ of 0.56%, and a quality factor $Q_s$ of 980 at its turnover temperature, 18.05°C.

Moreover, temperature-compensated LWRs operating at high temperatures based on the AlN/SiO₂ multilayered membranes have been designed, fabricated, and characterized. In order for the resonators to operate at high temperature up to 600°C, Pt was used as the
metal material for the bottom and finger electrodes. Based on different thickness ratios of AlN to SiO₂, complete thermal compensation for the LWRs was achieved at 214°C, 430°C, and 542°C, respectively. The turnover temperatures can be intentionally designed at higher temperatures by increasing the thickness ratio of SiO₂ to AlN. In addition, the intrinsic $Q$ and $R_m$ at high temperatures are extracted by using a simple equivalent circuit. These results demonstrate the potential of thermally stable AlN/SiO₂ LWRs for timing, frequency control, and sensing applications at high temperatures.

Finally, the power handling ability of the AlN LWRs with various bottom electrode conditions has been experimentally studied as well. The LWR with no bottom electrode showed better power handling than those with the bottom electrode since it suffers from less self-heating at resonance due to only the lateral electrical field in the resonator. The AlN/SiO₂ composite layer is experimentally demonstrated to be capable of achieving the zero first-order TCF, reducing the thermally induced nonlinearity, and then enhancing the power handling capability for the piezoelectric resonators. The temperature-compensated AlN/SiO₂ LWRs using the flat edge-type reflector, showing the low motional resistance, small size, potential for CMOS integration, good frequency-temperature stability, and possible power handling improvement, are promising to enable advanced oscillators and bandpass filters.
Chapter 6

High-Q AlN/3C–SiC Lamb Wave Resonators and Filters

Nano/micro mechanical resonators offer prospects for a variety of important applications including signal processing [3], mass sensing [174], biosensing [175], [176], quantum mechanism [177]–[179], and digital logic circuits [180], [181]. In general, high $Q$ and high $f_s$ are the required features for nano/micro mechanical resonators since the high $Q$ can offer the low loss for the electronics and supply the high resolution for the sensors. In addition, the high operating frequency can increase the data rate for the electronics and enhance the sensitivity for the sensors. However, while the mechanical resonators with small footprints enable the high resonance frequencies, the shrinking sizes significantly deteriorate their $Q$’s [55], [182], [183]. As a result, a long-standing challenge for the nano/micro mechanical resonators is to enable high $Q$ and high $f_s$ simultaneously, which is often quantified using the product of the two quantities ($f_s Q$). For both piezoelectric and electrostatic transduction methods, materials with large elastic constants and low densities are desirable for achieving high frequencies [184], [185] and materials with low acoustic losses provide high mechanical $Q$’s [92], [186]. In this chapter, we present that the composite plate including an AlN thin film and an epitaxial 3C–SiC layer has the remarkable capability to enable high-performance electroacoustic resonators and filters. The use of the epitaxial 3C–SiC layer is attractive since the SiC crystals have been theoretically proven to have an exceptionally large $f_s Q$ product due to its intrinsic low acoustic loss characteristic at microwave frequencies [93], [191]. In addition, AlN and 3C–SiC have well-matched mechanical and electrical properties [79], making them a suitable material stack for nano/micro mechanical electroacoustic resonators.

6.1 High-Order Lamb Waves in an AlN Membrane

In order to achieve a high resonance frequency above 3 GHz, advanced electron-beam lithography tool [55] and nano-imprinting technology [187] have been utilized to make tiny resonators, while the $Q$’s are usually diminished with the shrinking resonator sizes. However, the $Q$ of the AlN LWR utilizing the $S_0$ mode would be degraded to 500 while
the IDT finger width is downscaled to the nanometer scale for a super-high resonance frequency up to 3.46 GHz [55]. To utilize the high-order resonance modes [188], [189] or acoustic wave modes [52], [190] in the micromechanical resonators is an alternative to increase the resonance frequency \( f_s \) without sacrificing the \( Q \). Although the first-order symmetric (\( S_1 \)) Lamb wave mode in an AlN thin plate demonstrates a high phase velocity up to 26,400 m/s as well as a resonance frequency \( f_s \) of 2.2 GHz, its \( Q \) of 1,100 is not satisfied [52], [190]. So far, significant research efforts have concentrated on the AlN thin films for the designs of electroacoustic resonators, but researchers have overlooked that a multilayer plate structure can change the acoustic wave properties and the resonator performance remarkably. In this section, the high-order Lamb wave modes in the AlN membrane as well as AlN/3C–SiC composite plate will be theoretically investigated and compared and then employed in the designs of the electroacoustic resonators.

6.1.1 Phase Velocity

Based on the effective permittivity approach described in Chapter 2, Fig. 2–6 presents the simulated phase velocity dispersion of the first ten Lamb wave modes propagating in a piezoelectric AlN membrane with electrically free top and bottom surfaces. Although the high-order Lamb wave modes exhibit very high phase velocities in the AlN thin plate, the steep phase velocity dispersion is not preferred for manufacturing the LWRs since their resonance frequency would be very sensitive to the thickness of the AlN thin film. In contrast to the high-order modes, the \( S_0 \) Lamb wave mode exhibits much weaker phase velocity dispersion in the piezoelectric AlN membrane. This unique weak phase velocity dispersion of the \( S_0 \) Lamb wave mode is desirable for the Lamb wave devices since their resonance frequency is insensitive to the thickness variation of the AlN thin film.

![Simulated phase velocity dispersion of the first ten Lamb wave modes propagating in the AlN thin plate.](image-url)
6.1.2 Electromechanical Coupling Coefficient

As it is discussed above, two transducer configurations can be employed for the AlN LWRs as shown in Fig. 2–3, the bottom electrode arrangement would affect the intrinsic \( k^2 \) of the resonator. Figure 6–2 (a) shows the intrinsic \( k^2 \) of the first ten Lamb wave modes under the AlN plate with no backside metallization using the Green’s function. The simulation results indicate the \( S_0 \) mode exhibits a larger \( k^2 \) than the other Lamb wave modes for the type A configuration. Although the high-order Lamb wave modes show high phase velocity, their intrinsic \( k^2 \) is usually limited to around 1%. As shown in Fig. 6–2 (b), the \( S_1 \) Lamb wave mode exhibits a large \( k^2 \) up to approximately 4.5% while the AlN plate has the metallized bottom surface. Unfortunately though the conductive layer on the backside of the AlN thin film boosts the intrinsic \( k^2 \) of the \( S_1 \) mode, its steep phase velocity dispersion is unsuitable for the electroacoustic resonators. As a result, it is still of great interest to employ the \( S_0 \) mode for the AlN LWRs on the AlN thin plate.

6.2 High-Order Quasi-Lamb Waves in an AlN/3C–SiC Composite Plate

As it is mentioned in Chapter 2, 3C–SiC is the only polytype which can be grown on Si substrates [94]; therefore, the AlN/3C–SiC composite structure is studied for the LWRs. The effective permittivity and Green’s function are used to calculate the phase velocities and electromechanical coupling coefficients of the excitable Lamb wave modes in the AlN/3C–SiC composite plate. The material constants of the AlN and 3C–SiC employed in the theoretical simulations are listed in Table 2–3. Since the \( S_0 \) Lamb wave along the
[011] direction exhibit higher phase velocities and $k^2$ in the AlN/3C–SiC composite plate [86], the high-order Lamb wave modes are theoretically and experimentally investigated in the [011] direction in following sections [192].

6.2.1 Phase Velocity

Figure 6–3 shows the phase velocity dispersion of the first ten quasi-Lamb wave modes propagating in an AlN/3C–SiC composite plate while the 3C–SiC is 2.6-µm-thick and the wavelength is 11.08 µm, corresponding to a normalized 3C–SiC thickness $h_{3C–SiC}/\lambda$ equal to 0.235. It is noted that phase velocity dispersions of the high-order quasi-Lamb wave modes in the AlN/3C–SiC layered plate are smooth in comparison with the high-order Lamb wave modes an AlN thin plate. As a result, it is possible to design electroacoustic resonators utilizing the high-order quasi-Lamb wave modes in the AlN/3C–SiC layered plate since their high phase velocities are attractive to enable high-frequency piezoelectric resonators.

6.2.2 Electromechanical Coupling Coefficient

Figure 6–4 (a) depicts the intrinsic $k^2$ dispersion of the first ten quasi-Lamb wave modes propagating in an AlN/3C–SiC composite plate under the AlN plate with no backside metallization in the interface while the 3C–SiC is 2.6-µm-thick and the wavelength is 11.08 µm, corresponding to a normalized 3C–SiC thickness $h_{3C–SiC}/\lambda$ equal to 0.235. The simulation results indicate the QA$_0$ and QS$_0$ mode exhibits larger $k^2$ than the other modes while the AlN thickness $h_{AlN}$ is thinner than 0.3\lambda. As shown in Fig. 6–4 (b), similar to the

Figure 6-3. Simulated phase velocity dispersion of the first ten quasi-Lamb wave modes propagating in the AlN/3C–SiC composite plate while the normalized 3C–SiC thickness $h_{3C–SiC}/\lambda$ is equal to 0.235.
In an AlN thin plate, the QS0 Lamb wave mode still exhibits a large $k^2$ of approximately 2% while the AlN plate has the metallized interface.

In order to study the effect of the 3C–SiC layer on the intrinsic $k^2$, Fig. 6–5 (a) depicts the $k^2$ dispersion of the first ten quasi-Lamb wave modes propagating in an AlN/3C–SiC composite plate under the AlN plate with no backside metallization for the $h_{3C-SiC}/\lambda$ equal to 0.235. Some of the high-order quasi-Lamb wave modes in the AlN/3C–SiC composite plate (a) without and (b) with the backside metallization for the $h_{3C-SiC}/\lambda$ equal to 0.226.

$S_0$ mode in an AlN thin plate, the QS0 Lamb wave mode still exhibits a large $k^2$ of approximately 2% while the AlN plate has the metallized interface.
modes propagating along the [011] direction exhibit larger intrinsic $k^2$ due to the 3C–SiC layer than the corresponding Lamb wave modes in an AlN plate, enabling electroacoustic resonators utilizing the high-order quasi-Lamb wave modes, such as the second quasi-antisymmetric (QA$_2$) or third quasi-symmetric (QS$_3$) modes in the AlN/3C–SiC layered plate. As shown in Fig. 6–5 (b), the metallized interface is able to enlarge the intrinsic $k^2$ of some quasi-Lamb wave modes, such as the QS$_0$, QS$_1$, QA$_2$ modes in the AlN/3C–SiC composite plate. However, the conductive layer in the interface causes the electrical loss in the resonators and then degenerate the mechanical $Q$. As a result, in the following sections, it is of great interest to employ the AlN/3C–SiC LWRs with no bottom electrode in the interface to avoid an extra energy loss mechanism caused by the electrode layer.

6.3 AlN/3C–SiC Lamb Wave Resonators Utilizing High-Order Modes

Based on the above simulation results, the 3C–SiC layer not only enhances the coupling strength of some high-order modes but also smoothes the steep phase velocity dispersions of the high-order Lamb wave modes in the AlN thin plate. The AlN/3C–SiC composite plate is a promising multilayer structure for the high-frequency and high-$Q$ LWRs since the SiC crystals are proven to have intrinsic low acoustic loss characteristics and the high-order quasi-Lamb wave modes show very high phase velocities.

6.3.1 One-Port AlN/3C–SiC Lamb Wave Resonators

As shown in Fig. 6–6, the one-port LWR on the multilayer plate composed of an AlN thin film and an epitaxial 3C–SiC layer is studied in this section. In order to eliminate the undesired effects caused by the bottom electrode, the one-port AlN/3C–SiC LWRs are
intentionally designed with no metallized interface herein. In this study, we investigated
the excitable Lamb wave modes in the AlN/3C–SiC composite plate within a 4 GHz
frequency band using the effective permittivity method. Figure 6–7 shows the effective
permittivity for Lamb wave modes excitable in an AlN/3C–SiC composite layer as a
function of frequency (i.e. Lamb wave phase velocity) while the 3C–SiC layer thickness
$h_{3\text{C-SiC}}$ and AlN thin film thickness $h_{\text{AlN}}$ are 2.6 µm and 2.5 µm, respectively, and the
wavelength $\lambda$ corresponds to 11.08 µm. The solid line represents the real part of effective
permittivity and the dashed line represents the imaginary part. The effective permittivity
values of all excitable Lamb wave modes are real in this case, indicating that Lamb
waves would not attenuate since most surfaces of the AlN/3C–SiC Lamb wave resonator
are in contact with air.

In this work, the 2.6-µm-thick 3C–SiC layer was epitaxially grown on the silicon
(100) wafers using hot-wall CVD and chemomechanically polished by NOVASIC SA to
reduce surface roughness and remove surface defects. Highly $c$-axis oriented AlN thin
films were grown on the epitaxial 3C–SiC layers using AC reactive magnetron sputtering
at approximately 350°C. The cross-sectional SEM image of the AlN/3C–SiC composite
plate is shown in Fig. 6–8 (a) where the AlN and 3C–SiC film thicknesses are 2.5 µm and
2.6 µm, respectively. It is clear that the AlN thin film exhibits numerous columnar grains
perpendicular to the surface of the polished epitaxial 3C–SiC layer. As depicted in Fig.
6–8 (b), the crystalline structure was determined by the XRD normal coupled scan where
the diffraction peaks correspond to a hexagonal AlN (0002) thin film, a cubic SiC (100)
layer, and a cubic silicon (100) substrate, respectively. The presence of (0002) and
(0004) reflections at 36.06° and 76.45°, respectively, gives the indication of the highly $c$-
axis oriented AlN thin film grown on the epitaxial 3C–SiC layer. As shown in Fig. 6–8
(c), the rocking curve of the 2.6-µm-thick epitaxial 3C–SiC layer shows a FWHM value

![Figure 6-7](image_url) Figure 6-7. The effective permittivity for Lamb wave modes excitable in an AlN/3C–SiC composite layer without interfacial metallization while $h_{3\text{C-SiC}}/\lambda$ and $h_{\text{AlN}}/\lambda$ are 0.235 and 0.226, respectively.
of 0.21° which indicates the 3C–SiC layer with near single-crystal quality was epitaxially grown on the Si substrates. In addition, as shown in Fig. 6–8 (d), the 2.5-µm-thick AlN thin film shows a FWHM value of 1.28° which implies the AlN thin film has excellent crystallinity on the polished epitaxial 3C–SiC layer.

The one-port AlN/3C–SiC resonator which has different strips of 150-nm-thick Al IDT finger electrodes with the 2.77 µm finger width and 100 µm transducer aperture was fabricated using the process flow reported in section 3.4. To minimize the experimental errors resulting from the microfabrication processes, all the resonators were fabricated on the same wafer and placed in the vicinity. Figure 6–9 presents the SEM image of one fabricated AlN/3C–SiC LWR with the flat edge-type reflectors. The resonators were all tested in air at room temperature and $S_{11}$ parameters were extracted using an Agilent E5071B network analyzer. The measured $Q$ was extracted from the admittance plot by dividing the $f_s$ by the 3dB BW and the effective coupling coefficient $k^2_{\text{eff}}$ of the measured devices is defined by the IEEE standard definition. For the Lamb wave modes with weak

![Figure 6-8](image-url)
amplitudes, their measured $Q$’s were extracted by using the phase slope method.

In this work, the COMSOL FEA multiphysics software was employed to simulate the resonance mode shape of each quasi-Lamb wave mode propagating in the AlN/3C–SiC composite plate. All quasi-Lamb wave mode shapes at resonance are inserted as insets in

Figure 6-9. SEM image of a fabricated LWR on the AlN/3C–SiC composite plate.

Figure 6-10. Broadband frequency spectrum of the AlN/3C–SiC LWR measured from 100 MHz to 4 GHz. The insets show the resonance mode shape of each quasi-Lamb wave in the AlN/3C–SiC composite plate.
Fig. 6–10 which depicts the broadband frequency spectrum of the AlN/3C–SiC LWR measured from 100 MHz to 4 GHz. As predicted by the theoretical calculations, nine excitable Lamb wave modes with various resonance frequencies were measured in the UHF and SHF regions, respectively. A list of nine Lamb wave modes in the AlN/3C–SiC composite plate along with the corresponding measured $f_s$, $Q$, $R_m$, $k_{\text{eff}}^2$, and phase velocities is reported in Table 6–1. As shown in Fig. 6–10, the QA$_1$ mode is missing in measurement because its electromechanical coupling is theoretically predicted to be nearly zero while $h_{\text{AlN}}/\lambda$ and $h_{3\text{C–SiC}}/\lambda$ are 0.226 and 0.235, respectively. In addition, the experimental results show the QA$_2$ and QS$_3$ modes have their low $R_m$ of approximately 100 $\Omega$.

More specifically, as shown in Fig. 6–11, while the AlN and 3C–SiC thicknesses are 2.5 $\mu$m and 2.6 $\mu$m, respectively, the AlN/3C–SiC LWR utilizing the QS$_3$ mode, which has 33 strips of 150-nm-thick Al IDT finger electrodes, exhibits a low $R_m$ of 91 $\Omega$, a $k_{\text{eff}}^2$ of 0.23%, and a high loaded $Q$ of 5,510 at 2.92 GHz, demonstrating a high $f_s$-$Q$ product, $1.61\times10^{13}$ Hz. The experimental results indicate that the QS$_3$ Lamb wave mode shows a superior characteristic in $Q$ mainly thanks to the intrinsic low acoustic losses of the epitaxial 3C–SiC layer. It is also believed that the resonance mode shape of the QS$_3$ mode in the AlN/3C–SiC composite plate enables the high-$Q$ characteristics due to a decreased energy loss through the support tethers for the QS$_3$ mode leading to an isolation of displacement field in the plate body [193]. Moreover, the mode conversion loss of the QS$_3$ mode at the suspended free edges may be less than other Lamb wave modes while $h_{\text{AlN}}/\lambda$ and $h_{3\text{C–SiC}}/\lambda$ are 0.226 and 0.235, respectively. Figure 6–12 indicates while the number of IDT finger electrodes is less than 25, the measured $Q$ is dramatically decreased. Clearly, without the bottom electrode in the AlN/3C–SiC interface, more IDT electrode numbers can increase the IDT transduction efficiency but the series resonance

![Figure 6-11](image-url)
frequency $f_s$ shows a strong dependence on the number of the IDT electrodes due to the mass loading effect.

In order to investigate the effect of the epitaxial 3C–SiC layer thickness upon the $f_s$, $k^2_{\text{eff}}$, and $Q$, another LWR was fabricated with a 2.5-µm-thick AlN film grown on a 1.8-µm-thick epitaxial 3C–SiC layer. The same IDT design was utilized and the LWR using the QS$_3$ mode in the composite plate exhibits an $R_m$ of 218 Ω, a $k^2_{\text{eff}}$ of 0.15%, and a low

Figure 6-12. Dependence of measured $Q$ and $f_s$ on the number of the IDT finger electrodes.

Figure 6-13. Simulated and measured phase velocities of the first ten quasi-Lamb wave modes propagating the [011] direction of the AlN/3C–SiC multilayer plate.
$Q$ of 526 at 3.33 GHz while the $h_{\text{AlN}}/\lambda$ and $h_{3\text{C-SiC}}/\lambda$ are 0.226 and 0.162, respectively. Degradation in $Q$ and $k_{\text{eff}}^2$ is observed in the LWR with the thinner epitaxial 3C–SiC layer. Figure 6–13 shows the simulated phase velocity dispersion of the first ten quasi-Lamb wave modes propagating along the [011] direction while the $h_{\text{AlN}}/\lambda$ is 0.226. Obviously, the different resonance frequencies were resulted from the intrinsic phase velocity dispersion of the QS$_3$ Lamb wave mode propagating along the [011] direction of the AlN/3C–SiC composite plate. The phase velocities of the quasi-Lamb wave modes decrease with increasing 3C–SiC layer thicknesses even though 3C–SiC has a higher acoustic velocity than AlN. As presented in Fig. 6–13, the measured phase velocities of the quasi-Lamb wave modes show good agreement with the simulated results.

In addition, the QS$_3$ Lamb wave mode in the AlN/3C–SiC composite plate shows an ultra-high phase velocity up to 32,395 m/s, which is over 20,000 m/s higher than the phase velocity of the longitudinal wave (11,354 m/s) in an AlN thin plate. This ultra-high acoustic velocity enables the AlN/3C–SiC LWR with a high resonance frequency up to 2.92 GHz even though the wavelength is as large as 11.08 µm which is relatively larger than the 10-µm-wide support tethers in this work. It is worth noting that the ultra-high acoustic velocity also prevents the high-frequency LWR from the decrease in $Q$ which is usually caused by the mechanical energy loss through the support tethers [58] and the IDT finger widths being downscaled to sub-micron features [55]. That is to say, no strict photolithography technique is needed to narrow down the IDT finger widths to achieve a GHz resonance frequency since the QS$_3$ mode shows a high phase velocity in excess of 30,000 m/s. In particular, while the support tether widths are relatively narrower than the corresponding wavelength of the QS$_3$ mode, the mechanical energy loss through the support tether can be reduced and the $Q$ can be enhanced.

Figure 6–14 shows the measured fractional frequency variation for the AlN/3C–SiC

![Figure 6-14. Measured fractional frequency variation versus temperature of the AlN/3C–SiC LWRs using the QS$_3$ mode with the different thicknesses of the 3C–SiC layer.](attachment:image.png)
LWRs utilizing the QS\textsubscript{3} mode from room temperature to 100°C when the 3C–SiC layer thicknesses are 1.8 µm and 2.6 µm, respectively. As it is observed in the measured results, the resonator fabricated on the thicker 3C–SiC layer shows a smaller first-order TCF of –14.76 ppm/°C, implying the epitaxial 3C–SiC layer has smaller first-order TCEs than the AlN film and then reduces the first-order TCF [194]. Table 6–1 compares the overall performance of the LWRs utilizing various quasi-Lamb wave modes propagating in the AlN/3C–SiC composite membrane where the AlN and 3C–SiC thicknesses are 2.5 µm and 2.6 µm, respectively, corresponding to the wavelength of 11.08 µm.

### 6.3.2 Two-Port AlN/3C–SiC Lamb Wave Resonators and Filters

It is well known that two-port filters are applicable to frequency control and sensing applications and two-port resonators, with more flexible design constraints than their one-
port counterparts, are usable in oscillator applications [91], [195], [196]. This section will present the design and measured results of two-port Lamb wave filters and resonators on the AlN/3C–SiC plates for the first time. As illustrated in Fig. 6–15, a two-port Lamb wave filter employs two sets of IDTs for input and output signals, whereas Fig. 6–16 pictures a two-port resonator that is also formed using two sets of IDTs but in conjunction with two suspended free edges for acoustic wave reflection to form the standing waves in the resonance cavity.

The two-port Lamb wave filters and resonators under investigation were fabricated using the two-mask fabrication process described in section 3.4. The Lamb wave devices have 55 strips of 150-nm-thick Al finger electrodes for each pair of IDTs, the delay line is

![Figure 6-16. Illustration of a two-port AlN/3C–SiC Lamb wave resonator using the flat edge-type reflector with no bottom electrode.](image)

| Table 6-2. Dimensions of the two-port AlN/3C–SiC Lamb wave devices. |
|------------------|------------------|------------------|------------------|
|                  | Filter           | Resonator        | Units           |
| IDT electrode finger number | 55              | 55              | –               |
| Al electrode thickness      | 150             | 150             | (nm)            |
| Aperture W                   | 180             | 180             | (µm)            |
| Electrode finger width w     | 3               | 3               | (µm)            |
| Wavelength λ                 | 12              | 12              | (µm)            |
| Metallization ratio η        | 0.5             | 0.5             | –               |
| Delay line                   | 120             | 120             | (µm)            |
| Overhang distance            | –               | 1.5             | (µm)            |
| AlN thickness $h_{AlN}$      | 2.5             | 2.5             | (µm)            |
| 3C–SiC thickness $h_{3C-SiC}$ | 1.8, 2.6, 3.5   | 1.8, 2.6, 3.5   | (µm)            |
120 µm, the electrode width is 3 µm, and the aperture is 180 µm. The dimensions of Lamb wave filters and resonators are summarized in Table 6–2. All of the Lamb wave devices were tested at room temperature in air and the $S_{21}$ parameters were measured with 50 ohm terminations using an Agilent E5071B network analyzer. The time-gating method was employed to remove the unwanted Lamb wave reflections from the original transmission signals.

Figure 6–17 depicts the broadband frequency spectrum of a two-port AlN/3C–SiC Lamb wave filter which was measured from 100 MHz to 3 GHz while the AlN and 3C–SiC thicknesses are 2.5 µm and 2.6 µm, respectively, and the wavelength corresponds to 12 µm. In order to distinguish the Lamb wave modes propagating in the AlN/3C–SiC composite plate, the effective permittivity approach is employed to calculate the phase velocities of excitable Lamb wave modes in the composite membrane. Pursuant to their displacement symmetries, the Lamb waves are sorted into four quasi-symmetric and four quasi-antisymmetric modes, respectively, within the 3 GHz frequency band. In order to study the effect of the 3C–SiC layer thickness on the performance of the resonators and filters, the AlN film is fixed to 2.5 µm whereas the 3C–SiC thicknesses are 1.8 µm, 2.6 µm, and 3.5 µm, respectively.

As shown in Fig. 6–18 (a), a two-port filter utilizing the QA$_0$ mode achieves a large 3dB BW up to 3.15% and an out-of-band rejection of 23 dB while the AlN and 3C–SiC thicknesses are 2.5 µm and 3.5 µm, respectively. However, somehow the insertion loss (IL) of the filter utilizing the QA$_0$ mode is as large as −40.5 dB. As shown in Fig. 6–18 (c), another filter utilizing the QS$_0$ mode shows a 3dB BW of 2.12%, an IL of −17.6 dB, and an out-of-band rejection of 23 dB while the 3C–SiC layer is 1.8-µm-thick. Although the QA$_0$ mode exhibit a slightly larger $k^2$ than QS$_0$ mode as predicted in Fig. 6–5 (a), the filter utilizing the QA$_0$ mode presents the wider bandwidth but worse IL than that using
Figure 6–16 depicts the illustration of a two-port LWR where the Lamb wave modes are excited by one IDT and then the generated Lamb waves are reflected by the suspended free edges at the both sides. Consequently the standing wave resonance forms inside the composite plate cavity and is received by the other IDT. As illustrated in Fig. 6–18 (b), the two-port resonator utilizing the QA\(_0\) mode achieves a \(Q\) of 3,026 and an IL of –16.8 dB at 455.2 MHz while the AlN and 3C–SiC thicknesses are 2.5 \(\mu\)m and 3.5 \(\mu\)m, respectively. The spurious longitudinal modes on either side of the main response are also observed when the periodic gratings [147], [195] and phononic crystals [197] are employed as the acoustic reflectors. By optimizing the overhang distance between the IDTs and reflectors, the two spurious mode responses can possibly be reduced [195]. In
contrast to the two-port filter topology, the experimental results imply that the QA0 mode is more suitable for two-port resonators. As shown in Fig. 6–18 (d), a two-port resonator utilizing the QS0 mode shows a low Q of 316 but a small IL of −7.1 dB at 898 MHz while the epitaxial 3C–SiC layer is 1.8-µm-thick. Obviously, in comparison with the two-port resonator topology, the QS0 mode is more suitable for the two-port filter topology since it usually exhibits a large electromechanical coupling coefficient $k^2$ among various Lamb wave modes in the AlN/3C–SiC composite layer [196].

Moreover, as shown in Fig. 6–19 (a), since the high-order Lamb wave modes have intrinsic low electromechanical coupling coefficients, the two-port filter utilizing the QS3 mode show a small 3dB BW of 0.1%, an IL of −16.8 dB, and an out-of-band rejection of 18 dB while the 3C–SiC layer is 2.6-µm-thick. It should be noted that the QS3 mode shows an ultra-high phase velocity of 35,454 m/s, enabling a center frequency up to 2.95 GHz even though the wavelength is 12 µm. Obviously, in comparison with the QA0 mode, the QS0 and QS3 modes show the better performance for the two-port filter topology. Figure 6–19 (b) depicts a two-port LWR utilizing the QA1 mode which shows a high Q of 3,303 and an IL of −19.8 dB at 1,037.3 MHz while the epitaxial 3C–SiC layer is 3.5-µm-thick. In addition, the experimental results also imply that the high-order Lamb wave modes in the AlN/3C–SiC multilayer plate are promising for the designs of the two-port electroacoustic devices.

6.4 Conclusions

In summary, the 3C–SiC layer is employed in the electroacoustic devices since it has been theoretically proven to have a large $f_sQ$ product. Based on our simulation results,
the 3C–SiC layer not only enhances the intrinsic $k^2$ strength of some high-order quasi-Lamb wave modes but also offers the smooth phase velocity dispersions of the high-order quasi-Lamb wave modes in the AlN/3C–SiC composite plate. Moreover, the AlN/3C–SiC composite plate was demonstrated to enable a high-frequency, high-$Q$, and low-impedance acoustic resonator utilizing the QS$_3$ mode. The ultra-high phase velocity up to 32,395 m/s of the QS$_3$ Lamb wave mode raises the resonance frequency up to 2.92 GHz without strictly narrowing the IDT finger widths down to sub-micron features. The ultra-high phase velocity also prevents the resonator from the decrease in $Q$ at high resonance frequencies since the support tether widths are relatively smaller than the corresponding wavelength. The micromechanical LWR utilizing the QS$_3$ mode in the AlN/3C–SiC composite plate exhibits a low $R_m$ of 91 $\Omega$ and a high loaded $Q$ of 5,510 at 2.92 GHz, showing the highest $f_s\cdot Q$ product up to $1.61 \times 10^{13}$ Hz among the suspended piezoelectric thin film electroacoustic resonators reported to date.

In addition, two-port filters and resonators based on the AlN/3C–SiC plates are experimentally investigated. The two-port resonator utilizing the QA$_0$ mode exhibits a high $Q$ of 3,026 but the two-port filter using the same mode shows an IL of $-40.5$ dB at about 455 MHz while the AlN and 3C–SiC layers are 2.5 $\mu$m and 3.5 $\mu$m, respectively. On the contrary, the two-port filter utilizing the QS$_0$ mode exhibits an IL of $-17.6$ dB but the two-port resonator using the same mode shows a low $Q$ of 316 at approximately 899 MHz when the AlN and 3C–SiC layer thicknesses are 2.5 $\mu$m and 1.8 $\mu$m, respectively. Moreover, a two-port filter using the QS$_3$ mode shows a small 3dB BW of 0.1%, an IL of $-16.8$ dB, and an out-of-band rejection of 18 dB at 2.95 GHz. All of the experimental results herein reveal that both two-port filters and resonators can have good performance under the appropriate selection of the quasi-Lamb wave modes as well as the AlN and 3C–SiC thicknesses.
Chapter 7

Conclusions and Future Research Directions

To date, the piezoelectric LWRs present a promising resonator technology which offers high quality factor, low motional impedance, post-CMOS compatibility, and multiple frequencies from 100 MHz to over 3 GHz on the same chip. The AlN LWRs show the potential in terms of performance and scalability to revolutionize the current wireless communication systems, for example, the frequency references or bandpass filters. In contrast to the SAW resonator technology, the low deposition temperature of the AlN thin film and the Si-based fabrication processes of the LWRs show potential integration with the CMOS circuits. In comparison with the FBAR technology, the AlN LWRs can offer multiple frequencies on one die for future realization of a single chip RF transceiver. Moreover, the LWRs present a superior in low motional resistances to the electrostatic resonators, allowing interfacing with the standard 50 Ω RF systems. In order to enhance the performance of the electronic system, the integration of micromechanical resonators directly onto the circuitry is an excellent approach to avoid unnecessary energy loss. Therefore, the ultimate goal is the integration of the RF MEMS resonators directly with the CMOS circuits, leading to a single chip solution. So far, there are many research efforts concerning the improvement of the Q’ s of the MEMS resonators to surpass the quartz resonators but sometimes the motional impedance is increased. Moreover, most MEMS resonators cannot achieve the temperature stability as excellent as the crystal resonators perform. This dissertation presents potential solutions for the above problems. This chapter concludes our research efforts on the temperature compensation and Q enhancement of the AlN LWRs and suggests some possible future research directions.

7.1 Summary

This dissertation presents the theoretical analysis, design, fabrication, and experimental verification of the LWRs utilizing the S₀ mode propagating in an AlN thin plate and the QS₀ mode propagating in a piezoelectric multilayer plate. The acoustic characteristics of the Lamb waves in the piezoelectric AlN membrane and composite plate, such as phase
velocities and TCFs, were theoretically investigated using transfer matrix method. In order to attain the large $k^2$ for the piezoelectric resonators, the intrinsic $k^2$ was also analyzed using the phase velocity difference approach or Green’s function method. The baseline microfabrication processes for the LWR technology have been characterized and successfully employed to fabricate the AlN, AlN/SiO$_2$, and AlN/3C–SiC LWRs. The reactive sputtering deposition of the highly $c$-axis oriented AlN thin films was also characterized on various bottom metals such as Al, Mo, and Pt. The two-step deposition process can overcome the lattice mismatch between the AlN thin film and the substrates such as Al and 3C–SiC. Based on the experimental observations, the crystalline degree and surface roughness of the substrates greatly affect the growth of the highly textured AlN thin films.

The suspended convex free edges can be used to confined the mechanical energy and eliminate the energy loss occurring in the support tethers; thus the AlN LWR using the convex free edges yields a loaded $Q$ as high as 3,280, representing a 2.6× enhancement in $Q$ over a 517.9-MHz LWR with the flat free edges. Moreover, one-port AlN LWRs with the electrically open, grounded, and floating bottom surface conditions are theoretically analyzed and experimentally investigated. The employment of the floating bottom electrode results in the lower static capacitance $C_0$ than the grounded bottom electrode in the AlN membrane and accordingly enhances the effective coupling coefficient $k^2_{\text{eff}}$ of the resonator. The floating bottom electrode simultaneously offers a larger $k^2_{\text{eff}}$, an easier fabrication process, and a higher figure of merit than the grounded bottom electrode without sacrificing the transduction efficiency. Hence the AlN LWRs with the floating bottom electrode are suitable for synthesizing narrowband filters. In contrast to the resonators with the bottom electrode, the LWRs with no bottom electrode show a high $Q$ up to 3033 since they get rid of the electrical loss which is caused by the non-uniform strain distribution in the interface. In particular, it also exhibits better power handling capacity than that with bottom electrodes given the low level of the nonlinearity induced by the self-heating in the resonators. The results suggest the AlN LWRs with no bottom electrode are suited for the oscillators and sensors thanks to their high $Q$.

The temperature compensation of the AlN/SiO$_2$ LWRs using flat edge-type reflectors was also experimentally demonstrated at room temperature and high temperatures. The turnover temperatures can be intentionally designed at any temperature by changing the thickness ratio of SiO$_2$ to AlN. The results demonstrate the potential of the thermally stable AlN/SiO$_2$ LWRs for timing, frequency control, and sensing applications at high temperatures. The power handling capability of the AlN and AlN/SiO$_2$ LWRs has also been experimentally studied. The nonlinear mechanism in the LWRs mainly was caused by the thermally induced nonlinearity and directly related to their TCFs. The AlN/SiO$_2$ composite plate was demonstrated ability to achieve the zero first-order TCF, reducing the thermally induced nonlinearity, and improving the power handling capability of the piezoelectric resonators. The AlN/SiO$_2$ LWRs using the edge-type reflector, showing the low motional resistance, small size, stable thermal stability, and good power handling, are promising for advanced reference oscillators and bandpass filters.

In order to further boost the $Q$’s of the LWRs, the 3C–SiC layer was employed in the electroacoustic devices as it has the large $f_c Q$ product and high acoustic velocity. The micromechanical LWR utilizing the QS$_3$ mode in the AlN/3C–SiC composite plate shows
a low $R_m$ of 91 $\Omega$ and a high $Q$ of 5,510 at 2.92 GHz, presenting the highest $f_s Q$ product up to $1.61 \times 10^{13}$ Hz among the suspended piezoelectric resonators reported to date. The ultra-high phase velocity up to 32,395 m/s of the QS$_3$ mode can easily raise the series resonance frequency $f_s$ up to 2.92 GHz without strictly narrowing the IDT finger widths down to sub-micron sizes and prevent the resonator from the decrease in $Q$ at high resonance frequencies. In addition, two-port filters and resonators utilizing the high-order quasi-Lamb wave modes in the AlN/3C–SiC plates are experimentally investigated. The AlN/3C–SiC composite plate was shown their potential to enable the high-frequency, high-$Q$, and low-impedance electroacoustic resonators.

7.2 Future Research Directions

The fundamental viability of temperature-compensation and high-$Q$ AlN MEMS LWRs has been successfully demonstrated in this dissertation and this research work has also set the pathway for the development of advanced electroacoustic resonators. That is, a new class of piezoelectric resonators and filters could be enabled through the novel transducer design, better piezoelectric material synthesis, or advanced microfabrication processes. There are still a number of engineering challenges which must be addressed to optimize the performance of the Lamb wave devices on the piezoelectric thin plate or composite membrane. The final section in this dissertation will present some potential extended research works.

7.2.1 Lamb Wave Resonators on High-Coupling Piezoelectric Plates

Although AlN has been widely used for the piezoelectric LWRs, the maximum $k^2$ of the S$_0$ Lamb wave mode is around 3.5%, which is not enough for the modern transmission architecture using the wideband filters. To explore high-coupling piezoelectric thin films can address the low coupling issue of the AlN LWRs. Recently, scandium (Sc) doped AlN thin films have been used to manufacture the high-coupling FBARs [198], [199] and one-port SAW resonators [200]. The CVD-deposited LiNbO$_3$ thin film was employed for the LWRs utilizing the A$_1$ mode which experimentally showed a large effective coupling $k^2_{\text{eff}}$ up to 7.2% [201]. In addition, a smart-cut process has been used to slice the LiTaO$_3$ [202] and LiNbO$_3$ [203] thin films which exhibit large coupling coefficients than AlN, enabling the high-coupling LWRs. All the research works suggest that the exploration of the new piezoelectric thin plates and Lamb wave modes propagation in them lighten the research directions toward the high-$Q$ and high-coupling LWRs.

7.2.2 Novel Mechanical Energy Confinement Approaches

As it was discussed in Chapter 4, the electrical and tether losses would be the main loss mechanisms for the AlN LWRs. The electrical loss caused by the non-uniform strain
distributions could be eliminated by the well-controlled residual stress of the metal layer under optimized deposition conditions. The tether loss can be minimized using the in-plane acoustic reflectors [127], phononic crystal strips [128], or suspended convex free edges [58]; however, the loss-eliminated tethers and acoustic reflectors cause some other problems at the same time. For example, the convex free edges induced unwanted spurious modes in the resonator due to the different acoustic wave propagation lengths in the lateral direction as shown in Fig. 4–10. The support tethers based on the phononic crystal strips are only valid for a specific frequency range due to their limited band gap. It is believed that novel designs of the support tethers, edge-type reflectors, and grating reflectors can be employed in the resonators to realize high-$Q$ and low-impedance AlN LWRs in the future.

7.2.3 Advanced Temperature Compensation

Although the temperature-compensated AlN/SiO$_2$ LWR shows a first-order TCF of $-0.31$ ppm/$^\circ$C and a second-order TCF of $-21.5$ ppb/$^\circ$C$^2$ at room temperature, it still shows a total frequency drift up to around 100 ppm in the temperature window from $-40^\circ$C to $85^\circ$C, which is still worse than the AT-cut quartz as shown in Fig. 5–13. As a result, it is of strong interest to reduce the second-order TCF of the AlN/SiO$_2$ LWRs using materials with positive second-order TCEs. Recently, Mo has been reported to have a second-order TCF of $+7$ ppb/$^\circ$C$^2$ [67] so the use of Mo as the transducer electrodes is possible to further improve the frequency-temperature stability. In addition, the AlN/SiO$_2$ multilayer plate composed of 1-$\mu$m-thick AlN and 0.83-$\mu$m-thick SiO$_2$ was used to successfully reduce the first-order TCF of the 711-MHz LWR to $-0.31$ ppm/$^\circ$C at room temperature. However, the 460-MHz AlN LWR still showed a first-order TCF of $-7.61$ ppm/$^\circ$C due to the dispersive characteristics of the $S_0$ Lamb wave mode. According to the theoretical simulation, an AlN layer as thin as 250 nm can significantly reduce the intrinsically dispersive TCF behaviors of the Lamb waves, and it is possible to achieve nearly zero first-order TCFs for the LWRs operating at multiple frequencies fabricated on the same AlN/SiO$_2$ stack.

7.2.4 Temperature Compensation Using Other Materials

As it is discussed in Chapter 2, the silicon oxide layer significantly decreases the phase velocity and electromechanical coupling strength of the QS$_0$ Lamb wave mode in the AlN/SiO$_2$ composite layer. If a thinner thermal compensation layer is employed in the structure, the unwanted effects can be eliminated. To simultaneously achieve the zero first-order TCF, high phase velocity, and large electromechanical coupling coefficient, a more efficient temperature compensation layer is desired. Most recently, TeO$_2$ [70] and SiOF [73] are investigated to have more positive TCEs than the undoped SiO$_2$ thin films. As a result, it is interesting to integrate these new thermal compensation materials with the AlN LWRs to enhance the effective coupling strength and increase the resonance frequency. The synthesis of the new materials with positive TCEs for the temperature compensation is always of great interest.
7.2.5 100+ GHz Phase-Locked Loop Utilizing AlN LWRs

With the development of the CMOS millimeter-wave circuits, applications at tens of GHz range have drawn great interests not only in the academia but also commercial markets. For example, WiGig standard (802.11AD) operating at 60 GHz band allows the data transmission at a rate up to 7 Gb/s, solving the problem of ever increasing data demand in the modern world. Other examples include 77 GHz automotive radar system, aiming to improve driving safety, 94 GHz medical imaging for early-detection of breast tumor, and sub-THz chip-to-chip communication for instrumentation [204]. In the systems, a high-frequency local oscillator (LO) is necessary and it is often generated through the on-chip clock multiplying unit (CMU) via the phase-locked loop (PLL) technique. Unfortunately, recent development of PLLs at 60 and 100 GHz still exhibits high phase noise at their in-band (offset frequency less than PLL loop bandwidth). For example, the PLLs at 60 and 100 GHz exhibit the in-band phase noise of –82 and –92.5 dBc/Hz, respectively [205], [206]. Such high in-band phase noise is mainly caused by the high reference noise and large multiplication ratio. The phase noise of the reference oscillator can be improved by enhancing the $Q$ of the micromechanical resonator while the multiplication ratio (N) in the CMU can be reduced by increasing the reference frequency. It is noted that the in-band phase noise is gained up by $20\times\log(N)$ (in dB) when referred to the PLL output frequency. Therefore, it is of great interest to improve the phase noise by implementing the high-$Q$ AlN/3C–SiC LWRs at GHz frequencies into the CMOS reference oscillator for the 100+ GHz PLLs.

7.2.6 RF Voltage Transformers on Piezoelectric Plates

Since the Lamb wave modes in the AlN thin plate shows the high phase velocity up to 9,800 m/s, a large impedance ratio between the output and the input ports can be designed by using the different number of the input and output transducer fingers to enable high-frequency voltage transformer [207], [208]. The two-port Lamb wave device on the AlN thin plate with the different input and output interdigital fingers can function as a voltage transformer and a bandpass filter at the same time. Alternative novel designs on the acoustic resonators and piezoelectric materials are expected to decrease the insertion loss and achieve the higher transformation ratio.
Bibliography


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