Surface Acoustic Wave Characterization and Interdigitated Transducer Optimization for Studying Stress-Enhanced Phenomena

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SURFACE ACOUSTIC WAVE CHARACTERIZATION AND INTERDIGITATED TRANSDUCER OPTIMIZATION FOR STUDYING STRESS-ENHANCED PHENOMENA

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DISSERTATION
Submitted in Partial Fulfillment of the
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DEDICATION

I’d like to dedicate this work to my beautiful wife, Lauren. You are the most incredible partner any person could ask for, and I cannot imagine a happier life without you.

Also, for our dogs and all dogs everywhere.
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ABSTRACT

Surface acoustic wave devices have not yet achieved their full potential as the effects of standing acoustic fields on stress-sensitive phenomena in semiconductor systems have been largely unexplored. From this perspective, it is necessary to develop novel methods to characterize surface acoustic wave devices quantitatively and prepare an experimental platform to probe stress-enhanced processes. In this dissertation, interdigitated transducer devices are fabricated on gallium arsenide to evaluate their potential impact on strain-enhanced phenomena. A novel Raman characterization technique characterizes the surface stress induced by a standing acoustic field, revealing stress values on the order of $10^8$ Pa. FEM software models the electrical and mechanical behaviors of interdigitated transducer structures, and the simulated displacements are confirmed with atomic force microscopy at room temperatures. FEM modeling predicts device performance for temperatures as high as 177 °C, confirming that SAW devices are a robust experimental platform for studying strain-enhanced phenomena. A full-geometry parametric study suggests potential avenues to optimize SAW-resonator designs and produce intricate and powerful stress fields, which can then sculpt designer features for quantum devices via stress-enhanced atomic diffusion.
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CHAPTER 1: INTRODUCTION

1.1 Scalable Manipulation of Quantum Barriers in Semiconductor Device Structures

Developing methods to manipulate quantum barriers and form laterally organized nanostructures in a scalable way would impact a variety of technological fields, including optoelectronics[1], [2], telecommunications[3], [4], and solid-state data storage[1], [5]. Highly organized quantum structures facilitate complex semiconductor device designs, and the high-throughput manufacturing of such devices accommodates an ever-growing economic demand[6]. However, scalable lateral control of compound semiconductor nanostructures is a standing barrier in nanomanufacturing, limiting applications such as quantum computing and quantum information processing[7]. Developing novel fabrication techniques to extend device capabilities is an ongoing engineering endeavor that receives substantial attention from the research community.

Semiconductor device performance and applicability are determined predominately by the material’s electronic band structure, which establishes properties such as absorption/emission wavelength, carrier mobility, and critical breakdown voltage[8]. Modern semiconductor technologies exploit material bandgaps through solid-state engineering to achieve extraordinary functionalities for electronic, optoelectronic, and photonic applications. One such exploitation is the fabrication of quantum structures with reduced domain dimensionalities, depicted in Fig. 1.1, to introduce quantized energy states into the band structure. These quantized energy states can have an immediate effect on
device capabilities by enabling phenomena such as stimulated emission[9], 2-D electron
gasses[10], [11], and single-photon detection/generation[10], [12].

Figure 1.1: Quantum structures are formed through the spatial confinement of semiconductor
domains, introducing quantized energy levels within the material’s band structure. As the
dimensionality decreases from (a) to (d), the energy levels become more discrete.

Fabricating quantum structures requires precise control of material domain
boundaries at the nanoscale, and top-down manufacturing techniques are necessary to
address economic demand pragmatically. Modern large-scale fabrication methods can
produce semiconductor heterostructures by combining various semiconductor materials
within the same growth procedure[13]. Single-crystal growth techniques such as molecular
beam epitaxy (MBE) or chemical vapor deposition (CVD) are reliable approaches for
growing micro-and-nanometric structures. Such fabrication methods can lead to quantum
mechanical phenomena through the carrier confinement induced by quantum well/quantum dot structures or conjoining semiconductor interfaces[14].

Additionally, single-crystal epitaxial growth enables a range of compound semiconductor compositions, but lattice mismatch between heterostructures limits the materials palette due to the subsequent high defect densities. For applicable material systems, however, the results of single-crystal growth are exceedingly impactful. As seen

**Figure 1.2**: The bandgap (eV) vs. lattice constant relationship for various semiconductor systems is commonly referenced for device fabrication processes. Lattice mismatch hinders heteroepitaxial growth, limiting the applicability for many semiconductor material systems. The GaAs-AlAs system is popular for quantum devices due to their similar lattice constants. This figure is provided by Ref. [15]
in Fig. 1.3, the lattice constants of gallium arsenide and aluminum arsenide are practically identical[15], and therefore defect densities can be kept relatively low. Molecular beam epitaxy growth is thus a reliable technique to grow defect-free $\text{Al}_{1-x}\text{Ga}_x\text{As}$ quantum structures, enabling access to its wide range of electronic bandgaps. Devices that rely on the $\text{Al}_{1-x}\text{Ga}_x\text{As}$ system are popular as infrared photodetectors and laser diodes[16], which are otherwise difficult to produce by other means reliably. For reasons that are not currently well understood, III-nitride materials are difficult to grow using molecular beam epitaxy[17], so gallium nitride and aluminum nitride structures are typically grown using metal-organic chemical vapor deposition (MOCVD)[18]. Recent advancements in growing low-defect AlGaN structures have dramatically improved power conversion systems and power switching devices[19].

Access to such complex material structures enables more advanced semiconductor technologies, such as quantum information processing[20] or single-photon systems[2]. The ability for quantum dots to manipulate individual charge carriers and their potential integrability with more complex devices have made them popular candidates in various solid-state applications. For many decades, self-assembled epitaxial quantum dots have been a research topic of immense interest as their unique properties are valuable for quantum information and communication applications[20], [21]. Single-photon emitters/detectors are a natural direction for quantum dot technologies, as electrically-or-optically-pumped quantum dots generate excitons that often produce a single photon upon electron-hole recombination. The careful arrangement of an individual quantum dot within an optical cavity would provide suitable means for an efficient single-photon emitter[21]. Figure 1.2 illustrates the various atomic growth modes utilized in MBE. The Stranski-
Krastanov (SK) growth mode is the primary method for epitaxially growing quantum dots, which involves an atomic layering of lattice-mismatched systems to spontaneously form 3-D island structures[22]. A significant drawback for this popular strain-limited growth mode is the random island distribution, constraining the fabrication of highly organized devices.

![Figure 1.3](image)

**Figure 1.3**: The various MBE growth modes result from thermodynamic interactions of strained surfaces. The (a) FVM growth mode produces coherent atomic layers through either step-growth or island-growth. The (b) VW growth mode forms islands directly on the substrate surface. (c) The SK growth mode transitions from layer-by-layer growth to spontaneous 3-D island formation.

In general, strain-limited growth restricts the overall selection of accessible semiconductor materials, especially for highly organized device designs. As such, there is a pressing call for innovative methods to manipulate quantum barriers and form laterally organized nanostructures in a scalable way. While modern top-down fabrication approaches make many of the current industrial practices tenable, the complicated methods necessary for large-scale manufacturing limit economic supply. Additionally, highly ordered and addressable structures are even more challenging to obtain for large-scale manufacturing. The growing demand for an expanded materials palette and even more
complex structures requires novel fabrication techniques to advance the limits of present technological capabilities.

The principal objective of this work is to introduce an experimental platform to study stress-sensitive phenomena such as crystal growth and compound semiconductor interdiffusion by way of acoustic enhancement. The success of this research endeavor naturally leads to a scalable technique to form three-dimensional quantum structures in epitaxially grown III-V compound semiconductor layers by applying patterned stress fields at elevated temperatures. This approach is inherently more straightforward to control than, for example, Straniski-Krastanov growth because it does not require non-equilibrium processes such as nucleation and growth of new phases. It is also expected to be cheaper than other top-down fabrication approaches because the non-destructive mechanism does not require additional epitaxial growth and it relies on elastic strain to induce high-resolution patterning.

1.2 Previous Efforts to Explore Strain-Driven Diffusion

Strain effects on semiconductor diffusion processes have been largely unexplored and may be a practical route to locally alter diffusion rates in a compound semiconductor substrate. The standard continuum diffusion equation for species $i$ is given by

$$\frac{\partial c_i}{\partial t} = \sum_j \nabla \cdot (D_{ij} \nabla \mu_j) + \epsilon, \quad (1.1)$$

where $c_i$ is the concentration, $D_{ij}$ is the diffusion matrix, $\nabla \mu_i$ is the driving force due to a chemical potential $\mu_i$, and $\epsilon$ is a thermal noise term that satisfies the fluctuation-dissipation theorem\textsuperscript{22,26}. The diffusion matrix, $D_{ij}$, for compound semiconductor systems describes
the self-diffusivity of atomic species. It also describes atomic diffusion as being mediated by vacancies and interstitials whose concentrations and diffusivities are influenced by temperature, composition, and stress[23]. Furthermore, the generalized chemical potential, $\mu_i$, is fundamentally defined by the system’s free energy wherein elastic stress can significantly impact the mechanisms for pattern formation and phase separation[24].

**Figure 1.4:** (a) The silicon nanopillar array and SiGe wafer are placed into a mechanical press assembly. (b) The nanopillar array and SiGe wafer are pressed against each other and undergo a high-temperature processing step. (c) The mechanically induced compressive stress promotes preferential diffusion of the larger germanium atomic species, leaving behind a patterned array of germanium depleted, silicon-rich regions.
Our research group’s previous work has attempted to exploit the mechanisms of strain-enhanced semiconductor interdiffusion by way of point-defect mediation using a ‘Press-and-Print’ fabrication technique[23]. A mechanical press imposes a patterned strain field onto a silicon germanium (SiGe) substrate, and after high-temperature processing, produces a composite surface of Si-SiGe-Ge domains. As shown in Fig. 1.4, a silicon nanopillar array is pressed against the surface of the SiGe substrate and then heated to temperatures sufficient to induce atomic interdiffusion. The mechanically applied compressive stress alters point defect concentrations, promoting preferential diffusion of the larger Ge atomic species, leaving behind a patterned array of Si-rich regions. In theory, this technique would provide a means for large-scale patterned quantum dot fabrication and readily enable more complex device geometries.

**Figure 1.5:** The atomic percentage of Si (black) and Ge (white) near the surface of the indented SiGe substrate. (a) Under appropriate temperature conditions, preferential diffusion is thought to be observed. However, (b) with too much applied pressure, plastic deformation interferes with the supposed diffusion mechanism. This figure is provided by Ref. [23]
Figure 1.5 depicts transmission electron microscopy results and energy dispersive X-ray analysis that suggests preferential atomic diffusion has occurred beneath the contact junction of the silicon nano-indenter and the SiGe substrate. Swap et al. claim that mechanically imposed stress depletes the larger Ge atoms from the Si-Ge matrix, shown in Fig. 1.5(a), and leaves a tensile-strained and Si-rich region. Plastic deformation is said to interfere with the supposed diffusion mechanism, and Fig. 1.5(b) depicts no notable change in the Si-Ge matrix, which is attributed to an excess of applied pressure.

Rigorous characterization of the ‘Press and Print’ experiment is challenging to complete due to the plastic nature of the applied strain and the complicated diffusion mechanism that dictates this supposed process. Additionally, the magnitude of force applied directly to the surface of the SiGe substrate is extremely difficult to control and maintain at high temperatures. The work by Li et al. also suggests SiGe as an unfavorable material system for patterning via stress-induced diffusion due to the convexity of the free energy functional, which reflects the lack of miscibility gap in Si-Ge systems[24]. For these reasons, it is paramount to this research effort to develop a nondestructive and strain-based technique, which allows for precise control of the applied strain fields at high temperatures and is applicable for many material systems.

1.3 Interdigitated Transducers as an Experimental Platform

Interdigitated transducer (IDT) devices are among the most frequently used periodic electrode structures for nondestructive testing (NDT), microelectromechanical systems (MEMS), and telecommunications[25]. IDT sensors benefit from being passive elements that wirelessly interact and do not require a power supply, enabling remote
monitoring in harsh environments. The devices typically work in a frequency range of $10^6$-$10^9$ Hz and have a compact structure that offers high stability and sensitivity, low cost, fast and real-time response, and are extremely small. Wireless temperature, pressure, and chemical sensing IDT devices are in great demand in energy generation, automotive, and aerospace industries due to their robust capabilities in extreme environments [26].

![Figure 1.6: The simplistic design for a typical IDT structure consists of metal electrodes deposited onto a piezoelectric substrate which responds to an electrical input to produce a mechanical response. This mechanical response produces a coherent traveling acoustic wave, known as a surface acoustic wave at a specific resonance frequency.](image)

Despite their remarkable performance within various engineering applications, the current technological capabilities of IDT devices have not been extensively applied to studying stress-sensitive diffusion processes in semiconductor systems. An inherent capability of IDT devices is the ability to generate surface acoustic waves (SAWs), which
can produce powerful and coherent strain fields with sub-micron wavelengths. Furthermore, SAWs have many essential properties that make them attractive for studying strain effects on surface or near-surface phenomena at the micro or nanoscale. For one, the acoustic energy confinement near the surface of a solid implies the wave can be modified or characterized as it propagates[27], which enables a high degree of experimental versatility. Additionally, the velocity of surface acoustic waves is approximately $10^{-5}$ times smaller than that of electromagnetic waves, enabling suitable device sizes and compatible time scales [28]. Finally, the low attenuation of these waves in well-fabricated devices enables long delay lines minimally hindered by propagation losses [29]. These many reasons make SAW-based devices a primary candidate for studying stress-enhanced semiconductor phenomena.

Figure 1.7 depicts characteristic illustrations of select experimental endeavors exploring different SAW-enhanced phenomena by various research groups[30]–[33]. Most of the research found in the literature has been primarily computational [34]–[39]; however, Chen et al. and Sazan et al. have independently demonstrated highly oriented nanowire and nanoparticle assembly using standing SAW fields generated by interdigitated transducer devices [30], [31]. Theoretical modeling from various research groups suggests the potential for periodic stress fields to enhance crystal growth and localized diffusion in compound semiconductors[34]–[39], which, as discussed previously, is valuable for developing next-generation semiconductor technologies.
IDT devices offer an experimental stage to study interfacial phenomena such as surface/bulk atomic diffusion and crystal growth through the introduction of acoustic strain. The precise control of standing acoustic wave amplitudes and wavelengths provides an opportunity for new device fabrication techniques; however, current methods to probe these SAW-based devices are generally limited to electrical characterization. From this perspective, it becomes crucial to develop new techniques to interrogate the stress fields produced by surface acoustic waves and optimize device designs to provide tailored stress patterns for strain-enhanced fabrication processes.

**Figure 1.7**: Previous research has been completed to uncover the potential for SAW-enhanced phenomena[30]–[33]. Experimental work has demonstrated nanowire and nanoparticle assembly, while computational efforts have attempted to quantify the impact SAWs have on crystal growth and atomic diffusion processes.
1.4 Summary of Proposed Work

In this dissertation, newly developed characterization methods and rigorous computational modeling thoroughly probe the mechanical behaviors of IDT structures. A 2-D Raman imaging technique demonstrates a novel characterization method to study the surface stress induced by a standing acoustic field. Finite element method modeling accurately predicts the mechanical behaviors of the SAW-generating IDT assemblies and optimizes the IDT structures for improved device performance. The high-temperature response of SAW-resonator devices is measured and compared with simulated devices. The work discussed in this dissertation lays the groundwork for future endeavors involving SAW-enhanced phenomena to expand the selection of semiconductor fabrication methods.

‘Chapter 2’ reviews the fundamental principles for various fabrication and characterization techniques, especially those pertaining to fabricating and characterizing interdigitated transducers. The described methods are referenced throughout the remainder of the dissertation.

‘Chapter 3’ outlines acoustic theory within solid media and reviews the mathematical framework for SAWs in non-piezoelectric and piezoelectric domains. The discussion of acoustic theory in solid media begins with a technical description of longitudinal and transverse waves. The analysis continues into horizontal and vertical shear waves and how they couple with longitudinal waves to form surface acoustic waves under the appropriate boundary conditions. Finally, common attenuation mechanisms observed for acoustic waves within the studied frequency range and device size scale are discussed.
‘Chapter 4’ explores the technological impact of interdigitated transducers and their significance as electronic filters, environmental sensors, and micromechanical pumps. The fabrication procedure for interdigitated transducers deposited on gallium arsenide is reviewed in detail, covering the specific procedures for photolithography, metal deposition, inductively coupled plasma cleaning, and wire bonding. The devices are characterized using vector network analysis, RF power detection, and atomic force microscopy.

‘Chapter 5’ demonstrates how Raman microscopy can improve our quantitative understanding of the surface stress induced by the interdigitated transducer (IDT) devices. A novel technique using Raman microscopy is deployed in conjunction with atomic force microscopy to characterize the acoustic strain field of experimental interdigitated transducer devices. The relationship between the Raman peak broadening and the crystal strain induced by the standing surface acoustic waves is defined, and stress values are acquired using a unique Raman peak fitting scheme. 2-D Raman analysis directly measures the stress induced by SAWs, and atomic force microscopy independently verifies the Raman measurement results.

In ‘Chapter 6’, FEM modeling using COMSOL Multiphysics demonstrates the relevance of computational analysis as a viable technique for device design and characterization. IDTs are a potential platform to study the effects of stress on semiconductor diffusion, and a rigorous understanding of the device’s mechanical response is necessary for further investigation. The tuning of an IDT’s mechanical response through optimization of the device geometry is significantly aided by finite element method (FEM) modeling, as device fabrication and characterization can be an extensive and costly process.
In ‘Chapter 7’, high-temperature measurements are recorded for SAW resonators fabricated on gallium arsenide and compared with simulated data. Atomic force microscopy measures the room-temperature surface displacement values for the experimental device and validates the simulation results. Standing-wave stress analysis completed over the range of tested temperatures demonstrates how IDT devices are a promising platform for investigating stress-enhanced phenomena.
CHAPTER 2: FUNDAMENTALS OF FABRICATION AND CHARACTERIZATION TECHNIQUES

This chapter reviews the fundamental principles for various fabrication and characterization techniques, especially those pertaining to interdigitated transducers devices.

2.1 Fabrication Techniques

2.1.1 Photolithography

Photolithography techniques are among the most advanced and robust fabrication methods for micro-and-nano-devices in the semiconductor industry [40]. Photolithography is used in device fabrication to produce geometric patterns on a substrate by exposing a photosensitive polymeric chemical known as photoresist with an ultraviolet light source. Current state-of-the-art photolithography processes can produce wafer-scale geometries on the order of tens of nanometers across comparatively large regions with a high throughput[41]. The photolithography techniques used in this work are contact lithography and interferometric lithography.

Contact Lithography

In contact lithography, a photomask is brought into hard or soft contact with a photoresist layer, such that ultraviolet light can pass through the photomask and form a 1:1 image on the photoresist layer. Photomasks are manufactured using a quartz slide with negative or positive chromium images of the feature design. The image is often printed onto the mask using electron-beam lithography, introducing
a higher cost element to photomask manufacturing. Frequent use degrades a photomasks lifetime, as rubbing against the substrate or contamination by photoresist affects the image quality. An intimate contact must be made between the contact mask and the substrate surface to prevent air-gap-induced light diffraction and typically limits the pitch resolution for contact lithography to about 1 μm[40]. For systems capable of achieving a higher resolution, the ultimate limit for contact lithography when considering classical optics is defined as[42]:

\[ d_c = 0.61 \frac{\lambda}{NA}, \]  

(2.1)

where \( d_c \) is the critical-feature distance, \( \lambda \) is the wavelength of the incident light, and \( NA \) is the numerical aperture of the lens. The factor 0.61 is a product of the Rayleigh criterion and the analysis of Airy diffraction patterns[43]. Features smaller than the critical feature become obscured by the diffraction of light. The numerical aperture's dependence on the refractive index means that a higher index medium can be used, but this only further increases the cost of production. The laser used for the contact photomask setup in this work is a 355-nm 'i-line' laser with a wavelength of 365 nm. Contact lithography has been used in this work to fabricate the aluminum interdigitated transducer devices on gallium arsenide and demonstrated a minimum critical feature size of 2.5 μm.

**Interferometric Lithography**

Interferometric lithography is a mask-less photolithography technique that utilizes two or more coherent light beams and is favored for its inexpensive and easy-to-use setup[44]. The interference pattern produced by the converged light
beams has an intensity distribution that can be imprinted onto the photoresist pattern and achieves resolutions significantly smaller than what is offered by contact photolithography[45]. Multiple-exposure interference is also possible, which enables the production of complex 2-D patterns[45]. A simplified graphic detailing the two different setups used for interferometric lithography is shown in Fig. 2.1. The feature size for interferometric lithography is defined by the following equation:

\[ d = \frac{\lambda}{2n \sin \theta}, \]

where \( d \) is the pitch size of the interference pattern, \( n \) is the refractive index for the medium through which the incident light passes through, \( \theta \) is the angle of the stage with respect to the incident light, and \( \lambda \) is the wavelength of the laser. For air, \( n \) is approximately 1. A quartz prism, demonstrated in Fig. 2.1(b), or water immersion techniques decrease the interfering beam's pitch size further. In this work, two-beam interferometric lithography is used to produce a silicon nanopillar array with nanopillar diameters of 200 nm.
Physical vapor deposition (PVD) techniques typically involve a coating process in which a material is evaporated or sublimated in a vacuum chamber and condensed onto a substrate to form a thin film. PVD is a reliable technique to deposit single crystal, polycrystalline, or amorphous films (metal or non-metal)\[46\]. The two most frequently used techniques used in this work are thermal deposition and electron beam evaporation. Physical vapor deposition relies on a medium-to-ultra-high vacuum environment, depending on the film qualities necessary for deposition. Table 2.1 details the qualities and applications for each vacuum regime.

**Figure 2.1**: (a) A mirror and substrate stage setup are angled to produce a specified interference pattern pitch. (b) A prism is included to increase the refractive index of the medium in which the incident light interferes. Figure provided by Brueck et. al.[45].

### 2.1.2 Physical Vapor Deposition

Physical vapor deposition (PVD) techniques typically involve a coating process in which a material is evaporated or sublimated in a vacuum chamber and condensed onto a substrate to form a thin film. PVD is a reliable technique to deposit single crystal, polycrystalline, or amorphous films (metal or non-metal)[46]. The two most frequently used techniques used in this work are thermal deposition and electron beam evaporation. Physical vapor deposition relies on a medium-to-ultra-high vacuum environment, depending on the film qualities necessary for deposition. Table 2.1 details the qualities and applications for each vacuum regime.
The deposited film quality is a function of the vacuum system's mean free path, which is directly associated with the probability that a particle such as an atom or molecule collides with another particle. The mean free path, \( \lambda \), is defined as follows\,[47]:

\[
\lambda = \frac{k_B T}{\sqrt{2\pi Pd^2}},
\]

where \( k_B \) is the Boltzmann constant, \( T \) is the gas temperature, \( P \) is the gas pressure, and \( d \) is the particle diameter. For a high vacuum system, the mean free path is in the range of \( 10^{-1} \) to \( 10^3 \) m.

**Table 2.1:** Increasing vacuum types offer additional benefits but are harder to achieve and maintain. Applications require different vacuum types as longer mean free paths are required for robust processing\,[47].

<table>
<thead>
<tr>
<th>VACUUM TYPE</th>
<th>PRESSURE RANGE (PA)</th>
<th>OBJECTIVE</th>
<th>TYPICAL APPLICATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>LOW VACUUM</td>
<td>( 10^3 &lt; P &lt; 10^5 )</td>
<td>• Exploit pressure gradients</td>
<td>Holding, vacuum transport, forming</td>
</tr>
<tr>
<td>MEDIUM VACUUM</td>
<td>( 10^{-4} &lt; P &lt; 10^3 )</td>
<td>• Decrease heat transfer</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Remove contaminants and undesired gases</td>
<td>Sintering, freeze drying and dehydration, microbalance measurements</td>
</tr>
<tr>
<td>HIGH VACUUM</td>
<td>( 10^{-7} &lt; P &lt; 10^{-4} )</td>
<td>• Avoid molecular and atomic collisions</td>
<td>Electron beams and tubes, thin-film deposition, X-ray tubes, electron microscopes</td>
</tr>
<tr>
<td>ULTRA-HIGH VACUUM</td>
<td>( 10^{-10} &lt; P &lt; 10^{-7} )</td>
<td>• Obtain clean interfaces</td>
<td>Surface analysis, molecular-beam epitaxy, space research</td>
</tr>
</tbody>
</table>
Thermal Deposition

Thermal deposition occurs in a medium-to-high vacuum environment, and thermal heating controls the source material's vapor pressure and, therefore, the evaporation rate of a material. A diagram describing the deposition setup is shown in Fig. 2.2. The sample is mounted at the top of the vacuum chamber directly above the target-material-containing source, which is heated via resistive heating. The vapor that rises from the heated crucible forms a Gaussian plume that deposits the vaporized material onto the substrate. Thermal deposition provides high purity films with nanometer accuracy and homogenous thickness due to the vacuum environment[46]. In this work, indium is melted in a crucible in a "low" vacuum chamber and deposited onto gallium arsenide.
Electron-Beam Deposition

An electron-beam deposition involves bombarding a target anode with an electron beam generated by a tungsten-filament cathode and steered with a magnet in a high-vacuum environment. The tungsten filament is kept out of the line of sight from the target due avoid interactions between evaporated atoms and the cathode[47]. The electron-beam steering process is demonstrated in Fig. 2.3. The electron beam promotes atoms to evaporate or sublimate from the target and condense onto the substrate. An advantage offered by the direct-heating effect of the electron beam is that the highest temperature achieved within the target material-containing crucible occurs at the electron-beam area of contact[47]. Electron-beam deposition is often favored for its high degree of control and film quality and the many materials it can evaporate and deposit[47]. In this work, electron-beam deposition deposits Cr, Al, Au, Ti, and Ag films.

Figure 2.3: In an electron beam deposition, an energized tungsten filament produces free electrons which are guided by a steering magnet into the source-material-containing crucible to instigate resistive heating of the material.
2.1.3 Inductively Coupled Plasma Etching

Inductively coupled plasmas have many advantages, including high density and readily stable plasma, low ion damage, facile scalability, and tailored control. "Inductively coupled" implies the plasma is generated through inductive coupling, meaning the plasma density is robust enough to form a closed circuit[48]. An antenna coil induces a time-varying magnetic field, per Faraday's law, which produces an induction to generate and sustain the plasma[48]. The resulting plasma can then radicalize the plasma constituents for reactive interactions with the substrate surface or bombard the surface with positive ion species that then act to etch away at the surface material[49].

ICPs were initially introduced into the semiconductor manufacturing process for their etching capabilities but have since been developed for ashing, ion implantation, and deposition. In this work, ICP etching is used for photoresist etching, descumming, and silicon anisotropic etching using a fluorine-based plasma.

2.1.4 Plasma-Enhanced Chemical-Vapor Deposition

Plasma-enhanced chemical-vapor deposition (PECVD) extends the applicability of chemical vapor deposition (CVD) for the fabrication of higher quality thin films that are otherwise impractical to form using wet chemical or physical vapor deposition techniques (PVD) [50]. Precursor monomers (organic or inorganic) are exposed to a high-energy plasma field and undergo rapid disintegration and radical polymerization, contributing to the following thin film deposition step. Standard silicon-based films produced using PECVD are silicon dioxide (SiO$_2$), silicon nitride (Si$_x$N$_y$), silicon oxy-nitride (SiO$_x$N$_y$), silicon carbide (SiC), and amorphous silicon (αSi)[51]. PECVD offers a higher deposition
rate than typical PVD techniques, utilizes both organic and inorganic precursors, and does not require a high operating temperature. The deposited films' high thermal and chemical stability leads to a resistance to corrosion and solvent durability, and target substrates are less limited in their geometries and compositions. However, PECVD often relies on highly toxic or explosive gases within the plasma stream and requires a stable and humidity-free deposition environment[50].

Silicon nitride films, $\text{Si}_x\text{N}_y$, are used widely in the solar cell industry as they provide excellent anti-reflection properties and can act as a passivation layer for bulk and surface passivation[52]. In this work, however, $\text{Si}_x\text{N}_y$ layers were used as an arsenic-sublimation barrier during high-temperature gallium arsenide annealing. Silane ($\text{SiH}_4$) and ammonia ($\text{NH}_3$) are the reactive processing precursors, while $\text{N}_2$ or $\text{Ar}$ is typically included as a dilutant. The chemical reaction occurs within a plasma-glow discharge, and the resultants adsorb to the substrate in the following reaction[53]:

$$\text{SiH}_4 + \text{NH}_3 \rightarrow \text{SiN}_x : \text{H} + \text{H}_2$$

Ellipsometry analysis determines the refractive index and thickness of $\text{Si}_x\text{N}_y$ layers. The refractive index ($n$) of $\text{Si}_x\text{N}_y$ is typically in the range of 1.9 and 2.4 and details the stoichiometry of $\text{Si}_x\text{N}_y$ according to the following relationship, proposed by Dauwe[54]:

$$n = 1.35 + 0.74 \frac{[\text{Si}]}{[\text{N}]}, \quad (2.4)$$

Essential considerations during silicon nitride film deposition are the residual stress stored within the film and the degree of hydrogenation. Residual film stress becomes more apparent for thicker films, leading to cracking and thermal degradation. This residual stress
can also affect optical modes and introduce birefringence[55]. A common technique to measure residual stress is using the wafer curvature technique, which requires measuring the surface curvature of the substrate before and after deposition. The effects of residual stress can be mitigated through carrier-gas chemistry and using a lower frequency RF power[56].

Hydrogenation occurs because of the disassociation of Si – H and N–H bonds during film growth[57], which implants hydrogen within the film. The hydrogen content can severely affect film properties, especially concerning semiconductor device performance. Hydrogen can also affect the refractive index of silicon nitride and hinder the etch rate of nitride films. Hydrogenation is often associated with an incomplete gas reaction of NH$_3$ which leads to an increasing Si – H concentration during deposition[53]. Hydrogenation content is often characterized using FTIR analysis, and the effects of hydrogenation can be mitigated using low-pressure PECVD.

2.1.5 Wire Bonding

Gold wire bonding is the primary option for LED packaging and is among the most common techniques deployed for general semiconductor packaging processes[58]. In this work, wire bonding connects the SAW-generating interdigitated transducer devices to a gold-coated quarter-wavelength transmission line for impedance matching by way of gold bonding pads attached to the SAW devices. Au-ball wire bonding is typically mediated using an ultra-sonicating process to form an intermetallic compound and bridge the wire to its contact[59]. Initial intermetallic compound (IMC) formation occurs at the peripheral regions of the Au-ball contact, which then extends inward with increasing ultrasonication
The first wire bond forms a ball bond with the 1-μm gold pad connected to the aluminum device. The second wire bond connects to the quarter-wavelength transmission line and is formed with the gold layer deposited atop an electroless nickel (e-Ni) layer via an immersion gold (i-Ag) electrochemical process. The electroless nickel is about 2-μm thick, while the immersion gold layer is approximately 200-nm thick.

Gold-aluminum bonds on the device side can form an undesired intermetallic material known as "purple" plague during higher-temperature processes. Purple plague develops from an intermetallic AuAl₂ compound, which is purple in color[60]. Purple plague leads to contact weakening, susceptibility to failure with shock or vibration, higher saturation voltages, and increased series resistances[60]. For this reason, a 10-nm titanium layer is included in between the gold and aluminum layers, which additionally acts as an adhesion layer. Other intermetallic "plague" materials can form under the appropriate processing or operating conditions, such as "white" plague and "tan" plague.

**Figure 2.4**: Wire bonding is completed to connect the interdigitated transducer devices to the quarter-wavelength transmission line. Gold ball bonds are formed on the gold bonding pads incorporated into the SAW-generating devices and are then connected to the Cu-plated laminate, which has undergone electroless-nickel/immersion-gold electrochemical processing.
2.2 Characterization Techniques

2.2.1 Scanning Electron Microscopy and Energy Dispersive Spectroscopy

In scanning electron microscopy, a primary electron beam is focused onto the surface of a specimen and produces a variety of characteristic particles used in spatial imaging and characterization of the specimen[61], [62]. The primary components of an SEM are the electron source, the magnetic lens column, the electron detector, and the sample chamber. The most common electron source is a tungsten electron filament due to its low price, high reliability, and low magnification suitability. A solid-state crystal electron source can be used for higher resolution imaging; however, these crystals often require a significantly higher vacuum to avoid filament contamination. The focusing column for an SEM utilizes an electromagnet coil to control the trajectories of the electrons and is further adjusted by the current applied to the coils. The diameter of the electron beam can be magnified or de-magnified, resulting in a variable focal length[62].
The detectors used in SEM analysis are dependent on the particles of interest. Figure 2.5 details the different particles produced by scattering the primary electron particles and describes the scattering volume for each resulting particle. Secondary electron imaging is the primary technique used in this work to record surface topography. Secondary electrons are typically detected using a three-step process: (1) captured electrons are converted into a light signal using a scintillator; (2) the light is transferred away from the sample chamber, often outside of the vacuum chamber or column; (3) the transferred light is converted back into an electron signal where it undergoes an electron-multiplying process to boost the electronic signal[63]. This process allows for electrons to be analyzed far away from the sample chamber, otherwise leading to faster degradation of the detector and more frequent calibration due to sample chamber contaminates.

**Figure 2.5:** In electron microscopy, the incident-focused electron beam generates a variety of characteristic particles that are all used for their own form of analysis. In scanning electron microscopy, secondary electrons are studied to generate an electron image of the studied topology. Backscattered electrons can also be studied to determine compositional variations or to observe grain boundaries in polycrystalline specimen.
Backscattered electron imaging observes the compositional variation within a sample[64] or the different grains of a polycrystalline specimen[65]. Backscattered electron detection works on a principle like secondary electron detection, however, the bias applied to the detector is adjusted, or the detector position is changed to accommodate the backscattered electron signal and minimize secondary electron intrusion.

Energy dispersive spectroscopy (EDS) is used to gather the spectrum energy intensity of X-rays for chemical composition mapping. The characteristic X-rays produced during primary-electron bombardment produce a spectrum unique to each detectable element. The

**Figure 2.6:** The scattered characteristic particles produced during electron microscopy are used for various forms of analysis. The scattering volume within the bulk specimen determines the resolution of imaging, with auger electrons and secondary electrons producing the smallest scattering volume and characteristic X-rays producing the largest. The X-rays analyzed in electron microscopy are used in EDS for chemical composition mapping.
spectrum can then be differentiated to define the sample concentration. The most common X-ray detector used in EDS analysis is the Si(Li) detector.

### 2.2.2 Atomic Force Microscopy

Atomic force microscopy (AFM) profiles the parallel and perpendicular surface topography with atomic resolution by monitoring the interaction forces between a sharp tip mounted to a flexible cantilever and the specimen's surface. By analyzing tip-on-sample interaction forces, local material properties can also be investigated in addition to high-resolution topographical information, such as adhesion and material stiffness. AFM analysis is often coupled with other analytical techniques such as Raman microscopy or scanning-tunneling electron microscopy. There have been many modes of operation developed for AFM analysis that monitor the surface properties of the specimen, but within this work, only contact mode, non-contact mode, and intermittent-contact mode are discussed.

The monitored forces for these modes are the attractive van der Waals force and the repulsive electrostatic force as determined by Pauli's Exclusion principle[66]. The combined effect of these forces between the cantilever tip and the specimen surface is comparable to the bonding forces between two atoms. A bonding force, $E_b$, is measured at the equilibrium separation distance, which is described by the Lennard-Jones potential, as follows:

$$E_b = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right], \quad (2.5)$$
where $\varepsilon$ is the potential well depth and $\sigma$ is the hard-sphere radius. The first term is associated with the pseudo-repulsive force attributed to the Pauli Exclusion principle and increases precipitously for radii constituting overlapping electron clouds between atoms. The second term is attributed to the attractive van der Waals dispersion forces, dominating large distances.

**Figure 2.7:** The Lennard-Jones potential is used to describe the interatomic forces between the cantilever tip and the sample surface. The different modes of AFM analysis function within different regimes of the interatomic force diagram.

The measurement regimes for each described modes of operation have been illustrated in Fig. 2.7, which also describes the Lennard-Jones potential as a function of probe-to-surface distance. Contact-mode AFM is the primary technique used to image standing SAWs in this work due to the relatively small changes in surface topography and
the dynamic behavior of the acoustic surface, which would otherwise complicate frequency-driven contact modes of AFM analysis.

Contact Mode

In the contact mode, the sharp-tipped probe drags along the sample surface, with an approximate operating distance of an atomic radius. As the AFM probe approaches the sample surface, the van der Waals attractive force increases, such that the probe deflects towards the surface. Eventually, the net forces acting upon the probe's tip begins to decrease as the repulsive force increases. The repulsive forces from the surface atoms then cause the cantilever to bend according to changes in topography. The interacting forces between the probe tip and the sample surface are on the order of $10^{-8}$ to $10^{-6}$ N. Due to the hard contact of the AFM probe, the cantilever stiffness is required to be less than the effective spring constant holding the specimen atoms together, otherwise the cantilever tip affects the surface topography of the sample. In contact-mode AFM, the feedback system works in either constant-force or constant-height mode and the feedback system response time becomes the limiting factor in the scanning speed.

Non-Contact Mode

Contact mode AFM analysis requires low cantilever stiffness, relative to the sample's atomic effective-spring constant, otherwise the analysis can result in damage to the sample surface. Vibrating cantilever techniques have been developed to mitigate the damage to softer sample such as gels, liquids, or biological samples. In non-contact mode, a stiff cantilever is vibrated near its resonant frequency within
a proximity of the sample surface. A stiffer cantilever is necessary for this mode of operation to minimize the pulling effect on the cantilever from the van der Waals force and substantial pulling on the cantilever leads to an unstable feedback effect and requires slower scan speeds. The interacting forces between the probe tip and the sample surface is a function of probe proximity and tends to be small, typically on the order of $10^{-12}$ N[66]. The feedback system for non-contact AFM moderates a constant resonant frequency and vibrational amplitude to generate the sample topography[66].

**Intermittent/Tapping Mode**

Intermittent mode, or tapping mode, AFM analysis relies on a principle like non-contact mode, however, the amplitude of oscillation is often much larger, and the tip is expected to make brief contact with the sample surface during each oscillation cycle. The sample interactions change the amplitude, resonance frequency, and phase angle for the cantilever which are all used in this mode's analysis. Tapping mode can provide a resolution similar to contact mode, while mitigating surface damage to the sample. Tapping mode does exhibit some disadvantages compared to contact and non-contact modes, such as slower scan speeds and a more complex AFM setup. In general, tapping mode is ideal for softer samples requiring improved lateral resolution.
2.2.3 Vector Network Analyzer

A vector network analyzer (VNA) is an instrument that measures the frequency response and power of passive or active components using a high-speed signal, either as individual parts or as a network composed of many components[67]. The computer connected to the VNA calculates the key parameters such as return loss, insertion loss, and

Figure 2.8: (a) Contact mode AFM drags the tip of the cantilever across the surface to profile the topology. (b) Intermittent AFM taps the surface to mitigate the damage associated with contact mode AFM for softer materials. (c) Non-contact mode AFM vibrates the cantilever above the surface at a resonant frequency to further minimize damage at the cost of longer scan times.
the scattering or admittance parameters of a system using the measured amplitude and phase of the high-frequency signal. Zhang, et al. provide a simplified VNA architecture blog diagram[67], shown in Fig. 2.9. In this work, a VNA was used to measure the device performance of the interdigitated transducer devices before wire bonding.

![Figure 2.9: A simplified architecture block diagram for a vector network analyzer](image)

*Figure 2.9: A simplified architecture block diagram for a vector network analyzer describes how devices are characterized. A continuous-wave source is an input into the device-under-test, and signal amplitude and phase are measured.*

### 2.2.4 Photoluminescence Spectroscopy

Photoluminescence spectroscopy (PL) is a valuable technique to characterize materials and study the optical properties or processes. PL is often combined with
complementary analytical techniques to obtain a complete picture regarding the dynamic processes of a system. For example, indium gallium arsenide (InGaAs) quantum wells (QW) have been grown into a GaAs matrix, and PL is used to characterize the quantum well's bandgap after growth or thermal annealing. However, an additional analytical technique such as secondary ion mass spectroscopy (SIMS) is necessary to determine the precise concentration profile of the InGaAs QW, which readily changes during thermal annealing processes.

For semiconductor analysis, photoluminescence spectroscopy relies on the radiative emission and absorption of photons to provide information about bandgap energy levels. Photoluminescent spectroscopy is most effective for direct bandgap materials on account of the higher rate of stimulated emission. Due to the valleys and peaks of the conduction and valence band being positioned directly in line with each other, with respect to the wave vector axis, momentum is conserved during the emission process, thus significantly increasing the chances of photorecombination. This conservation of momentum is not as readily possible for indirect bandgap materials and requires a mediating particle such as a phonon to ensure[13]. The bandgaps for direct and indirect materials are depicted in Fig. 2.10.
Figure 2.10: Photoluminescent spectroscopy is most effective for direct bandgap materials on account of the higher rate of stimulated emission. Due to the valleys and peaks of the conduction and valence band being positioned directly in line with each other, with respect to the wave vector axis, momentum is conserved during the emission process, thus greatly increasing the chances of photorecombination.

2.2.5 Raman Spectroscopy

Raman spectroscopy is used extensively in this work for its demonstrated ability to measure the strain values of surface acoustic waves. A classical description of the Raman process begins by considering a light wave with an electric field that oscillates according to the following equation

\[ E = E_0 \cos(\omega t), \]  

(2.6)
where $E_0$ is the maximum value of the electric field, and $\omega$ is the field's oscillating frequency. When a molecule is present within this field, a dipole moment is induced due to the nuclei being attracted to the negative pole, while the electrons are attracted to the positive pole. This dipole moment can be expressed as

$$\mu_{ind} = \alpha E_0,$$  \hspace{1cm} (2.7)

where $\alpha$ is the proportionality constant known as the polarizability of the molecule. The magnitude of $\alpha$ can vary as molecular bonds are stretched or compressed from the bond's equilibrium position. This effect is most apparent at the natural vibrational frequency, $\omega_0$, of the bond, and for low amplitude vibrations, $\alpha$ can vary as follows[68]:

$$\alpha = \alpha_0 + (\Delta \alpha) \cos(\omega_0 t),$$  \hspace{1cm} (2.8)

where $\alpha_0$ is the equilibrium polarizability, and $\Delta \alpha$ is the susceptibility or the maximum polarization variation. Higher-order terms can exist for the polarizability of the molecule; however, for the case of small vibrations, the 1st order expansion term is the only included term[69]. Substituting Eq. (2.6) and (2.8) into Eq. (2.7) leads to

$$\mu_{ind} = [\alpha_0 + (\Delta \alpha) \cos(\omega_0 t)][E_0 \cos(\omega t)],$$  \hspace{1cm} (2.9)

and rearranging according to the cosine product identity yields

$$\mu_{ind} = \alpha_0 E_0 \cos(\omega t) + (1/2)\Delta \alpha E_0 [\cos(\omega + \omega_0) t + \cos(\omega - \omega_0) t].$$  \hspace{1cm} (2.10)

The induced dipole moment oscillates with components of frequency $\omega$, $\omega - \omega_0$, and $\omega + \omega_0$. The first frequency is the familiar Rayleigh scattering event, while the other two frequencies are the Stokes and anti-Stokes radiation scattering events. Stokes scattering events have a higher statistical likelihood of being observed than anti-Stokes
scattering events due to anti-Stokes scattering requiring a participating electron to already be in a higher energy state, which is statistically less likely. This simple approach to Raman scattering connects the vibrational nature of the molecular bonds and the oscillating electric dipole[68]. A more in-depth description of Raman scattering within crystal domains is provided in ‘Chapter 5’ of this work. Silicon and gallium arsenide are among the more commonly studied semiconductor materials. Figure 2.11 depicts the Raman modes for zinc-blende gallium arsenide and its 291 cm\(^{-1}\) Raman peak shift.

![Raman spectrum for GaAs](image)

**Figure 2.11:** The Raman spectrum for GaAs features a strong peak associated with the longitudinal optical phonon around 291 cm\(^{-1}\).
CHAPTER 3: ACOUSTIC WAVE THEORY AND SURFACE

ACOUSTIC WAVES

3.1 General Description of Acoustic Waves in Solid Media

3.1.1 Bulk Acoustic Waves

Within a solid material, elastic displacement denotes a change in the relative position of atoms or particles, often specified in terms of strain, with respect to a stated equilibrium position. The internal forces generated within this elastic displacement tend to return the material to its equilibrium and unstrained state\[70\]. Plastic (or inelastic) deformation occurs when the displacement within a solid material reaches a point in which the atomic arrangement is permanently changed. The internal forces within the medium cannot return the material to its equilibrium position.

Figure 3.1: Plane waves are described as a moving wavefront in which all values are constant over the coronal plane. (a) Longitudinal planes are polarized along the direction of the acoustic wave propagation vector. (b) Transverse waves are perpendicular to the propagation vector and are further described as vertical and horizontal shear waves.
Acoustic waves are a propagating phenomenon involving the stresses and strains associated with elastic displacement. Plane waves are the simplest form of acoustic waves in an isotropic medium. Plane waves are defined by moving planes called wavefronts within which all variables are constant over the plane normal to the direction of travel[27], [70]. In general, acoustic plane waves propagating through solid media are described as a linear combination of their longitudinal (pressure) and transverse (shear) wave components[29]. The vibrational mode of the longitudinal wave is polarized along the direction of the acoustic wave propagation vector, while the transverse waves are perpendicular to the propagation vector, as depicted in Fig. 3.1. An acoustic wave that is described as being purely longitudinal or purely transverse is referred to as bulk acoustic waves (BAW)[29]. BAW propagation in an elastic and isotropic medium gives rise to different phase velocities, \( V_l \) and \( V_t \), for the longitudinal and transverse (shear) wave modes. In zinc-blende gallium arsenide, for waves traveling in the \([100]\) direction, the expression for wave speed for both the longitudinal and transverse cases can be described as:

\[
V_l = \sqrt{\frac{c_{11}}{\rho}}, \\
V_t = \sqrt{\frac{c_{44}}{\rho}},
\]

where \( c_{ij} \) are the components of the elasticity matrix and \( \rho \) is the density of the substrate.

In a propagation direction in gallium arsenide that reveals the anisotropic nature of the crystal structure, such as the \([110]\) direction, the longitudinal velocity remains unchanged. However, the transverse mode splits into two orthogonally polarized modes such that the transverse wave velocities are defined as:
\[ V_{t\parallel} = \sqrt{\frac{c_{44}}{\rho}} , \quad (3.3) \]
\[ V_{t\perp} = \sqrt{\frac{(c_{11} - c_{12})}{2\rho}} . \quad (3.4) \]

These quasi-shear waves are referred to as fast-shear and slow-shear waves, and for a specified direction of propagation, there exist three independent acoustic waves, as shown below in Fig. 3.2. The fast-shear wave velocity remains unchanged for rotations about the (001) plane, while the slow-shear and longitudinal waves undergo steady changes in their respective velocities, demonstrating a 4-fold symmetry for both crystallographic orientations. This is due to the fast-shear wave's direction of polarization remaining unchanged with respect to the (001) crystal plane during the rotation, while the slow-shear and longitudinal waves phase velocity demonstrate a directional dependence.

**Figure 3.2**: The normalized slowness (inverse velocity, \( v^{-1} \)) of the different acoustic modes traveling on the (001) planes of (a) silicon and (b) tellurium oxide. The shear modes split due to the anisotropic nature of the diamond crystal structure of silicon, demonstrating the slow and fast shear wave modes in the <110> direction. This figure is provided by Ref. [29].
When considering the effect of a boundary on acoustic shear waves, Hashimoto explains that the polarization direction of bulk shear waves is often described as the relative direction with respect to the substrate surface[29]. Shear waves with a polarization perpendicular and parallel to the substrate surface are called shear-vertical (SV) and shear-horizontal (SH) BAWs. The velocity of these waves is a function of the anisotropy of the elastic medium.

![Diagram of BAW propagation](image)

**Figure 3.3**: As the BAW extends into the bulk of the substrate, the power density decreases inversely proportional to the square root of the propagation distance.

### 3.1.2 Surface Acoustic Waves

At the surface boundary of a semi-infinite substrate, one can consider the generation of BAWs into the surface because of an elastic impact on the substrate surface. In an isotropic medium, the BAW power spreads uniformly in all directions with equal speed and suggests the power density decreases inversely proportional to the square root of the
propagation distance[29], as shown in Fig. 3.3. The surface boundary condition does not allow SV- and L-type BAWs to generate parallel to the surface. However, assuming a traction-free surface, the boundary conditions allow for coupling the SV- and L-type BAW components near the surface called a Rayleigh-type surface acoustic wave (SAW). Figure 3.4 illustrates the SAW structure and depicts the decaying amplitude as the wave extends into the bulk.

![Figure 3.4: A coupling of SV-type and L-type BAWs form the Rayleigh-type SAW. The energy is confined to the surface in that the wave amplitude decays exponentially into the bulk of the substrate.](image)

Lord Rayleigh first described the SAW in 1885 in a publication that details the behavior of acoustic waves confined to the free surface plane of a homogeneous isotropic elastic solid of infinite depth[71]. SAWs propagate along the plane surface with an amplitude decaying exponentially away from the surface. SAW velocities are smaller than their SV-BAW component, and the resulting elliptical motion of the material is in the sagittal plane[70]. Figure 3.5 depicts the elliptical motion of the individual atoms of a
SAW. A comprehensive mathematical description of SAW fields is explored later in this chapter.

Rayleigh waves can further describe two other acoustic waves known as pseudo-surface acoustic waves (PSAW) and leaky surface acoustic waves (LSAW). PSAWs are possible in anisotropic media and exist only for propagation directions perpendicular to the displacement of the slow shear wave. As a result, the PSAW does not have a slow shear wave component, and the PSAW velocity is then slightly faster than the slow shear wave[70]. PSAWs are considered surface waves because they do not inherently attenuate as they propagate, and their wave amplitude decays exponentially with increasing depth. For example, Rayleigh-type waves exist on the Y-Z plane for quartz, but the presence of a PSAW is found for a propagation angle of 153° with respect to the z-axis[72].
LSAWs occur for a PSAW propagation direction slightly different from what the boundary condition requires. Deviation from the PSAW direction results in a small slow-shear bulk wave component that causes attenuation by carrying some wave energy into the bulk. Acoustic waves devices can be organized into three acoustic mode categories in bulk, solid material: bulk acoustic waves (BAW), surface acoustic waves (SAW), and pseudo-surface acoustic waves (PSAW).

### 3.1.3 Attenuation Mechanisms of Acoustic Waves in Solid Media

The intrinsic attenuation of acoustic waves imposes an upper limit to the quality factor of mechanical oscillators. The quality factor, $Q$-factor, is defined as $2\pi$ times the ratio between the total stored energy of the wave and the energy dissipated per cycle of oscillation. The $Q$-factor of a device is an essential parameter for mechanical oscillators in micro/nano-electromechanical systems (MEMS/NEMS)[73]. The attenuation of sub-THz acoustic waves in solid media is generally attributed to three separate mechanisms, the latter two being an intrinsic process and are closely associated with thermal phenomena[27]:

1. Inhomogeneity in propagation media from crystal defects or boundary layers results in waves scattering. This temperature-independent mechanism is typically avoided or mitigated through sufficient material preparation and device fabrication[27], [29].

2. Thermal relaxation due to temperature gradients brought about by the stretching and compression of the solid media is typically referred to as thermoelastic dissipation (TED)[73], [74].
Scattering of coherent waves due to thermal lattice vibrations, otherwise known as Akhiezer damping (AD), results in the relaxation of thermally excited phonons to a local equilibrium[73], [75].

In the case of thermoelastic dissipation, the temperature gradient incited by the volume-changing acoustic strain field results in heat flow, leading to entropy generation. This mechanism is only present in longitudinal waves as shear waves do not attribute to volume changes in the media. The $Q$-factor associated with TED is given by[75]:

$$Q^{-1}_{TED} = \frac{\alpha^2 ET}{C_v} \frac{\omega \tau_{td}}{1 + (\omega \tau_{td})^2},$$

where $C_v$ is the specific heat capacity at constant volume, $\alpha$ is the coefficient of thermal expansion, $E$ is the Young's modulus of the material, $T$ is the mean system temperature, $\omega$ is the angular frequency of the acoustic mode, and $\tau_{td}$ is the thermal diffusion time. For a temperature gradient across a length of characteristic width $w$ (often associated with the wavelength of the acoustic mode) and material with thermal conductivity $\kappa$, the thermal diffusion time of relaxation can be further expressed as $\tau_{td} = \frac{w^2 C_v}{\pi^2 \kappa}$. It should then be noted that for small characteristic widths, the $Q$-factor associated with thermo-elastic dissipation increases, and the mechanism of TED soon becomes negligible.

In the case of Akhiezer damping, attenuation occurs due to the flow of heat between different phonon modes, arising from strain fields modulating thermal phonon frequencies. Under the presence of an applied strain field, whether it is uniform or non-uniform, a temperature difference occurs between different phonon modes, which tend to relax toward
the mean temperature of the system. The $Q$-factor associated with Akheizer damping can be defined as:

$$Q^{-1} = \frac{C_p T a v^2}{\rho v^2} \frac{\omega \tau_{ph-ph}}{1 + (\omega \tau_{ph-ph})^2},$$

where $C_p$ is the specific heat capacity at constant pressure, $v$ is the acoustic velocity, and $\tau_{ph-ph}$ is a time constant associated with the phonon energy mean transfer time. $\lambda_{av}$ is the mean value of the Grünesian parameter. Grünesian parameters are mode-dependent material values proportional to the ratio between phonon energy dispersion and the locally applied strain. A crystal under compression would see an increase in this ratio, while a crystal experiencing expansion would see a decrease in this ratio\cite{76}. For $\omega \tau_{ph-ph} \leq 1$, the $Q$-factor decreases, implying this effect emerges as the main mechanism of acoustic attenuation for higher frequency systems.

### 3.2 Rayleigh Waves and Piezoelectric Materials

#### 3.2.1 The Wave Equation and Non-Piezoelectric SAW Formulation

The mathematical description of acoustic waves in solid media begins with the wave equation, which relates the displacement, $u$, of a particle from its undisturbed location to the local stress, $T$, acting upon the particle:

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial T_{ij}}{\partial x_j},$$

where $\rho$ is the substrate density, $u_i$ are the three spatial components ($i = 1,2,3$) of the substrate, and $T_{ij}$ are the components of the stress tensor.
While there are many sources to choose from to derive the solutions to the wave equation concerning surface acoustic waves in an isotropic medium, the primary sources for the theory outlined here are drawn from Shearer[77], Biryukev[78], and Auld[27]. In the case of a non-piezoelectric material, the right side of the wave equation can be expanded by including Hooke's Law for non-piezoelectric materials, defined as

$$T_{ij} = c_{ijkl}S_{kl}, \quad (3.8)$$

where $c_{ijkl}$ are the components of the elasticity tensor and $S_{kl}$ are the components of the strain tensor defined as
\[ S_{kl} = \frac{1}{2} \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right). \]  

(3.9)

For the case of a linear, isotropic substrate, Eq. (3.8) is first reformulated as

\[ T_{ij} = \lambda \delta_{ij} S_{kk} + 2 \mu S_{ij}, \]  

(3.10)

where the elasticity tensor has been broken down into the Lamé parameters, \( \lambda \) and \( \mu \). The linear case is not often practical in typical engineering applications; however, it is a reasonable approach for systems such as single-crystal silicon. After combining Eqs. (3.9) and (3.10) and substituting into Eq. (3.7), we obtain the 3-dimensional wave equation for a non-piezoelectric, isotropic medium:

\[ \frac{\rho}{2} \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial}{\partial x_j} \left[ \lambda \delta_{ij} \frac{\partial u_k}{\partial x_l \partial x_k} + \mu \left( \frac{\partial u_j}{\partial x_l} + \frac{\partial u_l}{\partial x_j} \right) \right]. \]  

(3.11)

Lastly, it can be shown that Eq. (3.11) can be split into solutions for longitudinal and shear waves using vector transformations, becoming

\[ \ddot{\mathbf{u}} = c_l^2 \nabla \cdot \mathbf{u} - c_t^2 \nabla \times \nabla \times \mathbf{u}, \]  

(3.12)

where \( \ddot{\mathbf{u}} \) is the 2\(^{nd} \) time derivative of the displacement vector, and the longitudinal wave velocity, \( c_l \), and the shear wave velocity, \( c_t \), are given by

\[ c_l = \sqrt{\frac{\lambda + 2\mu}{\rho}}, \]  

(3.13)

and

\[ c_t = \sqrt{\frac{\mu}{\rho}}. \]  

(3.14)
It is therefore convenient to separate the displacement vector into its independent longitudinal and transverse modes per the Helmholtz decomposition, which allows the displacement vector \( \mathbf{u} \) be defined as

\[
\mathbf{u} = \nabla \varphi + \nabla \times \boldsymbol{\psi},
\]

(3.15)

\[
\nabla \times (\nabla \varphi) = 0,
\]

(3.16)

and

\[
\nabla \cdot \boldsymbol{\psi} = 0,
\]

(3.17)

where the scalar potential, \( \varphi \), represents the curl-free longitudinal wave and the vector potential, \( \boldsymbol{\psi} \), represents the shear wave. Recognizing the independent longitudinal and shear waves must satisfy their respective wave equation, the equations for \( \varphi \) and \( \boldsymbol{\psi} \) have the form

\[
\nabla^2 \varphi = \frac{1}{c_l^2} \frac{\partial^2 \varphi}{\partial t^2},
\]

(3.18)

and

\[
\nabla^2 \boldsymbol{\psi} = \frac{1}{c_l^2} \frac{\partial^2 \boldsymbol{\psi}}{\partial t^2}.
\]

(3.19)

For the case of surface acoustic waves propagating along the sagittal plane \((x_1, x_3)\), the vector potential possesses only a single non-zero component, \( \psi_2 \), and the scalar potential does not change with respect to the \( x_2 \)-direction. Equation (3.15) is then described by the formulas
\[ u_1 = \frac{\partial \varphi}{\partial x_1} - \frac{\partial \psi_2}{\partial x_3}, \quad (3.20a) \]

\[ u_2 = 0, \quad (3.20b) \]

and

\[ u_3 = \frac{\partial \varphi}{\partial x_3} + \frac{\partial \psi_2}{\partial x_1}. \quad (3.20c) \]

Using the separation of variables technique, the solutions of Eq. (3.18) and (3.19) have the form

\[ \varphi = \varphi_0 \exp(px_3) \exp[i(k_{SAW} x_1 - \omega t)], \quad (3.21) \]

and

\[ \psi_2 = \psi_0 \exp(sx_3) \exp[i(k_{SAW} x_1 - \omega t)], \quad (3.22) \]

where \( \omega \) and \( k_{SAW} \) are the wave frequency and the SAW wave number, \( p \) and \( s \) are the attenuation coefficients for the longitudinal and shear waves propagating into the substrate, and \( \varphi_0 \) and \( \psi_0 \) are the amplitudes of the two respective waves. Substituting Eq. (3.20) and (3.21) into Eqs. (3.18) and (3.19) reveals the relationship \( p^2 = k_{SAW}^2 - k_l^2 \) and \( s^2 = k_{SAW}^2 - k_t^2 \), where \( k_l \) and \( k_t \) are the wave numbers for the longitudinal and transverse waves. Rearranging and simplifying both relationships gives

\[ p = \sqrt{1 - \left(\frac{c_{SAW}}{c_l}\right)^2}, \quad (3.23) \]

and
\[ s = \sqrt{1 - \left( \frac{c_{SAW}}{c_t} \right)^2}, \quad (3.24) \]

where \( c_{SAW} \) is the velocity of the SAW. It should be noted that for the attenuation of the longitudinal and shear waves to stay real, the SAW velocity must be slower than both the longitudinal and shear waves.

Combining Eqs. (3.20a) and (3.20c), with Eq. (3.10) we can define the non-zero components of the stress tensor:

\[ T_{11} = \lambda \Delta^2 \phi + 2\mu \left( \frac{\partial^2 \phi}{\partial x_1 \partial x_3} + \frac{\partial^2 \phi_2}{\partial x_1^2} \right), \quad (3.25) \]

\[ T_{22} = \lambda \Delta \phi, \quad (3.26) \]

\[ T_{33} = \lambda \Delta^2 \phi + 2\mu \left( \frac{\partial^2 \phi}{\partial x_3^2} + \frac{\partial^2 \phi_2}{\partial x_1 \partial x_3} \right), \quad (3.27) \]

and

\[ T_{13} = \mu \left( 2 \frac{\partial^2 \phi}{\partial x_1 \partial x_3} - \frac{\partial^2 \phi_2}{\partial x_3^2} + \frac{\partial^2 \phi_2}{\partial x_1^2} \right), \quad (3.28) \]

At the surface of the infinite half-space \((x_3 = 0)\), the boundary condition \( T_{13} = 0 \) must be held. By first recognizing

\[ k_t^2 = \frac{\mu}{\lambda + 2\mu} k_t^2 \]

and substituting Eqs. (3.21) and (3.22) into Eqs. (3.27) and (3.28) and simplifying into matrix form yields
\[
\begin{bmatrix}
(k_{SAW}^2 + s^2) & 2iqs \\
2iqp & -(k_{SAW}^2 + s^2)
\end{bmatrix}
\begin{bmatrix}
\varphi_0 \\
\psi_0
\end{bmatrix} = 0,
\] (3.30)

where the determinant of the characteristic matrix reveals the Rayleigh equation:

\[
(k_{SAW}^2 + s^2)^2 - 4k_{SAW}^2ps = 0,
\] (3.31)

whose solution for \(k_{SAW}\) details the velocity of the SAW. Further inspection of this solution reveals that the speed of the SAW is dispersion-less, and exact solutions require numerical solver methods.

### 3.2.2 The Crystal Structure of GaAs and the Piezoelectric Effect

The crystal structure of Gallium Arsenide is the cubic zinc-blende structure with a lattice spacing, \(a\), of 5.654 Å, and a space group of \(F\bar{4}3m\).[79], [80] In the unstrained zinc-blende unit cell, each atom is tetrahedrally oriented with four nearest neighbor counter-bonded atoms, as shown in Fig. 3.7.

The direct piezoelectric effect is the ability of a material to generate an electric charge in response to applied mechanical stress. The deformed internal structure of a piezoelectric material forces a separation of the crystal's positive and negative charge centers, resulting in a dipole-induced polarization. The nature of any piezoelectric material implies reversibility of the effect, such that an applied electric field produces a mechanical response; this is known as the indirect piezoelectric effect. The zinc-blende structure is among the most straightforward crystal structures to demonstrate the piezoelectric effect.
The Curie brothers discovered the direct piezoelectricity effect, in 1880, after recognizing the mechanical forces arising from an applied electric charge to materials like quartz, topaz, and Rochelle salt. The coinciding inverse piezoelectric effect was then mathematically deduced by Lippmann and soon confirmed experimentally by the Curie brothers the following year[81]. The first technological applications of the piezoelectric effect were realized in sonar technologies during the First World War by Langevin and Rutherford[82], [83].

**Figure 3.7:** The zinc-blende unit cell structure for Gallium Arsenide is a cubic structure with a lattice spacing of 5.654 Å and a space group of \( F\bar{4}3m \). Each atom is tetrahedrally oriented with four nearest neighbors of counter-bonded atoms. There are four gallium atoms and four arsenic atoms in a single unit cell.
The relationship between the elastic and dielectric behavior of piezoelectric materials is described through a set of coupled equations relating the crystal stress, \( T_{ij} \), and the electric displacement, \( D_i \).

\[
T_{ij} = c_{ijkl} S_{kl} + e_{ijk} E_k, \quad (3.31)
\]

and

\[
D_i = -\varepsilon_{ij} E_j + e_{ijk} S_{jk}, \quad (3.32)
\]

where \( c_{ijkl} \) are the components of the 4\(^{th}\)-rank elasticity matrix, \( e_{ijk} \) are the components of the 3\(^{rd}\)-rank piezoelectric coupling tensor, and \( \varepsilon_{ij} \) is the relative permittivity matrix. Equation (3.31) is an extension of Hooke's law to incorporate the indirect piezoelectric effect from the electric field, and Eq. (3.33) includes the polarization density, \( P_i \), induced by the dipole moments of the piezoelectric crystal, defined as:

\[P_i = \sum_j e_{ijk} E_j \]
\[ P_i = e_{ijk} S_{jk}, \] (3.33)

The elasticity matrix for the zinc-blende structure with respect to a crystallographic axis with \( \hat{x}_1 = [100], \hat{x}_2 = [010], \hat{x}_3 = [001] \), is given as

\[
c = \begin{bmatrix}
  c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\
  c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\
  c_{12} & c_{12} & c_{12} & 0 & 0 & 0 \\
  0 & 0 & 0 & c_{44} & 0 & 0 \\
  0 & 0 & 0 & 0 & c_{44} & 0 \\
  0 & 0 & 0 & 0 & 0 & c_{44}
\end{bmatrix}, \] (3.34)

where, \( c_{11} = 11.83 \times 10^{10} \text{ N/m}^2 \), \( c_{11} = 5.32 \times 10^{10} \text{ N/m}^2 \), and \( c_{11} = 5.95 \times 10^{10} \text{ N/m}^2 \) for GaAs at 300K. Birman, et al. show there exists only a single piezoelectric constant[84], \( e_{14} \), in the zinc-blende structure and, for GaAs, is equal to 0.16 \( C/m^2 \)[85].

The piezoelectric matrix for gallium arsenide is defined as:

\[
e = \begin{bmatrix}
  0 & 0 & 0 & e_{14} & 0 & 0 \\
  0 & 0 & 0 & 0 & e_{14} & 0 \\
  0 & 0 & 0 & 0 & 0 & e_{14}
\end{bmatrix}. \] (3.35)

Both \( c_{ijkl} \) and \( e_{ijk} \) are represented in the Mandel-Voigt notation, taking advantage of the crystalline symmetry necessary to describe the zinc-blende structure concisely.

### 3.2.3 Surface Acoustic Waves in Piezoelectric Media

The relationship between the elastic displacement and the piezoelectric potential of a surface acoustic wave is described by solving the acoustic wave equation in conjunction with a nondivergent electric displacement \( D \), in accordance with Gauss' law for electric insulators,

\[ \nabla \cdot D = 0, \] (3.36)
where Eq. (3.10) is to be expressed in terms of the modified Hooke’s law, described in Eq. (3.31), and Eq. (3.27) is expressed in terms of the electric displacement described in Eq. (3.32). It is essential to recognize that the velocities of elastic waves are typically five orders of magnitude slower than the velocities of electromagnetic radiation. This observation enables the quasi-static approximation of a curl-free electric field, $\nabla \times E = 0$, and allows for the electric field to be expressed as a time-varying scalar potential, $\phi$, such that

$$E = -\nabla \phi. \quad (3.37)$$

Substituting Eqs. (3.9), (3.31), (3.32), and (3.37) into Eqs. (3.7) and (3.36) provides the coupled set of equations describing the motion of acoustic waves in piezoelectric materials:

$$\rho \frac{\partial^2 u_i}{\partial t^2} - c_{ijkl} \frac{\partial^2 u_k}{\partial x_j \partial x_l} - e_{kl} \frac{\partial^2 \phi}{\partial x_k \partial x_l} = 0, \quad (3.38)$$

and

$$e_{ikt} \frac{\partial^2 u_l}{\partial x_t \partial x_k} - \epsilon_{ik} \frac{\partial^2 \phi}{\partial x_i \partial x_k} = 0. \quad (3.39)$$

The solutions to Eqs. (3.38) and (3.39) are assumed to have the form

$$u_i = A_i \exp(i k_{SAW} l_3 x_3) \exp[i k_{SAW}(l_1 x_1 - vt)] , \quad (3.40)$$

and

$$\phi = A_4 \exp(i k_{SAW} l_3 x_3) \exp[i k_{SAW}(l_1 x_1 - vt)] , \quad (3.41)$$

where $A_i$ is the maximum wave amplitude, $l_1$, and $l_3$ are attenuation coefficients, and $k_{SAW}$ and $v$ are the wavenumber and wave velocity, respectively. Substituting Eq. (3.40) and
(3.41) into Eqs. (3.38) and (3.39) reveal a 4-by-4 square matrix, parameterized by the vector \( A_i \). Solving the characteristic equation associated with this matrix reveals an 8\(^{th}\) order polynomial that must be solved for \( l_3 \), for which there are eight solutions, all of which are functions of \( k_{SAW} \). Four of these solutions are complex and therefore are ignored as this would result in non-decaying waves into the substrate. The remaining four solutions then allow for Eqs. (3.40) and (3.41) to be written as a linear combination of the four \( l_3 \) parameters provided here as

\[
u_i = \sum_{r=1}^{4} A_{l,r} \exp(ik_{SAW}l_3,r x_3) \exp[ik_{SAW}(l_1 x_1 + l_2 x_2 - vt)], \quad (3.42)
\]

and

\[
\phi = \sum_{r=1}^{4} A_{4,r} \exp(ik_{SAW}l_3,r x_3) \exp[ik_{SAW}(l_1 x_1 + l_2 x_2 - vt)], \quad (3.43)
\]

Like the boundary condition described in the previous section, the stress-free boundary condition can be applied at the surface:

\[
T_{l3} = c_{l3kl} \frac{\partial u_i}{\partial x_k} + e_{kl3} \frac{\partial \phi}{\partial x_l} = 0, \text{ at } x_3 = 0. \quad (3.44)
\]

In addition, the continuity of normal electric displacement must be recognized at the surface boundary between the free space above the dielectric and the dielectric itself:

\[
D_3 = \epsilon_0 \frac{\partial \phi}{\partial x_3}, \text{ for } x_3 > 0, \quad (3.45)
\]

and
\[ D_3 = \varepsilon_{3kl} \frac{\partial u_k}{\partial x_l} - \varepsilon_{3k} \frac{\partial \phi}{\partial x_k}, \text{ for } x_3 < 0. \]  

(3.46)

This relationship is further simplified as

\[ \varepsilon_{3kl} \frac{\partial u_k}{\partial x_l} + \varepsilon_{3k} \frac{\partial \phi}{\partial x_k} - \varepsilon_0 k_{SAW} \phi = 0, \text{ at } x_3 = 0. \]  

(3.47)

Substituting Eqs. (3.42) and (3.43) into Eqs. (3.44) and (3.47) produce a 4-by-4 matrix that for any practical scenario, explicit solutions of surface wave fields in this system are not possible, and numerical computations are necessary. Numerical computations describing the behavior of SAWs generated by interdigitated transducer devices are discussed in Chapters 6 and 7 of this dissertation.

3.3 Conclusion

The acoustic theory, which outlines the mechanical and electrical behavior of SAW fields, is outlined for both non-piezoelectric and piezoelectric materials. Acoustic attenuation mechanisms are also discussed with respect to the frequency domain of interest in this study. Analytical expressions are difficult to acquire for both the non-piezoelectric and piezoelectric material cases, and numerical methods must be utilized to provide a complete picture of surface acoustic fields. The next chapter of this dissertation discusses techniques and device designs for generating powerful acoustic waves using IDT devices fabricated on gallium arsenide substrates. Vector network analysis characterizes the device’s electrical performance, and AFM measures surface acoustic fields generated by interdigitated transducers.
CHAPTER 4: INTERDIGITATED TRANSDUCER DEVICE

FABRICATION AND CHARACTERIZATION

4.1 Piezoelectric Sensors and Their Applications

Piezoelectric sensors and actuators play a vital role in various practical engineering applications. Sensors convert a mechanical or chemical input into an electric output, while actuators utilize a contrasting function in that an electric input produces a mechanical output. Technologies that function with a bidirectional conversion principle are referred to as transducers. The principles of conversion between mechanical and electric quantities of sensors and actuators make piezoelectric materials desirable systems for developing these technologies[82].

Piezoelectric sensing principles exploit the impact of physical quantities of interest on electrical sensor characteristics. For example, mass loading shifts the resonant frequency of a specific vibration mode inside a quartz crystal microbalance (QCM)[86]. This makes a QCM and other thickness-shear mode resonators reliable devices for measuring film thicknesses or determining liquid densities and viscosities. Additionally, time measurements of wave propagation between transducers allow time-of-flight calculations to characterize physical or chemical interactions with the traveling wave's surface. Antlinger et al. demonstrate a sensing technique to determine the acoustic impedance of an imposing liquid for condition monitoring applications using time-of-flight measurements[87].

Acoustic-based piezoelectric sensors are typically passive components readily coupled with wireless electronic systems. These small and robust sensors do not require
any embedded electronics, which presents many advantages for a wide range of applications, particularly in extreme environments. SAW sensors are particularly useful for temperature, pressure/strain, and chemical sensing applications. Various material factors are considered in selecting a suitable substrate for SAW-based sensors, such as the electromechanical coupling coefficient ($k^2$), SAW velocity or high-frequency response, and temperature coefficient of delay ($TCD$).[88]

Campbell et al. provide an exhaustive list of the application of SAW devices concerning their signal processing capabilities, but only a select choice is provided in the following table. The merits of SAW-based devices as practical signal processing technologies are worth noting due to numerous excellent characteristics compared to competing technologies. For example, SAW bandpass filters provide exceptional response characteristics in a routine design that would otherwise require an impractical network of inductors and capacitors in conventional LC-filter designs[28], [89]. Furthermore, SAW devices can provide complex signal processing capabilities within a single package design containing a single set of input and output interdigitated transducers. Their small, durable, light, and power-efficient modules enable mobile and space-borne communication systems, and their analog nature allows them to be employed as digital communication devices[90]. Additionally, the simple design of these devices enables mass production using standard semiconductor microfabrication techniques, which promotes competitive product pricing.
**Table 4.1:** Interdigitated transducer devices are readily utilized for their signal processing capabilities. Campbell et al. provide an exhaustive list of their signal processing applications, and only a select few are shown here for the (1) bidirectional, (2) unidirectional, and (3) resonator IDT modes.

<table>
<thead>
<tr>
<th>Bidirectional SAW IDTs</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Wideband delay lines for recirculating digital storage</td>
</tr>
<tr>
<td>• Intermediate frequency (IF) filters for TV receivers</td>
</tr>
<tr>
<td>• Bandpass filters for linear and prescribed non-linear phase response</td>
</tr>
<tr>
<td>• Nyquist filters for digital radios</td>
</tr>
<tr>
<td>• Comb filters for multiplexer filter banks</td>
</tr>
<tr>
<td>• Fourier-transform processors for spectral identification</td>
</tr>
<tr>
<td>• Acousto-optic spectrum analyzers</td>
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<table>
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<tr>
<th>Unidirectional IDTs</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Low-loss bandpass filter applications</td>
</tr>
<tr>
<td>• Communications receiver “front-end” circuit stages</td>
</tr>
<tr>
<td>• Comb filters with low insertion loss</td>
</tr>
<tr>
<td>• Multimode oscillators for frequency-agile radar</td>
</tr>
<tr>
<td>• Duplexers for cellular devices</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Resonators</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Very narrow-band filter applications</td>
</tr>
<tr>
<td>• Cable TV filters</td>
</tr>
<tr>
<td>• Fixed frequency oscillators with high short-term stability</td>
</tr>
<tr>
<td>• Resonators for garage door transmitter control circuits and medical alert</td>
</tr>
<tr>
<td>transmitter circuits</td>
</tr>
</tbody>
</table>

In SAW temperature sensors, temperature changes lead to thermal expansion and contraction of the finger spacing of the SAW device, thus increasing the acoustic
wavelength. Temperature changes also affect the material properties of the piezoelectric substrate and therefore change the acoustic mode velocities. The piezoelectric system's chemical or mechanical stability typically imposes temperature sensing limitations in piezoelectric sensors. Figure 4.1 illustrates a simplified diagram of a SAW-based temperature sensor.

Figure 4.1: SAW sensors are particularly useful for their wireless communication applications in temperature and pressure sensing. Changes to the SAW-device environment alter the resonant frequency of the device, which can then be relayed to a remote location for analysis.

Temperature sensing as high as 1400 °C is possible in Langasite (LGS, La$_3$Ga$_5$SiO$_{14}$) or Langatate (LGT, La$_3$Ga$_{5.5}$Ta$_{0.5}$O$_{14}$) materials[91], though these materials exhibit high acoustic propagation losses with the temperature at higher frequencies and are thus limited to lower frequency (< 1 GHz) applications[92]. Li et al. demonstrated an AlN-based SAW resonator for temperature sensing purposes as an alternative to typical Langasite-dependent devices, capable of achieving accurate temperature readings up to 500 °C for high-frequency applications[93]. The resonance frequency dependence exhibits a
linear dependence with pressure for constant temperatures. Lucia et al. designed and fabricated SAW pressure sensors capable of handling pressures as high as $1.5 \times 10^5$ psi on an ST-Cut quartz substrate using low-cost production methods to replace typical BAW-sensors for oil exploration applications[94].

![Figure 4.2: In a typical SAW-based chemical sensor design, the delay line of a SAW device is coated with a concentration-sensitive thin film. SAWs that are launched from IDT-1 interact with the concentration-sensitive thin film in a predictable way and measured are by IDT-2.](image)

SAW devices are also well known for their high surface-mass detection sensitivity for chemical sensing[95]. In a typical SAW-based chemical sensor design, the delay line of a SAW device is coated with an organic or inorganic thin film, and the chemical species of the ambient environment are adsorbed or desorbed, ultimately altering the device response predictably. SAW-based chemical sensors have been attractive for chemical detection due to their sensitivity, low cost, portability, and excellent selectivity. Wohltjen et al. first introduced the concept of chemical analysis probes using SAW devices in 1979, noting that these sensors' amplitude response depends on the pressure of gaseous molecules of specified molecular weight[96], [97]. Huang et al. demonstrated a passive and wireless SAW system with remarkable sensitivity and reliable repeatability for detecting hydrogen in ambient conditions in the presence of variable humidity and fluctuating
temperatures[98]. Recently, Chen et al. developed a SAW-based vapor sensor utilizing a graphene IDT for TNT detection and shows a marked improvement over typical aluminum-based sensors[99]. Figure 4.2 illustrates a simplified diagram of a SAW-based temperature sensor.

These acoustic devices have seen marginal application to stress-sensitive phenomena such as compositional patterning in crystalline semiconductors[36], catalytic reactions[100], and crystal growth[101]. Theoretical modeling from various research groups suggests the potential for periodic stress fields to enhance crystal growth and localized diffusion in compound semiconductors[34]–[39], which would be valuable for developing next-generation semiconductor technologies. Notwithstanding their notable performance within various industrial applications, the current technological capabilities of SAW-based devices have not been entirely realized.

4.2 Interdigitated Transducer Principles and Design

Interdigitated transducer (IDT) devices are among the most frequently used periodic electrode structures for nondestructive testing, microelectromechanical systems (MEMS), telecommunications, chemical sensing, piezo-acoustics, and biotechnology applications[25]. IDT sensors benefit from being passive elements that do not require a power supply and wirelessly interact, enabling remote monitoring in harsh environments. The devices typically work in a frequency range of $10^6$-$10^9$ Hz and have a compact structure that offers high stability and sensitivity, low cost, fast real-time response, and are extremely small and lightweight.
An IDT is constructed of two interweaving comb-shaped arrays of metal electrodes and responds to an electrical input at a specific resonant frequency. The device resonant frequency, $f_r$, can be predicted by $f_r = \frac{v_{SAW}}{\lambda}$, where $\lambda$ is the acoustic wavelength or device finger pitch, and $v_{SAW}$ is the SAW velocity. Single-electrode IDT's offer a simplistic design for photolithography techniques or screen-printing processes due to the relatively wide strip width ($\lambda/4$). Contact-mask lithography is the typical fabrication technique used to fabricate IDT's for MHz applications, though more complex designs reliant on feature
sizes smaller than 1 μm require more expensive or complicated techniques, such as electron-beam lithography[102]. Figure 4.2 depicts the simplistic design of an IDT structure.

IDT devices are often used in wireless network systems[28], [29], acousto-optic technologies[103], [104], and chemical[105], [106], pressure[107], [108], and temperature[109], [110] sensors. However, they have seen minimal application for the analysis of stress-sensitive phenomena such as compositional patterning in crystalline semiconductors[36], catalytic reactions[100], and crystal growth[101] applications. Theoretical modeling has suggested the potential for periodic stress fields to enhance crystal growth and localized diffusion in compound semiconductors[34]–[39], which would be valuable for developing next-generation semiconductor technologies. IDTs are a potential platform to study the effects of stress on semiconductor diffusion, and a rigorous understanding of these devices' mechanical responses is necessary for further investigation.

4.2.1 SAW Reflections and Mass Loading

The metal strips used for the finger pairs and the mirror strips produce a damping and frequency distortion effect that alters the center frequency position and frequency response shape for the fabricated device[111]. Mass loading from the finger pairs introduces damping and shifts the center frequency to lower values, while acoustic Bragg reflectors distort the frequency response and introduce asymmetric artifacts. These mass loading effects are undesirable in electronic signal processing applications. The simplest way to mitigate issues associated with mass loading is to use a low-density metal, such as aluminum, or to ensure the metal strip thickness is considerably smaller than the
wavelength of the acoustic wave. Mass loading effects from the metal strips are ignored for a sufficiently small film-thickness ratio. However, an adequate metal thickness is necessary to provide complete electrical contact and low sheet resistance[28].

Other techniques to minimize mass loading effects have been demonstrated, such as a double-finger design or embedding the fingers into the piezoelectric substrate. These strategies are not employed in this work but may be potential options to explore in the future. The use of a double-finger design does not suffer from Bragg reflections[112], but the fingers' width is reduced by 50% to generate a SAW of the same frequency as a single-finger design. SAW reflections are shown to be reduced by a factor of 5 by embedding the metal fingers in the substrate[113], which requires a brief plasma-etching step before metal deposition.

4.2.2 Second-Order Interference Effects

Bulk wave interference within the delay line region occurs due to BAWs being excited by the IDT structures. Bulk waves can constructively interfere during the operation of the SAW resonator device and alter the electrical response. The frequency of the bulk wave is a function of the radiation angle, $\phi_r$, and bulk wave velocity, $v_{BAW}$, and is described by

$$f_b = \frac{v_{BAW}}{\lambda \cos \phi_r}.$$  \hspace{1cm} (4.1)

Like bulk wave interference, multi-transit interference can distort the scattering response of the SAW resonator device. Multi-transit interference occurs when an acoustic wave is launched from one side of the device, travels across the delay line region, and then
reflects off the electrodes on the other side of the device. This effect produces ripples in the filter passband response at frequencies described by

\[ f_{\text{MTI}} = \frac{1}{n\tau}, \]  

(4.2)

where \( n \) is the transit number, \( \tau = d/v_{\text{SAW}} \) is the time it takes for the SAW to travel across the delay line region of the device.

### 4.2.3 Wave Diffraction

The aperture of the IDT structure is an important parameter to bear in mind when considering the diffraction of the acoustic wave. Diffraction of the acoustic wave, with respect to the intention of the current experiment, can significantly alter the quality of the standing acoustic field and is, therefore, an effect that should be minimized. In a manner analogous to the Fresnel number for the diffraction of light waves, a diffraction parameter, \( F \), or 'Figure of Merit' is used to describe the degree of diffraction observed for acoustic waves:

\[ F = \frac{\lambda_{\text{SAW}} D(1 - 2A_d)}{(W/2)^2}, \]  

(4.3)

where \( D \) is the distance from the aperture of the device to the point of interest, \( W \) is the aperture of the IDT (illustrated in Fig. 4.3), and \( A_d \) is an empirical anisotropy parameter. In the case of GaAs, \( A_d \) is equal to zero for acoustic waves traveling along the \([110]\) direction on the \(\langle001\rangle\) crystallographic plane[28].

For an \( F < 1 \), acoustic diffraction is within the Fresnel region and the energy of the acoustic wave is primarily contained within the delay line region of the device. Eventually, the acoustic wave extends far enough away from the aperture of the device such that \( F > \)
1, and the diffraction is within the Fraunhofer region, and acoustic energy escapes outside of the delay line region of the device[111]. The aperture of the IDT is the only practical way to control the $F$ parameter for the acoustic wave and should be appropriately wide for the consideration of the experiment.

4.2.4 Standing Surface Acoustic Wave Resonator Design

Standing wave resonator structures produce a coherent interference from the incident and reflected traveling waves and can be configured to act as a narrow-band resonant circuit[28]. SAW resonators can exhibit relatively high Q and low insertion loss[114] and find applications as highly selective bandpass or notch filters. These mirror gratings enable the low insertion loss for these devices (typically < 6 dB). An electromagnetic waveguide resonator allows for constructive interference of electromagnetic waves within a bounded cavity defined only by metal reflector plates. This simple boundary condition does not suffice for acoustic waves due to the elliptical displacement behavior of the substrate surface, which is made of a parallel and a perpendicular displacement component with respect to the SAW propagation direction (described earlier in this chapter). A single metal reflector is insufficient to provide a total reflection of both displacement components[28]. The SAW grating is necessary as each weakly-reflecting element combines to provide near-total SAW reflection, similar to a distributed Bragg reflector in an optical cavity. SAW reflections from a reflection grating are most significant at the center frequency for which the individual reflections are additive. An IDT stop-band filter utilizes a similar design as there is a narrow frequency over which the grating reflects SAW waves with reduced efficiency[28]. The width of the
stopband can be specified and is dependent on several design parameters such as (a) substrate material, (b) reflection grating geometry, and (c) grating quantity.

Figure 4.4 shows a simplified schematic of the design used in this work. SAW resonators can be configured as a one-port or a two-port network and rely on acoustic mirror gratings to form the resonating structure. The IDT structures (grey) that produce the standing SAW structure (red) are positioned between an array of acoustic Bragg reflectors (blue). The device is powered by electrically connected a frequency generator to the gold bonding pads (yellow) via wire bonding.

![Figure 4.4: A simplified schematic of the SAW device used in this work depicts the dual IDT structure (grey), the acoustic mirror assembly (blue), and the gold bonding pads (yellow). The standing wave structure is observed in the center of the device (red).](image)

The IDT devices used in this work are fabricated on GaAs(100) and positioned such that the waves propagate in the ⟨110⟩ direction. The device is based on a SAW
resonator design. However, fingers are removed from the device’s center to provide a 100-µm to 200-µm-wide delay line for an unimpeded standing-SAW strain field to form, as shown in Fig. 4.5(a). The delay line length is kept small so diffraction effects can be ignored; otherwise, considerations would need to be made for the cases of Fraunhofer and Fresnel diffraction.

Each side of the IDT structure is made up of 50-150 aluminum finger pairs and an acoustic Bragg reflector consisting of 50-200 grounded aluminum metal strips. The transition from finger pair electrodes to acoustic Bragg reflectors is depicted in in Fig. 4.5(b). There are 1000 electrode strips and 600 grounded metal strips for the largest SAW-resonator device fabricated. This quantity of metal strips implies a length of more than 8 mm. The finger pitch of the IDT device determines the SAW wavelength, and therefore approximately determines the resonant frequency of the device in accordance with \( \lambda_{SAW} = \frac{v_{SAW}}{f} \), where \( v_{SAW} = 2863 \text{ m/s} \) in the \( \langle 110 \rangle \) direction for GaAs. The width of the fingers, relative to the finger pitch is designed to be \( \lambda_{SAW}/4 \).

Ground-signal-ground (GSG) pads are included at the periphery of the device for VNA testing and electrical contact via wire bonding. The aluminum GSG-pad layer (before gold deposition) is shown in Fig. 4.5(c). The pads expand outwards to increase the wire bonding area for more accessible electrical contact. For high-frequency devices (>10 GHz), a careful bonding pad design is necessary to minimize impedance effects. However, no noticeable parasitic capacitance or inductance effects were observed in introducing the large-area bonding pads for the current design.
Figure 4.5: (a) The delay line region of the SAW resonator device is included in the device design to allow for unimpeded observation of the standing SAW structure. (b) The finger-pair electrodes and the acoustic mirror assembly are positioned for maximum acoustic reflection. (c) The wire bonding pads begin as small G-S-G pads for VNA testing but expand to facilitate an easier wire bonding procedure.
4.3 Device Fabrication

4.3.1 Photolithography and Metal Deposition Procedure

The IDT structure is fabricated using optical lithography and electron-beam metal evaporation. First, a positive photoresist (Ultra-i-123-0.8) is spun onto a 2-inch GaAs(100) wafer with a spin speed of 2250 RPM. According to the material datasheet, the photoresist thickness is approximately 800nm thick. The coated wafer undergoes a soft bake on a hotplate at 90 °C for 90 seconds to evaporate the remaining solvent within the photoresist. The resulting structure is illustrated in Fig. 4.6(a).

The coated wafer is then placed into a MicroTech SUSS Mask Aligner and exposed to a 355nm 'i-line' laser for approximately 6 seconds at a laser power of around 350 W. The exposed wafer undergoes a hardbake process in which a hotplate heats the wafer to 112 °C for 90 seconds to accelerate the photochemical reaction. The exposed-and-baked wafer is then submerged in a puddle of MF CD-26 developer at room temperature for 60 to 90 seconds, depending on the amount of exposure. Figure 4.7 illustrates the effects of an over-developed photoresist layer, which was seen only for a single device among an array of ten.

![Figure 4.6](image.png)

*Figure 4.6: (a) The first photoresist layer is deposited via spin coating onto a 2” GaAs wafer. (b) The photoresist layer undergoes photolithography, which opens areas for metal deposition. (c) E-beam metal deposition deposits a thin aluminum layer to form the first layer of the IDT device.*

The coated wafer is then placed into a MicroTech SUSS Mask Aligner and exposed to a 355nm 'i-line' laser for approximately 6 seconds at a laser power of around 350 W. The exposed wafer undergoes a hardbake process in which a hotplate heats the wafer to 112 °C for 90 seconds to accelerate the photochemical reaction. The exposed-and-baked wafer is then submerged in a puddle of MF CD-26 developer at room temperature for 60 to 90 seconds, depending on the amount of exposure. Figure 4.7 illustrates the effects of an over-developed photoresist layer, which was seen only for a single device among an array of ten.
devices. The exposed photoresist areas are immediately etched away during the initial developing stage and the photo-developer begins to etch the un-exposed photoresist areas. This result may have occurred due to an uneven distribution of photoresist as this particular device was close to the edge of the 2-inch wafer.

![Image of photoresist processing](image.png)

**Figure 4.7:** The exposed photoresist is etched away (yellow area), and the unexposed photoresist begins to be etched (green and red areas) during the developing procedure if the wafer is developed for too long.

An adequately exposed-and-developed sample undergoes a de-scumming step via O2 ICP cleaning for 20-60 seconds to remove carbon residue or widen device features. A shorter ICP cleaning step removes carbon residue, while a longer ICP step removes photoresist material. Figure 4.8(a) depicts the results of an under-exposed device. An under-exposed device does not receive a large enough laser dose to alter the chemical
structure of the photoresist sufficiently. As a result, the finger widths are smaller than desired, leading to a potentially underperforming device. Figure 4.8(b) demonstrates the effects of using an isotropic O₂ plasma for etching the photoresist and increasing device feature sizes in the case of an under-exposed lithography step. The finger-widths were measured to be 2.2 µm before the plasma etch. After the isotropic oxygen plasma etching step, the finger widths expanded to 2.5 µm.

![Figure 4.8](image)

*Figure 4.8: (left) An under-exposed photoresist layer results in excessively thin metal finger widths, which adversely impacts the performance of the IDT structure. (right) An oxygen plasma etching step widens the underexposed structures.*

During metal deposition, the vacuum chamber is pumped down to 2x10⁻² Pa using a roughing pump and is then further pumped down to 2x10⁻⁶ Pa using a cryopump. A 10 kV power supply powers the electron beam and the beam current is increased to approximately 0.85 A. The aluminum metal is deposited at a rate of 0.8 Å/sec for a total of 800 to 2000 Å. After aluminum deposition, the samples are unloaded from the chamber and submerged in acetone in an ultrasonication bath to begin the lift-off procedure. A mixture of acetone, methanol, isopropyl alcohol, and DI-water removes the photoresist and
the undesired aluminum metal. It is worth mentioning that a 5-nm titanium layer may be beneficial to incorporate between the bare GaAs surface and the deposited aluminum layer to improve device adhesion, especially for instances when the devices need to undergo lengthy ultrasonication bath times. Figure 4.6(c) illustrates the completed SAW device structure after the first photolithography and metal deposition procedure. Optical microscopy is used to ensure complete removal of the photoresist and deposition of aluminum that forms the base layer of the IDT devices. Figure 4.9 depicts shorted electrodes bridged by a defect produced during the lithography process. These defects are due to poor photoresist adhesion or particles on the photomask that prevents proper exposure on the wafer for this device.

*Figure 4.9: Fabrication defects in the device structure can lead to an electrical short in the electrode structure. This specific defect resulted from a defect in the photomask design.*
For the case when a thin film structure is deposited in the delay line region of the standing SAW structure, a similar procedure to the first photolithography step is completed. A positive photoresist (Ultra-i-123-0.8) is spun onto the wafer with a spin speed of 2500 RPM. The photoresist thickness is approximately 700nm thick. The coated wafer undergoes a soft bake on a hotplate at 90 °C for 90 seconds to evaporate the remaining solvent within the photoresist. The resulting structure is illustrated in Fig. 4.10(a).

Figure 4.10: (a) The second photoresist layer is deposited via spin coating onto a 2” GaAs wafer. (b) The photoresist layer undergoes a lithography step which opens areas for thin film deposition. (c) Metal deposition via thermal evaporation is used to deposit an indium layer in the delay line region of the device.

The coated wafer is then placed into the same MicroTech SUSS Mask Aligner and exposed to a 355nm 'i-line' laser for approximately 10 seconds at a laser power of around 350 W. Overexposure is no longer a concern due to the large area of the exposed area. The exposed wafer undergoes a hardbake process in which it is heated on a hotplate at 112 °C for 90 seconds to accelerate the photochemical reaction. The exposed and baked wafer is then submerged in a puddle of MF CD-26 developer at room temperature for 90 seconds. The resulting developed structure is illustrated in Fig. 4.10(b).
In the case of depositing an indium thin film, a thermal evaporator is utilized instead of the electron beam metal evaporator. The thermal deposition vacuum chamber is pumped down to $2 \times 10^{-2}$ Pa using a roughing pump and is then further pumped down to $2 \times 10^{-6}$ Pa using a cryopump. Resistive heating heats the crucible containing indium pellets, and the indium metal is deposited at a rate of 2 Å/sec for a total of 100 to 1500 Å. Figure 4.11 shows an SEM image of various indium depositions on the surface of bare gallium arsenide. An illustration of the thin film deposited in the delay region of the device is shown in Fig. 4.10(c).

Figure 4.11: Indium particles undergo coarsening as the deposited “film thickness” increases, eventually coalescing to form a sheet of indium. During experiments that would test the effects of a standing-SAW field on liquid metal fluid flow, the indium “film” is deposited in the delay line of the SAW resonator device.
After the delay-region film is deposited, the photolithography procedure is repeated using the GSG-specific photomask. The final lithography step to fabricate the completed IDT structure utilizes optical lithography and electron-beam metal evaporation. A positive photoresist (AZ-4210) is spun onto a 2-inch GaAs(100) wafer with a spin speed of 2000 RPM. According to the material datasheet, the photoresist thickness is approximately 4000nm thick. A thicker photoresist layer is used to ensure the deposited gold layer does not overtake the photoresist layer. The coated wafer undergoes a soft bake on a hotplate at 90 °C for 90 seconds to evaporate the remaining solvent within the photoresist. The resulting structure is illustrated in Fig. 4.12(a).

Figure 4.12: (a)The final photoresist layer is deposited via spin coating onto a 2” GaAs wafer. A significantly thicker photoresist is used for this step. (b) The photoresist layer undergoes a lithography step which opens areas for metal deposition. (c) E-beam metal deposition is used to deposit a thin titanium layer for improved adhesion followed by a 1000-nm gold layer to form the bonding pads for the device.

The coated wafer is then placed into the same MicroTech SUSS Mask Aligner and exposed to a 355nm 'i-line' laser for approximately 10 seconds at a laser power of around 350 W. Overexposure is no longer a concern due to the large area of the exposed area. The exposed wafer undergoes a hardbake process in which it is heated on a hotplate at 112 °C for 90 seconds to accelerate the photochemical reaction. The exposed and baked wafer is
then submerged in a puddle of MF CD-26 developer at room temperature for 90 seconds. The resulting structure is illustrated in Fig. 4.12(b).

A 10-nm film of titanium is deposited using the electron beam deposition tool followed by a 1000-nm-thick gold layer. The titanium acts as an adhesion layer between the aluminum and the gold and a diffusion barrier to prevent harmful intermetallic formation. In the case of high-temperature applications, gold and aluminum can form a gold-aluminum intermetallic (Au$_2$Al), often referred to as 'purple plague'. The intermetallic has lower electrical conductivity and therefore increases electrical resistance, leading to total device failure[60]. The final SAW resonator structure is illustrated in Fig. 4.12(c).

### 4.3.2 Alignment Mark Design

Figure 4.13 illustrates the printed alignment mark after the first lithography step, which aids in matching the device orientation for the second lithography step. The minimum feature size is approximately 1 µm, and the photolithography alignment and photo-development quality can be gauged using optical microscopy. The photoresist used for the first two photolithography steps is on the order of 1 µm, which is an ideal thickness for the size of the alignment mark geometries. During the second photolithography step, the alignment marks are found using the mask aligner camera, and the photomask can be appropriately oriented by overlapping the positive and negative alignment mark patterns. There are four alignment marks placed near the periphery of the photomask, and a single alignment mark is placed at the very center of the photomask.
Figure 4.14 shows the effects of designing an alignment mark with features that are too small compared to the photoresist thickness being used. The minimum feature size of the alignment mark in Fig. 4.14 is 1 µm, which is too small relative to the thickness of the photoresist used in the final photolithography step, which is 4 µm. While it may be possible to resolve the finer details of the alignment mark with a photoresist of this thickness, the

Figure 4.13: The alignment mark for the first photolithography step shows clear geometries of varying sizes. The alignment mark allows a user to check the photo development results qualitatively and allows for future photomask alignments to be correctly oriented.
exposure time and developing time required to form the bonding pad areas is too long, and the alignment mark details are obscured.

![Figure 4.14](image)

**Figure 4.14**: The 1 µm feature size for the final lithography step’s alignment mark is too small to account for the photoresist thickness. The features of the alignment mark are obscured as a result.

### 4.3.3 Impedance Matching and Wire Bonding

Impedance matching is a necessary step in constructing power-efficient high-frequency interdigitated transducer structures. Impedance matching networks minimize power reflections and maximize the power dissipated in the load, and play an important
role in many electrical systems operating at radio or optical frequencies. In this work, a coplanar quarter-wave transmission line changes the load impedance to match the source impedance (50Ω). This is accomplished through careful consideration of the geometry and material of the impedance matching structure, which in this experiment, is a copper laminated Rogers PCB, which has undergone an ‘electroless Ni/immersion Au’-plating process.

Figure 4.15: (top) The geometric mean of the transmission impedance, $Z_{in}$, and the load impedance, $Z_L$, should “match” the source impedance, $Z_0$. (bottom) The length of the transmission line is $\lambda/4$ for phase matching of the incoming signal.

Figure 4.15 depicts how a transmission line acts as an impedance transformer for the devices used in this work. A quarter-wave transformer uses a section of line of
characteristic impedance $Z_{in}$ of $\lambda/4$ long, where $\lambda$ is the wavelength of the incoming frequency. For ideal matching, $Z_0 = \sqrt{Z_{in}(\lambda/4) \cdot Z_L}$, which indicates that the length-dependent impedance of the matching network should be chosen such that the geometric mean of the load impedance and the matching network’s impedance will equal in source impedance. Device impedance is measured via vector network analysis and the quarter wavelength transform is designed using CST Studio Suites, which includes the additional coplanar grounding strips and ground plane. The physical gold wires used in the wire bonding procedure are not considered in the impedance matching network design, as there is no reliable method to introduce these effects with the current laboratory setup. However, wire bonded devices seem to suggest there is a negligible amount of impedance introduced by the wire bonds for the current device frequencies. The impedance mismatch effects would likely be more substantial for higher-frequency devices, so wire bonding capacitance and inductance effects must be considered for future higher-frequency devices.

**Figure 4.16:** Wire bonding connects the interdigitated transducer devices to the impedance matching network. Gold ball bonds are formed on the gold bonding pads incorporated into the SAW-generating devices and are then connected to the Cu-plated laminate, which has undergone electroless-nickel/immersion-gold electrochemical processing.
A gold wire, attached via a wire bonding procedure, connects the SAW-generating interdigitated transducer devices to a gold-coated quarter-wavelength transmission line for impedance matching. Au-ball wire bonding is typically mediated using ultra-sonication to form an intermetallic compound and bridge the wire to its contact[59]. Initial intermetallic compound (IMC) formation occurs at the peripheral regions of the Au-ball contact, which then extends inward with increasing ultrasonication power[58]. The wire bonded IDT assembly is illustrated in Fig. 4.16.

Figure 4.17: The final wire bonded SAW resonator structure is depicted, showing the wire bonds extending from the gold bonding pads to the quarter wavelength transmission line. The aluminum device layer is visible as a dark grey and sits atop an even darker GaAs substrate. The delay line region of the device is also visible in the center of the device.
The first wire bond forms a ball bond with the 1-μm gold pad connected to the aluminum device. The second wire bond connects to the quarter-wavelength transmission line and is formed with the gold layer deposited atop an electroless nickel (e-Ni) layer via an immersion gold (i-Ag) electrochemical process. The electroless nickel is about 2-μm thick, while the immersion gold layer is approximately 200-nm thick. More detail concerning wire bonding and the adverse effects of intermetallic species that can form during this process is discussed in Chapter 2 of this dissertation. The resulting wire-bonded structure is illustrated in Fig. 4.17.

4.4 Device Characterization Methods and Design Analysis

In this dissertation, the two primary modes of device characterization are vector network analysis and atomic force microscopy. Vector network analysis provides insight into the electrical nature of these devices, while atomic force microscopy is used to characterize the mechanical response of the standing acoustic field generated by the devices. Additional methods have been introduced to characterize these devices, such as Raman microscopy and finite element method modeling, but these characterization results are discussed in later chapters.

4.4.1 Vector Network Analysis

The admittance, $Y_{11}$, and impedance, $Z_{11}$, matrix components for an IDT device, along with the remaining admittance and impedance matrix components, can calculate scattering responses per the following two-port network equations[115]:

$$S_{11} = \frac{(Y_0 - Y_{11})(Y_0 - Y_{22}) + Y_{12}Y_{21}}{(Y_0 + Y_{11})(Y_0 + Y_{22}) - Y_{12}Y_{21}}$$

(4.5)
\[ S_{21} = \frac{-2Y_{21}Y_0}{(Y_0+Y_{11})(Y_0+Y_{22})-Y_{12}Y_{21}} \]  

(4.6)

where \( S_{11} \) is the input voltage reflection coefficient, \( S_{21} \) is the input voltage transmission coefficient, and \( Y_0 \) is the device reference impedance (50Ω). However, using a Keysight 5247a RF Performance Vector Network Analyzer (VNA), scattering parameter components can be directly measured to provide the four components of the scattering matrix for the two-port SAW resonator device.

Figure 4.18 shows the scattering response measured by the VNA for an optimally performing SAW resonator structure made of 150 fingers pairs and 200 mirror strips per side of the device. A substantial \( S_{21} \) magnitude is observed near the resonance frequency.

**Figure 4.18:** The \( S_{11} \) signal implies minimal signal/power reflection at the resonant frequency of the device, while the \( S_{21} \) signal implies strong signal/power transmission. The additional modes observed in the scattering response are attributed to reflections in the delay line region of the device.
of the IDT device, which implies a high-power throughput and is enabled by the SAW resonator design used in this experiment. The coinciding $S_{11}$ magnitude is very small near the resonant frequency, implying minimal signal reflection. Additional modes are observed at slightly higher frequencies than the device's resonant frequency, which are attributed to acoustic reflections or triple-transit interference in the delay line region of the device.

Due to the symmetry of the IDT design, the device functions as a reciprocal and symmetrical network such that $S_{11} = S_{22}$ and $S_{12} = S_{21}$. In the case of a reciprocal and lossless network,
\[ S_{11}^2 + S_{21}^2 = 1. \] (4.7)

However, this is not the case for practical IDT structures, and mechanisms associated with acoustic attenuation, resistive heating, and inefficient mirror assemblies lead to measurable power loss within the device. Figure 4.19 shows the measured power loss for the device discussed in Fig. 4.18.

![Graph showing S21 components for different finger-pair quantities per side of the IDT resonator and no acoustic mirrors to contain the SAW field.](image)

**Figure 4.20:** As finger-pair quantity is increased, so does the magnitude of the \( S_{21} \) response across the entire tested frequency domain, which implies a stronger acoustic field amplitude.

In the absence of computational modeling of these devices, it is necessary to study different device design parameters such as finger-pair quantity, acoustic reflector array size, and impedance matching to the quarter wavelength transmission line. Figure 4.20 shows the \( S_{21} \) components for different finger-pair quantities per side of the IDT resonator and no acoustic mirrors to contain the SAW field. As the finger-pair quantity increases, so does the \( S_{21} \) component over the entire frequency domain, which furthers increases the
standing acoustic wave amplitude. For this reason, the number of finger-pair electrodes is increased to 150 finger pairs per side of the SAW resonator device. Continuing to add finger pairs to each side of the device increases the magnitude of the standing SAW field. However, as the device size grows, there is an increased likelihood of introducing fabrication errors, like the defect shown in Fig. 4.9.

![Figure 4.21: Increasing the size of the mirror array significantly improves the quality of the S21 response.](image)

Figure 4.21 depicts the effects of varying acoustic mirror array sizes within fabricated resonator devices. The quality of the scattering response for the device with only 50 mirror strips per side of the resonator is significantly worse than the device, which contains 200 mirror strips per side of the device. Similar behavior is observed in Fig. 4.20 where no mirror strips were incorporated. The resonator's quality is course diminished due to the device's inability to contain the acoustic field, leading to an increased power loss and
a minimized ability to perform as a stop-band filter. For this reason, a maximum number of mirror strips is an important design consideration to ensure an optimally performing device.

Following the VNA measurements, the best performing devices are wire bonded to respective quarter-wavelength transmission lines for impedance matching, and the full assemblies are powered using a Windfreak Synth NV frequency generator (with a power detector) with a maximum applied power of 20.85 dBm. $S_{21}$ measurements can be performed using the calibrated power detector incorporated with the Windfreak Synth NV frequency generator. This procedure allows the wire bonded assemblies performance to be compared to the VNA-tested device. The results of this comparison are shown in Fig. 4.22.

**Figure 4.22:** The VNA-test device scattering response nearly matches the scattering response for the wire bonded device which implies a sufficiently designed impedance matching network.
The agreeing measurements suggest that the impedance matching network that the device is wire bonded to is sufficiently designed to enable maximum power throughput.

### 4.4.2 Atomic Force Microscopy Analysis

Atomic force microscopy is used to measure the acoustic displacement induced by the standing SAW field. The dynamic nature of the acoustic strain field restricts the AFM cantilever to profile only the absolute displacement of the standing SAW. Contact-mode analysis may impart an impression that the AFM cantilever would attempt to track the motion of the acoustic wave and thus provide an inaccurate, time-averaged measurement. This is not the case, however, as the vibrational frequency of the silicon cantilever used in this experiment is on the order of $10^5$ Hz, while the frequency of the SAW is on the order of $10^8$ Hz. The response time of the cantilever is too slow to track the acoustic wave and can only measure the approximate-maximum positive excursion of SAWs.

Contact-mode atomic force microscopy (AFM) measurements are recorded at room temperature over a range of applied frequencies about the resonant frequency at a maximum applied power of 20.85 dBm. A 2-D AFM image recorded at the resonant frequency of 287.2 MHz for the 150-finger pair and 200-mirror strips per side of the device is shown in Fig. 4.23. Due to the phenomenon described previously, the standing wave structure is recorded as an absolute sine wave. Thus the 10-µm acoustic wavelength is represented as a 5-µm repeating structure.
Figure 4.23: The 10 µm acoustic wavelength is imaged as a 5-µm repeating structure due to the dynamic nature of the acoustic wave’s surface and the comparatively slow-moving AFM cantilever with which it makes contact.

Figure 4.24: An absolute sine wave function is fit to the resulting averaged line scan to reveal an average vertical displacement of 5.17 nm and an acoustic wavelength of 10.02 µm.
The 2-D AFM image is compiled into an averaged line scan and is fit to an absolute sine function, as shown in Fig. 4.24. Fitting reveals an average vertical displacement value of 5.17 nm, and the acoustic wavelength is calculated to be 10.02 nm. More discussion regarding the stress and strain imparted by standing acoustic fields can be found in Chapter 6 of this work.

AFM imaging presents an opportunity to study acoustic attenuation, as line-averaged data can extend over great distances to observe the changing acoustic amplitude associated with acoustic loss mechanisms. Additionally, the window for 2-D imaging can be expended to attempt to observe the effects of Fresnel or Fraunhoffer diffraction, which can either hinder or help the acoustic field structure for studying stress-enhanced phenomena. Either way, the implications of measuring acoustic fields using 2-D AFM are significant, and more studies should be completed using this simple technique to study the behavior of standing surface acoustic wave fields.

The surface displacement response as a function of applied frequency is shown in Fig. 4.25. The maximum displacement is recorded near the device's resonant frequency, but there is still a readily measurable acoustic field present at off-resonant frequency positions. The decaying amplitude of vertical displacement as a function of frequency is not as abrupt as one may expect, and the displacement is measured to be as large as 3 nm when the applied frequency was shifted by to 281 MHz and 295 MHz. The surface displacement is nearly zero at an applied frequency of 265 MHz and 310 MHz. Future studies should more closely inspect the change in acoustic amplitude as a function of frequency, near the resonance frequency of the device.
Conclusion

SAW resonator devices are fabricated on GaAs(100) using photolithography and electron-beam metal deposition. The devices are wire bonded to a quarter wavelength transmission line for impedance matching purposes. The completed SAW resonator assembly produce standing-SAW fields to study how acoustic fields can alter stress-enhanced phenomena. Before wire bonding, electrical device characterization is completed using a VNA to record scattering matrix components and determine device performance. VNA testing reveals the importance of including many finger pairs and mirror strips to promote a small filter bandwidth and strong acoustic response. Including additional finger pairs and mirror strips only serves to improve device performance. After wire bonding, contact-mode AFM measures the standing SAW fields, which show the SAW device
achieves a vertical surface displacement of 5.17 nm in the delay region of the device with an applied power of 20.85 dBm. A frequency sweep around the device resonant frequency demonstrates that low-amplitude SAWs are still produced when slightly off-resonance. However, a definitively more substantial wave is produced close to the device resonance frequency. The next chapter of this dissertation discusses a novel Raman imaging technique, which directly measures the crystalline stress induced by the standing acoustic field.
CHAPTER 5: RAMAN THEORY AND SAW DEVICE

MEASUREMENTS

5.1 A Classical Review of Raman Theory

While the first theories of the inelastic scattering of light were introduced in 1923 by Adolf Smekal[116], the first observations of the inelastic scattering of visible light were reported by C.V. Raman and his graduate student K.S. Krishnan in 1928[117], [118]. Raman would later receive the Nobel Prize for Physics in 1930 for achievements in the field of light scattering and the discovery of the Raman effect. In Raman spectroscopy, the transmitted light is not observed but rather the light scattered by the sample. Light of a single, monochromatic source must be used for a Raman experiment and the chances of a Raman scattering event occurring are on the order of 1/1,000,000. The typical scattering event, in which light of frequency $\nu_0$ is scattered from a point in all directions at the same frequency, is referred to as Rayleigh scattering. The light that scatters from this point does not have a frequency of $\omega$ but rather a frequency $\nu_t$, is referred to as Raman scattering. The energy difference between $\omega$ and $\omega_0$ is represented by $\Delta E = h|\omega - \omega_0|$, where $h$ is Planck’s constant, and $\Delta E$ refers to the energy absorbed or imparted by the scattering source. The case in which $\omega > \omega_0$ is referred to as Stokes radiation, and the case in which $\omega < \omega_0$ is referred to as anti-Stokes radiation[68]. A general case of Raman scattering is described in Chapter 2.

In this work, Raman microscopy is used to improve our quantitative understanding of the surface stress induced by the interdigitated transducer (IDT) devices. IDT devices are most commonly used in wireless network systems[28], [119]-[123] and acousto-optic
technologies[103], [124]-[127]. These SAW-based devices have also found significant use as bio[112], gas[105], [106], pressure[107], [108], and temperature[109], [110] sensors as well as actuators, pumps, and mixers in microfluidic applications[128], [129]. IDTs are often analyzed through electrical characterization, providing limited insight into the mechanical nature of surface acoustic waves. An improved understanding of mechanics and quantitative analysis would prove very useful in harnessing the benefits of stress-induced phenomena, such as compositional patterning in crystalline semiconductors[130], increase in catalytic reaction rates[100], and crystal growth applications[101].

5.2 Crystal Vibrations and Polarization Selection Rules

In the case of Raman spectroscopy in crystal structures, it is not typical to describe the vibrations of individual atoms but rather describe the collective motion of atoms in the form of waves[69]. These waves, or lattice vibrations, can be characterized by a wavevector, \( \mathbf{q}_j \), and a frequency, \( \omega_j \). The spatial amplitude of this vibration is described by:

\[
Q_j = A_j \exp \left[ \pm i (\mathbf{q}_j \cdot \mathbf{r} - \omega_j t) \right],
\]

where \( Q_j \) is the normal coordinate of the vibration, \( A_j \) is the vibration amplitude, and \( \mathbf{r} \) is the position within the crystal structure. These lattice vibrations are also useful to think of as phonon particles. Separately, we can describe an electric moment, \( \mathbf{P} \), induced at position, \( \mathbf{r} \), of a crystal by monochromatic light of frequency \( \omega_l \) incident on a crystal in a direction \( \mathbf{k}_l \) as:

\[
\mathbf{P} = \varepsilon_0 \chi \cdot \mathbf{E} = \varepsilon_0 \chi \cdot \mathbf{E}_0 \exp [i (\mathbf{k}_l \cdot \mathbf{r} - \omega_l t)],
\]
where \( \mathbf{E} \) has been expanded to represent the electric field induced by a monochromatic light source, \( \chi \) is the susceptibility tensor, and \( \varepsilon_0 \) is the vacuum permittivity. The electrical susceptibility describes the crystal's response to the electric field. Nearly identical to the way bond oscillations can alter the polarizability in a molecule as discussed in the previous section, these lattice vibrations, \( Q_j \), can affect the electrical susceptibility of the crystal, ultimately giving rise to the phenomena of Raman scattering in crystal structures.

The impact of lattice vibrations on the susceptibility tensor of the crystal can be explored in a Taylor series of the susceptibility with respect to the lattice vibrations:

\[
\chi = \chi_0 + \left( \frac{\partial \chi}{\partial Q_j} \right)_0 Q_j + \left( \frac{\partial \chi}{\partial Q_j \partial Q_k} \right)_0 Q_j Q_k + \cdots. \tag{5.3}
\]

Each term of the expansion refers to a different order of scattering; the first term, \( \chi_0 \), refers to the phenomena of Rayleigh scattering, and the following terms refer to first-order Raman scattering, second-order Raman scattering, and so forth. Each increasing order of Raman scattering implies the addition of a phonon in the light/vibration interaction. For example, the second-order Raman scattering event involves two phonons[131], greatly reducing the probability of the event occurring. First-order Raman scattering is already a low probability event, so terms higher than the first-order event are ignored for this discussion. Finally, combining Eq. (5.2) and (5.3) gives

\[
P = \varepsilon_0 \chi_0 \cdot \mathbf{E}_0 \exp[i(\mathbf{k}_i \cdot \mathbf{r} - \omega_i t)] + \varepsilon_0 \chi_0 \left( \frac{\partial \chi}{\partial Q_j} \right)_0 A_j \times \exp[-i(\omega_i \pm \omega_j)t] \exp[-i(\mathbf{k}_i \pm \mathbf{q}_j) \cdot \mathbf{r}]. \tag{5.4}
\]

It follows from this equation that describes the electric moment within a crystal, illuminated by a monochromatic light source of frequency \( \omega_i \), in the presence of crystal
vibrations of frequency $\omega_j$, that light re-emitted by the induced moment can have multiple
distinct frequency components: $\omega_i$, $\omega_i - \omega_j$, and $\omega_i + \omega_j$. We have again arrived at
Rayleigh scattering, Stokes Raman scattering, and anti-Stokes Raman scattering,
respectively, but for light scattered within a crystal structure.

Whether or not Raman scattering is observed for specific lattice vibrations depends
on whether the electrical susceptibility is affected by the presence of the lattice vibration
or, more specifically, if $\left( \frac{\partial \chi}{\partial q_j} \right)$ is non-zero. The Raman tensors, $R_j$, of the $j^{th}$ phonon are
proportional to $\left( \frac{\partial \chi}{\partial q_j} \right)$ and are used to calculate the polarization selection rules for Raman
scattering events. Loudon derived the Raman tensors for each of the 32 crystal
classes[132], which includes the diamond structure of silicon, and the zinc-blende structure
of gallium arsenide.

5.3 The Effects of Crystal Stress on Raman Scattering

The relationship between crystal strain and Raman peak shifts is widely established
and well understood, especially for semiconductor systems[132]–[134]. Mechanical strain
often affects the frequencies of the Raman modes in many crystal structures and follows a
linear relationship between strain magnitude and Raman peak shift. Ganesan et al. [135]
show that the frequencies of the three optical modes for diamond structures are linearly
dependent on strain by solving the following secular equation:

$$
\begin{vmatrix}
  p\varepsilon_{11} + q(\varepsilon_{22} + \varepsilon_{33}) - \lambda_0 & 2r\varepsilon_{12} & 2r\varepsilon_{13} \\
  2r\varepsilon_{12} & p\varepsilon_{22} + q(\varepsilon_{33} + \varepsilon_{11}) - \lambda_0 & 2r\varepsilon_{23} \\
  2r\varepsilon_{13} & 2r\varepsilon_{23} & p\varepsilon_{33} + q(\varepsilon_{11} + \varepsilon_{22}) - \lambda_0
\end{vmatrix} = 0. \ (5.5)
$$
Here p, q, and r are material constants known as the phonon deformation potentials, and \( \varepsilon_{ij} \) are the individual components to the strain tensor. Bell et al. [136] discuss how zinc-blende structures can be treated similarly, provided that the crystal electrostatic forces induced by the piezoelectric nature of the crystal are sufficiently small. The secular equation refers to a crystallographic axis with \( \hat{x}_1 = [100], \hat{x}_2 = [010], \hat{x}_3 = [001] \).

The change in Raman frequency for each mode in the presence of stress can be calculated from the eigenvalues:

\[
\lambda_{0,j} = \omega_j^2 - \omega_{j,0}^2,
\]

or

\[
\Delta \omega_j = \omega_j - \omega_{j,0} \approx \frac{\lambda_{0,j}}{2 \omega_{j,0}},
\]

\( \Delta \omega_j \) is the difference between the Raman frequency of each mode in the absence of stress, \( \omega_{j,0} \) and in the presence of stress, \( \omega_j \). For the simple case of uniaxial stress along the [100] direction, the stress matrix’s only non-zero value is the \( \sigma_{11} \) component. This then translates to the components of the strain matrix (written in Voigt notation) as \( \varepsilon = (S_{11} \sigma_{11}, S_{12} \sigma_{11}, S_{12} \sigma_{11}, 0, 0, 0) \)

5.4 SAW Mediated Raman and Biaxial Surface Stress Analysis on [100] GaAs

In the case of a SAW travelling parallel to the \( \hat{x}' \|[110] \) direction, it is useful to apply a coordinate transformation on the secular equation in which the strain field can be expressed as \( \varepsilon = (\varepsilon'_{11}, 0, \varepsilon_{33}, 0, \varepsilon'_{13}, 0) \). \( \varepsilon_{ij} \) are the strain components and
\(\hat{x}'_1\|[110], \hat{x}'_2\|[\bar{1}10]\), and \(\hat{x}'_3\|[001]\) define the axes of the transformed crystallographic orientation.

\[
\begin{pmatrix}
\frac{p}{2} \varepsilon'_{11} + \frac{q}{2} (\varepsilon'_{11} + 2 \varepsilon_{33}) - \lambda_0 & r \varepsilon'_{11} & \sqrt{2} \varepsilon'_{13} \\
r \varepsilon'_{11} & \frac{p}{2} \varepsilon'_{11} + \frac{q}{2} (\varepsilon'_{11} + 2 \varepsilon_{33}) - \lambda_0 & \sqrt{2} \varepsilon'_{13} \\
\sqrt{2} r \varepsilon'_{13} & \sqrt{2} r \varepsilon'_{13} & p \varepsilon_{33} + q \varepsilon'_{11} - \lambda_0
\end{pmatrix} = 0. \hspace{0.5cm} (5.8)
\]

The strain components can then be described as a function of the transformed SAW stress field distribution:

\[
\varepsilon'_{ij} = \begin{bmatrix}
S_{11} \sigma'_{11} + S_{12} \sigma'_{22} + S_{12} \sigma_{23} \\
0 \\
S_{12} \sigma'_{11} + S_{12} \sigma'_{22} + S_{11} \sigma_{33} \\
0 \\
S_{44} \sigma'_{13} \\
0
\end{bmatrix} \hspace{0.5cm} (5.9)
\]

Hooke’s Law is used, applying the similar assumption made by Bell et al. [136]. Additionally, the mechanical requirement for a surface wave is a stress-free surface, which can be stated as \(\sigma'_{13}\mid_{x_3=0} = 0\). The penetration depth of the 532 nm laser into the GaAs substrate is \(~1\%\) of the wavelength of the SAW, so there is a very minimal contribution from the \(\sigma'_{13}\) components to the Raman peak shift relative to the other non-zero components and are thus ignored. This makes the \(\varepsilon'_{13}\) effectively zero, reducing the remaining two strain components to be functions of only \(\sigma'_{11}\) and \(\sigma'_{22}\).

The solutions to Eq. (5.8) yield three eigenmodes, \(\lambda_{0,j}\), as well as their respective eigenvectors, \(\varphi_j\). Two of the eigenmodes described by the 2x2 diagonal block in the upper region of Eq. (5.8) are associated with the transverse character and result from a mixing of the unperturbed transverse optical (TO) phonon modes[137]. The symmetry of the z-
polarized mode is unmodified, and the Raman cross-section of the longitudinal optical (LO) phonon mode remains equal to the case of the unperturbed crystal[137]. Additionally, the TO modes are not Raman active given the [001] backscattering geometry[133], [137], so the only LO frequency variations are considered for the variations in the Raman signal. The relationship between the crystalline stress induced by a surface acoustic wave and the frequency of the LO GaAs phonon mode is

\[
\Delta \omega_{LO} = \frac{1}{2\omega_0} [(pS_{12} + qS_{11})\sigma'_{11} + S_{12}(p + q)\sigma'_{22}],
\]

(5.12)

where \(S_{ij}\) are the elastic compliance tensor elements of GaAs. The near-surface analysis of this technique allows \(\sigma'_{22}\) to be described as a linear combination of \(\sigma'_{22}\). The mechanical boundary condition \(\varepsilon_{22} = 0 = S_{12}\sigma'_{11} + S_{11}\sigma'_{22}\) can be rearranged, and Eq. (5.12) can be rewritten as

\[
\Delta \omega_3 = \frac{\sigma'_{11}}{2\omega_0} \left( \frac{S_{11} - S_{12}}{S_{11}} \right) (pS_{12} + q(S_{11} + S_{12})).
\]

(5.13)

Using the values \(S_{11} = 1.17 \times 10^{-11} \text{ Pa}^{-1}\) and \(S_{12} = -3.70 \times 10^{-12} \text{ Pa}^{-1}\) for the elastic compliance components and \(p = -1.10\omega_0^2\), \(q = -1.58\omega_0^2\), and \(r = 0.51\omega_0^2\) for the phonon deformation potentials[138], we find

\[
\Delta \omega_3 (\text{cm}^{-1}) = -1.63 \times 10^{-9} \sigma'_{11} (\text{Pa}).
\]

(5.14)

Under the presence of an acoustic wave, the surface of the crystal undergoes a rapid oscillation between compressive and tensile strain on the order of \(10^6\) and \(10^9\) oscillations per second, corresponding to the frequency of the acoustic waves. To determine the magnitude of strain induced by the SAW without using lock-in amplifier or interferometric
techniques, it would be necessary to revisit the interpretation of Raman peak fitting. Typically, Raman peaks are fit using a Lorentzian function,

\[
L = \frac{\left(\frac{c_0}{2}\right)^2}{\left((\omega - \omega_0)^2 + \left(\frac{c_0}{2}\right)^2\right)},
\]

(5.15)

where \(c_0\) is the full width at half max (FWHM), \(\omega\) is the Raman shift position, and \(\omega_0\) is the peak position at its maximum. Iikawa et al. proposed that the Raman signature of a surface containing SAWs would result in a symmetrically broadened Raman peak at the anti-nodes of the standing wave due to the time averaging of the compressive and tensile states of the surface[137]. Since the Raman peak shape can no longer be adequately fit with a Lorentzian function, it is ideal to use a time averaged Lorentzian in which the peak position is represented by the strain modulated peak position, \(\omega'_0(t) = \omega_0 + \Delta \omega_0 \sin(2\pi t / \tau_{SAW})\), where \(\Delta \omega_0\) is the maximum peak shift achieved by the standing SAW for any given point in time and \(\tau_{SAW}\) is the temporal period of the SAW. The time average integral reveals

\[
F = \frac{A}{2\Delta \omega_0} \left[ \tan^{-1} \left( \frac{\Delta \omega_0 + (\omega - \omega_0)}{c_0/2} \right) + \tan^{-1} \left( \frac{\Delta \omega_0 - (\omega - \omega_0)}{c_0/2} \right) \right],
\]

(5.16)

where the proportionality factor, \(A\), has been introduced to account for the amplitude of the Raman peak and can be ignored after normalization of the Raman data.

The purpose of this analysis is to improve our quantitative understanding of the surface stress induced by the SAWs. SAWs are often analyzed through electrical characterization, providing limited insight into the mechanical nature of surface acoustic wave devices. An improved understanding of mechanics and quantitative analysis would
prove helpful in harnessing the benefits of stress-induced phenomena, such as compositional patterning in crystalline semiconductors, increased catalytic reaction rates, and crystal growth applications. We use 2D Raman analysis to directly measure the stress induced by SAWs and independently verify this approach with atomic force microscopy (AFM). The two techniques are used in tandem to characterize and verify the stress and displacement imposed by SAWs.

5.5 Experimental Setup and Spectra Collection

The 2D Raman spectra, shown in Fig. 5.1, are gathered using a WITec Confocal-Raman 532 nm Microscope. The laser light was focused to an 850-nm spot size using a 50x objective. The laser power used for this experiment was approximately 1 mW. Eight equally spaced, 40 µm line scans were recorded and stitched together to produce the Raman image. The acquisition time for each point of the line scan is 15 seconds, and the point acquisition is repeated three times to reduce the noise.

The spacing between adjacent points is 1 µm. The mapping data are recorded over a 10x40 µm² area, for a total of 329 points, in the center of the viewing window region of the device. The total acquisition time is approximately 4 hours. Stress analysis is completed by examining the 291.7 cm⁻¹ LO phonon Raman peak. First, scans are recorded while the device is turned off, where the Raman data show homogeneous behavior. The device is then turned on and tuned to the resonant frequency to activate the SAW field, and the same image procedure is completed. Figure 5.1 depicts the difference in peak width observed for the one and off states of the IDT device in the anti-node region of the standing SAW field. The spectrum for each data point was fit using the scheme described in previously in this
chapter. The line scans were analyzed separately in using the MATLAB software and stitched together to form the image shown in Fig. 5.2.

![Graph showing Raman spectra](image)

**Figure 5.1**: Raman spectra of GaAs showing the TO peak at 268.3 cm\(^{-1}\) and the LO peak at 291.7 cm\(^{-1}\). The inset depicts the widening of the LO Raman peak (blue) when measured from the antinode region of the standing SAW.

### 5.6 Raman Imaging Results and Stress Field Analysis

Figure 5.2 depicts the apparent peak widths of the GaAs LO phonon Raman peak. The broadening of the Raman peak is observed at intervals of 5 µm, implying an acoustic wavelength of 10 µm, as expected, and the apparent width increases to values as high as 4.25 cm\(^{-1}\) in the anti-nodal regions of the standing SAW. The Raman peak width image is averaged into a single line scan, shown in Fig. 5.3. While the device is off, the peak width is observed to be around 4.00 cm\(^{-1}\) at a peak position of 291.76 cm\(^{-1}\). When the device is
turned on, peak widths, on average, oscillate between $4.09 \text{ cm}^{-1}$ and $4.20 \text{ cm}^{-1}$ at a relatively stagnant peak position of $291.69 \text{ cm}^{-1}$.

One might expect the Raman peak to show no broadening in the nodal regions of the standing wave; however, there is instead a $0.09 \text{ cm}^{-1}$ increase. There are a few reasons why this homogenous broadening of the Raman peaks would occur:

1. Heating of the GaAs substrate from the IDT device[139],

2. The spatial average of the strain field due to the relatively large lateral resolution of the Raman laser,

**Figure 5.2**: 2D mapping of Raman peak widths of the LO phonon mode of GaAs associated with the standing wave structure of the SAW. The peak width is broader in the anti-node region of the standing wave due to the combined effects of the red-shifting and blue-shifting Raman peaks associated with compressive and tensile stress.
(3) The coupling of the phonon wave vectors is induced by the non-homogeneous distribution of the SAW fields.[137]

This constant beam broadening effect would make the analysis of a traveling SAW field difficult, so additional studies should be completed to determine the cause of this effect.

Figure 5.3: Raman measurements are recorded over a 10x40 um² area and then averaged into a single 40 um line scan. Raman peak widths are observed to be stagnant when the device remains off; however, the peak widths periodically broaden in the anti-node region of the standing SAW when the device is turned on. A constant peak-width shift is observed when the device is turned on compared to when the device is turned off.

After fitting the Raman curves with the new fitting procedure defined by Eq. (5.16), we discover that, in the anti-nodal regions of the SAW, the Raman peak shifts as much as 0.42 cm⁻¹ to the left and right, during the tensile and compressive states of the SAW, respectively. As shown in Fig. 5.4, this translates to maximum $|\sigma'_{11}|$ and $|\sigma'_{22}|$ values of
260 MPa and 87 MPa. Applying these values to Eq. (5.9), provides strain values of $2.9 \times 10^{-3}$ and $1.4 \times 10^{-3}$ for $|\varepsilon'_{11}|$ and $|\varepsilon'_{33}|$, respectively.

Contact-mode atomic force microscopy is employed to confirm the magnitude of surface displacement caused by the standing SAWs. The dynamic nature of the acoustic strain field restricts the AFM cantilever to profile only the absolute displacement of the standing SAW. Contact-mode analysis may impart an impression that the AFM cantilever would attempt to track the motion of the acoustic wave and thus provide an inaccurate, time-averaged measurement. However, this is not the case as the vibrational frequency of the silicon cantilever used in this experiment is around $10^5$ Hz, while the SAW frequency is on the order of $10^8$ Hz. The response time of the cantilever is too slow to track the acoustic wave and can then measure the maximum positive excursion of SAWs. Figure 5.5 shows the 2D imaging results of the AFM profile of the standing SAW field.

Figure 5.4: The oscillation in the peak width is translated into surface stress values, which predict nearly 250 MPa of stress for $\sigma_{11}$.
Figure 5.6(a) shows the vertical line average of the 2D AFM image and the corresponding fitted and corrected profile. The vertical displacement induced by the SAW is fit with an absolute sine function, which agrees with the analytical solution for a SAW[111]. The red curve shows the fitting results for the absolute sine function and predicts a SAW wavelength of 10 µm and an amplitude of 3 nm. Combining the fitted data with the mechanical boundary conditions for a SAW and Hooke’s Law, the stress values induced by the SAW are calculated and shown in Fig. 5.5(b). The AFM analysis predicts maximum $|\sigma'_{11}|$ and $|\sigma'_{22}|$ values of 178 MPa and 60 MPa, respectively, in the anti-nodal regions of the standing SAW. For a more precise comparison, it would be ideal to measure...
the displacement induced by the standing SAW using interferometry techniques and acquire Raman data using a higher resolution spectrometer.

Figure 5.6: (a) The line average (solid black line) of the atomic force microscopy image is fit with an absolute sine function (red dashed line) and then corrected (dashed blue line) to reflect the sinusoidal nature of the standing SAW profile. (b) The displacement measurements translate to surface stress values for the standing SAW field, which agree well with the Raman measurements.
5.7 Conclusion

The relationship between the Raman peak broadening and the crystal strain induced by the standing surface acoustic waves is defined, and stress values are acquired using a unique Raman peak fitting scheme. The Raman peak fitting suggests that a higher resolution spectrometer may be necessary to accurately translate Raman peak broadening to the SAW displacement amplitude. Nevertheless, the Raman stress values agree well with the data collected from the AFM, thus demonstrating the potential of 2D Raman microscopy to characterize SAW fields and devices. Future studies should address the potential effects of substrate heating from the device and should acquire more accurate surface displacement data. In the next chapter, an FEM model simulates an IDT structure that accurately predicts standing SAW displacements. The FEM model aids in optimizing the device design for improved device performance.
CHAPTER 6: COMPUTATIONAL MODELING OF INTERDIGITATED TRANSDUCERS

6.1 The Relevance of FEM Modeling of IDT Devices

Theoretical modeling has suggested the potential for periodic stress fields to enhance crystal growth and localized diffusion in compound semiconductors[34]–[39], which would be valuable for developing next-generation semiconductor technologies. IDTs are a potential platform to study the effects of stress on semiconductor diffusion, and a rigorous understanding of these devices’ mechanical responses is necessary for further investigation. IDTs are often modeled using phenomenological methods like the coupling-of-modes (COM) method[140], P-matrix model[141], and equivalent circuit model[142], which adequately predict key RF-filter parameters such as device admittance and filter bandwidth.

The most popular among the phenomenological methods for SAW devices is the COM method, which considers the multiple reflections and acoustoelectric interactions between the propagating SAW and the numerous electrode charges[143], [144]. Despite its relative accuracy for narrowband devices, the COM model relies on numerous approximations and experimentally or numerically determined parameters[144], limiting its ability to capture the complete physics of the device. The COM model equations are founded on device structure periodicity, and abrupt changes in the periodic geometry occurring at gaps between transducers, reflectors, and at the ends of structures cause unaccounted effects such as phase changes, additional reflections, and scattering into bulk waves[143]. Additionally, the COM model can only describe two identical
counterpropagating waves, and other interactions within the system, such as delay line obstructions, bus bar radiation, and dynamic environments, make the model invalid[143]. Lastly, comprehensive mechanical analysis of the acoustic field is unattainable using any phenomenological method, which severely limits meaningful analysis of surface and bulk strain generated by IDT devices.

Finite element method (FEM) modeling considers the detailed physical description of the entire IDT device geometry and provides both the electrical and mechanical response characterization needed to predict more complex device behaviors. With ever-increasing and widely distributed computational resources, FEM modeling is becoming a more and more practical method for IDT device design and optimization. As of this study, very few high-fidelity computational works have been demonstrated. In this work, an interdigitated transducer and acoustic mirror assembly form a surface acoustic wave cavity resonator, subsequently modeled using COMSOL Multiphysics 5.6.

Within this chapter, COM theory as it applies to interdigitated transducer modeling is discussed and compared with FEM modeling. The shortcomings of COM theory are recovered using FEM modeling, and the simulation results are compared with experimental devices. Experimental device scattering parameters are measured using a vector network analyzer and are then compared to the agreeing simulated results. Maximum standing surface wave displacements for the experimental device are measured using atomic force microscopy, which corroborates the simulation’s mechanical response predictions. Finally, a parametric analysis is completed to study the effects of device geometry parameters on key device performance factors such as the device resonance frequency, effective coupling coefficient, quality factor, and maximum acoustic surface displacement.
6.2 The Coupling-of-Modes Model for Interdigitated Transducers

For many cases of IDT modeling, phenomenological methods such as the coupling-of-modes (COM) method are adequate for predicting key device parameters. While finite element simulations are of interest for optimizing and designing IDT devices, this form of analysis has long been considered too time-consuming to be practical until recently. The COM method is reviewed to discuss a standard method for IDT device design and analysis. The primary sources for the coupling-of-modes model outlined here are the texts by Plessky[143] and Chambon[144].

![Diagram of IDT structure with labels for device thickness, wavelength, and device aperture.]

**Figure 6.1:** (a) the schematic illustrates the various design considerations for an IDT structure such as the device thickness, h, the wavelength, \( \lambda \), and the device aperture, \( W \). (b) The COM parameters are extracted by assuming the IDT device mechanically responds to an electric potential by generating two opposing mechanical waves, \( u_+ \) and \( u_- \).

The COM model is an efficient and relatively accurate method to simulate SAW devices but requires knowledge of either experimentally or numerically determined parameters, known as COM parameters. The COM parameters are determined through analysis of acoustic fields, propagating within an infinite grating, defined by a set of device geometry parameters, illustrated in Fig. 6.1(a): the finger-pair pitch (\( \lambda \)), the device aperture
(W), and the electrode thickness (h) and width (a). The five COM parameters necessary to complete the analysis of a SAW device are the SAW velocity (v_{SAW}), reflection coefficient (k_{12}), finger transduction coefficient (\xi), finger capacitance coefficient (C), and the attenuation coefficient (\gamma).

It is worth noting that \gamma serves only as a convenient value that summarizes the many contributions to SAW attenuation such as thermal phonon interactions, surface or near-surface defects, surface loading, attenuation due to metal fingers, and acousto-electric interactions. In addition, close to the stopband frequency of the modeled structure, the attenuation coefficient is difficult to measure due to Bragg reflections. For this reason, this value is solved entirely through experimental or computational means and is otherwise assumed to equal zero for the remainder of this discussion.

The COM theory assumes two mechanical waves (u_+ and u_-) are propagating in opposing directions and individually undergo reflections at electrode interfaces, contributing an increasing amplitude to the opposing mechanical wave. The COM model considers first harmonic reflections, assumes acoustic attenuation leads to decreasing wave amplitudes, and assumes the transduction coefficient is a linear system due to the piezoelectric effect. These conditions are summarized in the form of the following equations

\[
\frac{du(x)}{dx} = -j \left( \frac{\omega}{v_{SAW}} - j\gamma \right) u_+(x) - jk_{12}u_-(x)e^{-j2\pi x/p} + j\xi Ve^{-j\pi x/p}, \quad (6.1)
\]

\[
\frac{du(x)}{dx} = j\kappa_{12}u_+(x)e^{j2\pi x/p} + j \left( \frac{\omega}{v_{SAW}} - j\gamma \right) u_-(x) - j\xi Ve^{j\pi x/p}, \quad (6.2)
\]
\[
dl(x) = -2j\xi u_+(x)e^{j\pi x/p} - 2j\xi u_-(x)e^{-j\pi x/p} + j\omega CV. \tag{6.3}
\]

which describes wave behavior mechanics and current density. A periodic function approximately describes the mechanical waves with respect to the finger-pair pitch, and therefore the general solution for the mechanical waves are

\[
u(x)_+ = R(x)e^{-j\pi x/p}, \tag{6.4}
\]

\[
u(x)_- = S(x)e^{j\pi x/p}, \tag{6.5}
\]

where \(R(x)\) and \(S(x)\) describe spatial variations of the field governed by slow varying amplitudes.

Equations (6.1)-(6.3) are summarized as the following COM linear system:

\[
\begin{align*}
\frac{dR(x)}{dx} & = \begin{bmatrix}
-j\theta_u & -j\kappa_{12} & j\xi \\
 j\kappa_{12} & j\theta_u & -j\xi \\
-2j\xi & -2j\xi & j\omega C
\end{bmatrix} \begin{bmatrix} R(x) \\ S(x) \\ V(x) \end{bmatrix}, \\
\frac{dS(x)}{dx} & = \begin{bmatrix}
-j\theta_u & -j\kappa_{12} & j\xi \\
 j\kappa_{12} & j\theta_u & -j\xi \\
-2j\xi & -2j\xi & j\omega C
\end{bmatrix} \begin{bmatrix} R(x) \\ S(x) \\ V(x) \end{bmatrix},
\end{align*}
\tag{6.6}
\]

where \(\theta_u = \frac{\omega}{v_{SAW}} \frac{\pi}{p} j\gamma\) is a detuning factor.

Determining the COM parameters requires considering three separate sets of electrical boundary conditions: (1) a short-circuit condition, (2) an open-circuit condition, and (3) a harmonic driving voltage condition. Each set of electrical boundary condition assumptions alters Eq. (6.6) such that the COM parameters can be extracted through numerical methods.

**Short Circuit Condition**
In the short-circuit condition, it is convenient to consider no attenuation \((\gamma = 0)\) and the system of equations describes a short-circuit model, which results in no electric field, such that \(V = 0\) and \(\xi = 0\). Equation (6.6) is then presented as

\[
\begin{pmatrix}
\frac{dR(x)}{dx} \\
\frac{dS(x)}{dx}
\end{pmatrix} = \begin{bmatrix}
-j\theta_u & -j\kappa_{12} \\
-j\kappa_{12} & j\theta_u
\end{bmatrix}\begin{bmatrix}
R(x) \\
S(x)
\end{bmatrix},
\] (6.7)

and the solutions for \(R(x)\) and \(S(x)\) are of the form

\[
\begin{pmatrix}
R(x) \\
S(x)
\end{pmatrix} = \begin{bmatrix}
R_0 \\
S_0
\end{bmatrix} e^{-jqx}.
\] (6.8)

Substituting Eq. (6.8) into Eq. (6.7) provides a matrix system that has non-zero solutions only if the matrix determinant is equal to zero,

\[
\theta_u^2 - q^2 - |\kappa_{12}|^2 = 0.
\] (6.9)

The general solutions for the short-circuit condition are then

\[
\begin{pmatrix}
R^{SC}(x) \\
S^{SC}(x)
\end{pmatrix} = A \begin{bmatrix}
\frac{1}{j\kappa_{12}} \\
\frac{\kappa_{12}}{1}
\end{bmatrix} e^{-jqx} + B \begin{bmatrix}
\frac{j\kappa_{12}}{\kappa_{12}} \\
\frac{1}{1}
\end{bmatrix} e^{jqx},
\] (6.10)

where \(A\) and \(B\) are constants determined by boundary conditions of the modeled device and \(q\) is the wave number of the existing mode, defined as

\[
q = \begin{cases} 
\pm \sqrt{\theta_u^2 - |\kappa_{12}|^2} & \text{if } \theta_u^2 > |\kappa_{12}|^2 \\
\pm j \sqrt{|\kappa_{12}|^2 - \theta_u^2} & \text{if } \theta_u^2 < |\kappa_{12}|^2 \end{cases}.
\] (6.11)

The short circuit frequencies which define the stop band edges of the dispersion relation are the solutions to the quadratic polynomial produced by substituting \(\theta_u\) into Eq. (6.11),
\[ f_{SC}^\pm = \frac{v_{SAW}}{\lambda} \left( 1 \pm \frac{\lambda |\kappa_{12}|}{2\pi} \right). \]  

(6.12)

Averaging Eq. (6.12) provides the \( v_{SAW} \) and the difference gives the reflection coefficients,

\[ v_{SAW} = \lambda \left( \frac{f_{SC}^+ + f_{SC}^-}{2} \right) \]  

(6.13)

\[ |\kappa_{12}| = \frac{\pi}{v_{SAW}} (f_{SC}^+ - f_{SC}^-). \]  

(6.14)

The magnitude of the normalized reflectivity \( (\kappa_p = \kappa_{12}\lambda) \) determines the relative width of the stopband, \( \Delta f/f_0 = |\kappa_n|/\pi \). The sign of \( \kappa_n \) can be either negative or positive and the phase of \( \kappa_{12} \) provides the center of reflectivity of the period.

**Open Circuit Condition**

In the open circuit condition, the current is zero such that the voltage can be expressed as

\[ V = \frac{2}{C\omega} \left( \bar{\xi}R(x) + \xi S(x) \right), \]  

(6.15)

according to Eq. (6.6). Substituting Eq. (6.15) into the remainder of Eq. (6.6) yields

\[
\begin{align*}
\left\{ \begin{array}{c}
\frac{dR(x)}{dx} \\
\frac{dS(x)}{dx}
\end{array} \right\} &= \begin{bmatrix}
-j \left( \theta_u - \frac{2|\xi|^2}{C\omega} \right) & -j \left( \kappa_{12} - \frac{2\xi^2}{C\omega} \right) \\
+ j \left( \bar{\kappa}_{12} - \frac{2\bar{\xi}^2}{C\omega} \right) & + j \left( \theta_u - \frac{2|\xi|^2}{C\omega} \right)
\end{bmatrix} \begin{bmatrix}
R(x) \\
S(x)
\end{bmatrix}.
\end{align*}
\]  

(6.16)

Again, a non-trivial solution only exists if the matrix determinant of Eq. (6.16) is equal to zero such that:
which further provides the stop band edge frequencies for the open circuit condition,

\[
f_{OC}^\pm = \frac{v_{SAW}}{2\pi} \left( \frac{\pi}{p} + \frac{2|\xi|^2}{C\omega} \pm \left| \kappa_{12} - \frac{2\xi^2}{C\omega} \right| \right). \tag{6.18}
\]

Assuming the values for the coupling coefficients and the transduction coefficients are real, the sum of the stop band frequencies for the open circuit condition yields

\[
f_{OC}^+ + f_{OC}^- = \frac{v_{SAW}}{\pi} \left( \frac{\pi}{p} + \frac{2|\xi|^2}{C\omega} \right). \tag{6.19}
\]

Rearranging Eq. (6.19) and substituting Eq. (6.13) provides a clear relationship between \( \xi \) and \( C \), such that

\[
\frac{|\xi|^2}{C} = \frac{\pi\omega}{2} \frac{(f_{OC}^+ + f_{OC}^-) - (f_{SC}^+ + f_{SC}^-)}{v_{SAW}}. \tag{6.20}
\]

The normalized transduction coefficient, \( \xi_p \), measures the excitation of waves due to piezoelectric coupling in a unit cell of length \( \lambda \), which is generally outlined by the length of a single electrode pair. The absolute value of the transduction coefficient is thus equal to the wave magnitude generated by the period under the drive voltage. The phase of the transduction coefficient defines the transduction center location.

On the other hand, the normalized capacitance parameter, \( C_p \), measures the electrostatic storage of energy in the structure per unit period. The capacitance depends on device geometries and substrate properties due to the long range of electrostatic forces, even for higher frequencies. For materials of sufficiently weak piezoelectric coupling like
quartz or gallium arsenide, the COM capacitance parameter may be sufficiently defined by
the static capacitance of the transducer per electrode pair. This assumption, however, does
not hold for stronger piezoelectric materials and requires the appropriate measures to fit
the parameter accordingly.

**Harmonic Driving Voltage Condition**

Finally, applying the harmonic driving voltage in the case of no attenuation ($\gamma = 0$)
determines the harmonic admittance parameter. The electrode finger potential does not
have $x$-dependence such that

$$\{\tilde{R}(x)\}^\alpha \{S(x)\}^\beta = \{A_+\} V. \quad (6.21)$$

Substituting Eq. (6.21) into the first two rows of Eq. (6.6) and simplifying yields

$$\begin{bmatrix} -j\theta_u & -j\kappa_{12} \\ j\kappa_{12} & j\theta_u \end{bmatrix} \begin{bmatrix} A_+ \\ A_- \end{bmatrix} = \begin{bmatrix} -j\xi \\ j\xi \end{bmatrix}. \quad (6.22)$$

Inverting this system and substituting the solution for $\{A_+, A_-\}$ into Eq. (6.21) leads to

$$\begin{bmatrix} \tilde{R}(x) \\ S(x) \end{bmatrix} = \frac{1}{\theta_u^2 - |\kappa_{12}|^2} \begin{bmatrix} \theta_u^2 - |\kappa_{12}|^2 \xi - \kappa_{12}\xi \\ \theta_u \xi - \kappa_{12}\xi \end{bmatrix} V. \quad (6.23)$$

Finally, substituting Eq. (6.23) into the third row of Eq. (6.6) provides the harmonic
admittance coefficient,

$$Y(f) = \frac{1}{V} \frac{dI(x)}{dx} = -2j\frac{2\theta_u^2 |\xi|^2 - 2\text{Re}(\kappa_{12}\xi^2)}{\theta_u^2 - |\kappa_{12}|^2} + 2j\pi f C. \quad (6.24)$$

Substituting the previously solved COM parameters into Eq. (6.24) provides the
capacitance coefficient, $C$, using numerical fitting techniques. Additionally, the resonance
and anti-resonance frequencies for the modeled structure are apparent when plotting Eq. (6.24), as shown in Fig. 6.2.

![Figure 6.2](image)

**Figure 6.2:** The resonance and anti-resonance pattern is observed in the admittance for an infinitely long periodic transducer. The solid line represents the real part of the admittance, while the dashed line represents the imaginary part of the admittance.

Due to the phenomenological nature of the COM model, the COM parameters \((v_{SAW}, \kappa_1, \zeta, C, \gamma)\) cannot be determined directly from the theory. The parameters must be defined using experimental measurements or FEM techniques and then inserted into the model. A typical FEM model considers an infinite grating geometry of sufficiently thin height. However, a significant amount of work has been dedicated to determining these parameters using perturbation theory or variational approaches.

Several practical cases exist in which the COM method fails to represent an IDT structure and its transduction mechanisms accurately. For example, internal perturbations,
acoustic interactions, and acoustic reflections must be small, and the finger reflectivity must be appropriately small. Additionally, the COM model only represents systems defined by identical counter-propagating waves. However, added interactions such as bulk waves or asymmetric counter-propagating waves lead to noticeable device responses, especially in the case of transverse surface waves. And as mentioned in previous discussions, the parasitic effects unrelated to surface interactions such as internal crystal reflections, resistive losses, parasitic capacitance/inductance from packaging geometries can alter the predicted device responses. Therefore, for finite structures containing more complex geometries, non-periodic elements, delay lines, excessively thick electrodes, etc., the COM model is tedious to solve and insufficient in its accuracy. Consequently, other methods should be explored to model SAW resonator devices accurately.

6.3 Simulation Description and Scattering Matrix Components

With ever-increasing and widely distributed computational resources, FEM modeling has become a more and more practical method for IDT device design and optimization. Two-dimensional device simulations are completed using COMSOL Multiphysics 5.6. Figure 6.3 depicts a simplified schematic of the simulated device. The simulated device geometry consists of two opposing sets of 150 finger pairs and 200 mirror strips. A 100-µm delay line region is included at the center of the device, mimicking the experimental device, which allows for analysis of the free-surface displacement field produced by the standing SAW. The substrate and metal strips are assumed to be 200-µm-deep to emulate the experimental device aperture. The substrate is four wavelengths (40 µm) in height and utilizes a low-reflecting boundary condition and a perfectly matched domain around the bottom and sides of the perimeter to mitigate mechanical wave
boundary reflections. Admittance and impedance simulations are completed by assigning a unique voltage terminal to the ‘Port 1’ and ‘Port 2’ electrodes, while power-dependent mechanical analysis is completed by assigning power terminals in place of the voltage terminals. The acoustic mirror strips are grounded for both forms of analysis.

As discussed in Chapter 3, a piezoelectric IDT device's electrical and mechanical behavior is governed by an extension to Hooke’s law that couples the system's mechanical stress and electric displacement. The stress tensor, $T$, and electric displacement, $D$, within a piezoelectric domain are related to the strain tensor, $S$, and the electric field, $E$, by the following mathematical framework[27], [28], [111]:

**Figure 6.3:** A diagram of an IDT resonator shows a standing SAW pattern (red) is produced in the center of the DIIT device (grey) and is contained by the distributed acoustic Bragg reflectors (blue). Electrical contact is made by way of wire bonding to the G-S-G pads (gold).
\[ T_{ij} = c^{E}_{ijkl} S_{kl} - e_{klj} E_k \]  
\[ D_i = e_{ijk} S_{jk} + \varepsilon_{ij} E_j \]  

where \( c^{E}_{ijkl} \) are the components of the elasticity tensor for a constant electric field, \( \varepsilon_{ij} \) are the components of the permittivity tensor for constant strain, and \( e_{ij} \) are the components of the piezoelectric tensor. Acoustic attenuation effects associated with thermoelastic attenuation[74], Akhiezer damping\(^\text{19}\), and device fabrication defects are approximated using an isotropic loss coefficient, \( \eta_s \), which modifies the elasticity tensor components to be complex values, and is experimentally determined to be \( 1.25 \times 10^{-4} \). \( c^{E}_{ijkl} \) then becomes:

\[ c^{E'}_{ijkl} = (1 + i\eta_s) c^{E}_{ijkl} \]  

The piezoelectric substrate material is modeled after GaAs\((100)\) and the device material is modeled after aluminum. The material orientation for GaAs\((100)\) is defined by a general rotation input using the Euler angle \((Z-X-Z)\) orientation of \((90^\circ - 45^\circ - 90^\circ)\) to match the experimental device orientation.
Admittance, $Y_{11}$, and impedance, $Z_{11}$, matrix components, depicted in Fig. 6.4, are simulated, along with the remaining admittance and impedance matrix components, and scattering responses are calculated in post-processing per the following two-port network equations:

$$S_{11} = \frac{(Y_0 - Y_{11})(Y_0 - Y_{22}) + Y_{12}Y_{21}}{(Y_0 + Y_{11})(Y_0 + Y_{22}) - Y_{12}Y_{21}} \quad (6.28)$$

$$S_{21} = \frac{-2Y_{21}Y_0}{(Y_0 + Y_{11})(Y_0 + Y_{22}) - Y_{12}Y_{21}} \quad (6.29)$$

where $S_{11}$ is the input voltage reflection coefficient, $S_{21}$ is the input voltage transmission coefficient, and $Y_0$ is the device reference impedance ($50\Omega$). Performance characteristics of piezoelectric resonators are often described with figures of merit, such as an effective

Figure 6.4: The simulated real (solid line) and imaginary (dashed line) parts of the device (a) admittance and (b) suggest the relative locations of the resonance and anti-resonance frequencies for the IDT device. The conductance and resistance peak positions refer to the series and parallel resonance frequencies, $f_s$ and $f_p$. 

Admittance, $Y_{11}$, and impedance, $Z_{11}$, matrix components, depicted in Fig. 6.4, are simulated, along with the remaining admittance and impedance matrix components, and scattering responses are calculated in post-processing per the following two-port network equations[115]:
The effective coupling coefficient, \( k_{\text{eff}}^2 \), is largely a function of resonator geometry and substrate material, and is used as a convenient measure of the bandwidth for a bandpass filter, which is defined as follows[89], [145], [146]:

\[
k_{\text{eff}}^2 = \frac{(f_p^2 - f_s^2)}{f_s^2}
\]

(6.30)

where \( f_s \) and \( f_p \) are the series and parallel resonance frequencies of the piezoelectric resonator. The location of \( f_s \) and \( f_p \) correspond with the maximum admittance and impedance positions, shown in Fig. 6.4.

The quality factor, \( Q \), describes the ratio of maximum stored strain energy to the dissipated energy per acoustic cycle[89], [145]–[149], and is defined as[147]:

\[
Q = \frac{\omega_r W_s}{P_d}
\]

(6.31)

where \( \omega_r \) is the resonant angular frequency, \( W_s \) is the total stored elastic strain energy, and \( P_d \) is the power dissipation within the device. Post-processing utilizes the simulated admittance, impedance, and strain field values, and a parametric analysis of the IDT device is performed to study the effects of electrode width and device thickness on various device performance factors, such as \( f_p \), \( k_{\text{eff}}^2 \), quality factor, and anti-node surface displacement.

### 6.4 COMSOL Materials and Physics Discussion

The piezoelectric substrate material is modeled after GaAs(100) and considers the temperature effects for the density, elasticity matrix, and relative permittivity. The material orientation for GaAs(100) is defined by a general rotation input in a ‘rotated system’
definition using the Euler angle (Z-X-Z) orientation of (90° − 45° − 90°) to match the experimental device orientation. The device material is modeled after aluminum and considers the temperature effects of density[150], Young’s modulus[151], and Poisson’s ratio[152]. Thermal expansion coefficients are incorporated for both materials to account for resonant frequency shifts attributed to thermal expansion of the substrate and metal fingers[153], [154]. The material properties for aluminum and gallium arsenide and their respective temperature dependences are detailed in Table 6.1. Customized ‘component materials’ are generated for aluminum and gallium arsenide, considering the temperature effects by linking the properties to the user-defined ‘Device Temperature’ input parameter. It is important to note that material properties are carefully selected for well-matching simulation and experimental results.

**Table 6.1**: Aluminum and gallium arsenide are defined by a set of temperature-dependent material properties. The table details the material properties required by the simulation and their respective temperature dependence.

<table>
<thead>
<tr>
<th>Material</th>
<th>Unit</th>
<th>Temperature Dependence</th>
<th>Value @ 293K</th>
<th>Temperature Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum</td>
<td>Young’s Modulus</td>
<td>GPa</td>
<td>85.8 − 0.054 × T</td>
<td>70.0</td>
</tr>
<tr>
<td></td>
<td>Poisson’s Ratio</td>
<td>--</td>
<td>0.172 + (5.38 × 10^{-4})T</td>
<td>0.330</td>
</tr>
<tr>
<td></td>
<td>Density</td>
<td>kg/m³</td>
<td>2745.1 − 0.15 × T</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>Thermal Expansion</td>
<td>--</td>
<td>--</td>
<td>29.0 × 10^{-6}</td>
</tr>
<tr>
<td>GaAs(100)</td>
<td>C_{11}</td>
<td>GPa</td>
<td>121.7 − (1.44 × 10^{-2})T</td>
<td>117.48</td>
</tr>
<tr>
<td></td>
<td>C_{12}</td>
<td>GPa</td>
<td>54.6 − (0.64 × 10^{-2})T</td>
<td>52.72</td>
</tr>
<tr>
<td></td>
<td>C_{44}</td>
<td>GPa</td>
<td>61.6 − (0.70 × 10^{-2})T</td>
<td>59.55</td>
</tr>
<tr>
<td></td>
<td>Relative Permittivity</td>
<td>--</td>
<td>12.79 + (1.28 × 10^{-4})T</td>
<td>13.165</td>
</tr>
<tr>
<td></td>
<td>Density</td>
<td>kg/m³</td>
<td>5344.6 − 0.092 × T</td>
<td>5317.55</td>
</tr>
<tr>
<td></td>
<td>Thermal Expansion</td>
<td>--</td>
<td>--</td>
<td>5.73 × 10^{-6}</td>
</tr>
<tr>
<td></td>
<td>e_{14}</td>
<td>C/m²</td>
<td>61.6 − (5.11 × 10^{-4})T</td>
<td>0.159</td>
</tr>
</tbody>
</table>
The simulation geometry is created by forming a union between the substrate and the finger and mirror arrays. The gallium arsenide’s substrate geometry width considers the number of fingers, mirrors, and the length of the delay line as well as an additional two-wavelength buffer on each side of the device. The substrate geometry height is defined to be four wavelengths tall to account for a fully developed SAW field adequately. The substrate is also equipped with a ‘Perfectly Matched Layer’ artificial-domain definition to simulate an infinite-space boundary condition for the sides and bottom of the substrate geometry. An additional rectangular domain is generated below the surface of the delay line, which is two wavelengths deep. This additional domain enables a higher quality mesh for the delay region for stress analysis, which is otherwise unnecessary for the remaining substrate domain.

The aluminum fingers are defined as four separate groups of entities to account for each side of the device and each terminal of the device. The finger-strip height is defined to be 80 to 200-nm thick and the finger-strip width is defined to be a quarter wavelength wide. The fingers are located at the surface of the substrate geometry. The fingers are then subject to a geometry array transform that multiplies and evenly spaces identical fingers for 150 fingers per entity group. This produces 300 finger pairs or 600 individual metal finger strips. The aluminum mirror strip geometries are produced like the finger strips but were only defined as two separate groups of entities to account for each side of the device. The mirror strips are of identical size and shape to the finger strips and underwent a similar geometry array transform to produce 200 mirror strips per side of the device for a total of 400 mirror strips. Between the two halves of finger sets, in the center of the device geometry surface, is the delay line region which contains no finger or mirror strips. Instead
of the complete simulation geometry, which cannot be readily displayed in this document due to its impractical aspect ratio, a simplified layout of the device simulation is depicted in Fig. 6.5.

![Figure 6.5: A simplified schematic of the XY-plane details the different components of the simulated IDT. The actual simulated device features 300 finger pairs, 400 mirror strips, and a 100 μm delay line region.](image)

The physics modules utilized in the simulation were the ‘Solid Mechanics’ module and the ‘Electrostatics’ module. Together, these modules formed the ‘Piezoelectric Effect’ Multiphysics module. The ‘solid mechanics’ domain consists of each geometry entity. The aluminum finger and mirror strips are assigned a ‘linear elastic material,’ which assumes an isotropic solid model and utilizes the user-defined Young’s modulus, Poisson’s ratio, and density for aluminum. Hooke’s Law defines the mathematical framework, and while the simulation is prepared to account for inelastic constraints, these are not considered for this simulation. The gallium arsenide substrate is assigned the ‘Piezoelectric Material’ domain, within which the coordinate system is defined as a rotated system to match the experimental device crystal orientation. The mathematical framework is defined by the extended version of Hooke’s Law to account for the electric field’s effect on the stress matrix and the strain matrix’s effect on the electric displacement vector. The piezoelectric material properties rely on the ‘stress-charge’ constitutive relation and utilize the user-
defined elasticity matrix, coupling matrix, and relative permittivity for gallium arsenide. The substrate is also assigned a ‘low reflecting boundary’ about its bottom and side perimeters, while the substrate surface and finger and mirror surfaces are assigned the ‘free’ boundary condition.

The electrostatic domains are assigned to the aluminum finger and mirror strips and omit the gallium arsenide substrate. The mirror strips are assigned a ‘charge conservation’ domain and a ‘grounded’ boundary constraint. The finger strips are split into two ports which are assigned a ‘terminal’ domain constraint for each element of a finger pair, like the assignments displayed in Fig. 6.5. For the admittance and scattering response simulations, the terminal types are defined as ‘voltage’ terminals. The input terminal is assigned a voltage of 1 V, and the output terminal is assigned a voltage of 0 V. The voltage terminal analysis is like running the device in the single ‘forward’ direction and would only generate the $Y_{11}$ and $Y_{21}$ admittance matrix components. For the power sweep and resulting surface displacement simulations, the terminal types are defined as ‘terminated’ terminals. A ‘manual terminal sweep’ performs a terminal sweep over both terminals to generate scattering responses with the appropriate user-defined applied power.

6.5 Geometry Mesh and Quality

The simulation mesh is generated within COMSOL and is defined as ‘mapped,’ ‘free quadrature,’ and ‘free triangular’ mesh definitions. The order in which the mesh is applied is essential for completing the mesh generation. The first mesh generated is a ‘mapped’ mesh for the finger and mirror strips. The mapped mesh consisted of two distribution nodes outlining the perimeter of the metal strips and split the strips into a 3-
by-3 segmented domains. Figure 6.6(a) depicts the geometry of the mapped mesh. The second generated mesh is the delay-line domain which contained two distribution nodes and split the domain into a 150-by-100 segmented domain.

**Figure 6.6**: (a) The finger and mirror strips are meshed using a mapped mesh, which breaks each strip into a 3-by-3 segmented geometry. (b) The substrate is meshed using a triangular mesh, but the region below the delay-line surface is meshed using a free quadrature mesh.
The remainder of the substrate is meshed with a ‘free triangular’ mesh. The previous mesh constraints define the distribution of the substrate mesh. The element size is set to the ‘extremely fine’ mesh condition, and the ‘maximum element growth rate’ is set to the value of 1.15. Figure 6.6(b) depicts the geometries of the ‘free quadrature’ and ‘free triangular’ meshes. The finalized geometry consists of 1,001 domains, 5,005 boundaries, and 4,005 vertices. The completed mesh consists of 25,892 domain elements and 7,930 boundary elements.

![Image of mesh geometry](image)

**Figure 6.7:** The health of the mesh geometry is determined using the ‘Mesh’ results feature, which quantifies the skewness of each mesh element. As the skewness for a mesh element increases, the mesh quality is penalized and decreases the mesh quality value, which is rated between 0 and 1.

The mesh quality is assessed using the ‘mesh results’ feature, which quantifies the skewness of each mesh element. The skewness quality measure is a default quality measure option and penalizes elements with large or small angles compared to the angles in an ideal
element. The mesh quality measure results for a simplified geometry are shown in Fig. 6.7 and allude to a healthy mesh throughout the entire domain.

6.6 Device Fabrication and Experimental Procedure

The IDT assembly used in this experiment is based on a SAW resonator design and is fabricated on semi-insulating GaAs(100), positioned such that SAWS propagate in the \( \langle 110 \rangle \) and \( \langle 1\overline{1}0 \rangle \) direction. Each side of the SAW resonator is equipped with 150 finger pair electrodes and 200 grounded metal strips, which function as a distributed acoustic mirror. The finger pitch of the IDT device is 10 \( \mu \)m, and the grounded metal strips are spaced one-half wavelength apart. The 10-\( \mu \)m finger pitch of the IDT device corresponds to the SAW wavelength. The device aperture is 200 \( \mu \)m, and a 100-\( \mu \)m delay line region is included in the middle of the device to allow for an unimpeded standing SAW field to form. The 160-nm aluminum IDT structure is fabricated using optical lithography and electron-beam metal evaporation. Underdevelopment or under-exposure of the device-layer photoresist resulted in an electrode width of approximately 2.3 \( \mu \)m. A 5-nm-thick adhesion layer of titanium and a 750-nm-thick layer of gold are additionally deposited to form ground-signal-ground (GSG) contact pads to allow for durable wire bonding.

Device scattering response measurements are recorded using a Keysight 5247a RF Performance Network Analyzer. The device is then wire bonded to a quarter wavelength transmission line for impedance matching and powered using a Windfreak Synth NV signal generator with an applied power of 20.85 dBm. Contact-mode atomic force microscopy measures the surface displacement amplitude produced by the generated standing SAW at the device resonance frequency.
6.7 Comparing Simulated and Experimental Results

Figure 6.8 depicts the measured scattering response magnitudes for the 300-finger pair IDT device compared to the simulated response calculated in COMSOL. Due to the symmetry of the IDT design, the device functions as a reciprocal and symmetrical network such that $S_{11} = S_{22}$ and $S_{12} = S_{21}$. The measured input voltage reflection coefficient, described by the $S_{11}$ parameter in Fig. 6.8(a), shows excellent agreement with the simulated response in both off-resonance and on-resonance frequency domains. A similar statement can be made for the input voltage transmission coefficient, described by the $S_{21}$ parameter in Fig. 6.8(b). However, there is a slight disagreement in the off-resonance magnitude at the edge of the measured frequency domain, which is attributed to unaccounted ohmic losses in the device.
Figure 6.8: The simulated scattering responses, (a) $S_{11}$ and (b) $S_{21}$, are calculated with Eqs. (4) and (5) and agree well with the experimental measurements. Additional resonant modes are observed at frequencies slightly higher than the anti-resonance frequency.
The FEM simulation predicts additional acoustic modes at frequencies higher than the anti-resonance frequency, confirmed by the experimental device. Similar modes have been observed in other two-port IDT studies\[^{[155], [156]}\]. Powlowski et al. suggest these additional modes could result from SAW reflections and multi-transit interference\[^{[156]}\], though no substantial evidence is provided to validate these claims. Within the FEM simulation, increasing the electrode thickness leads to an increasing magnitude of the additional modes, while removing the delay-line region of the SAW device virtually eliminates the modes. The investigation results are shown in Fig. 6.9, and support the claims made by Powlowski et al.. The FEM simulation has therefore demonstrated its

\[ \text{Figure 6.9: The additional resonant mode observed in the experimental and simulated results is associated with SAW reflections within the delay line region of the device. Removing the delay line (red) within the simulation removes the additional mode, and doubling the device thickness (blue) greatly increases the magnitude of the additional resonant mode.} \]
ability to predict complicated acoustic behaviors that are otherwise unaccounted for in typical phenomenological models.

![Displacement Profile](image)

Figure 6.10: The simulated displacement field predicts a vertical displacement at the surface of approximately 5.8 nm and a maximum displacement occurring just below the surface.

Figure 6.10 portrays the simulated displacement profile at the peak of SAW oscillation over a single wavelength in the delay line region of the device. Due to the dynamic nature of standing SAW field, the crystal domain undergoes a rapid oscillation corresponding to the frequency of the acoustic wave. The anti-node displacement oscillates between compressive and tensile values every half temporal period. The figure depicts a single snapshot of the dynamic wave at a moment of maximum displacement and
demonstrates an antisymmetric displacement profile. Maximum displacement is observed near the series resonance frequency, which is around 287.24 MHz.

The 2-D contact mode AFM imaging results of the standing SAW field are shown in Fig. 6.11. Described more thoroughly in previous work[157], the dynamic behavior of the acoustic wave restricts the AFM cantilever to outline only the absolute vertical displacement of the standing SAW. AFM measurement fitting reveals a standing-wave displacement amplitude of 5.2 nm and a SAW wavelength of 10.02 μm. Compared to the simulated device, the slight variation in the mechanical response of the experimental devices can be readily attributed to impedance mismatch introduced by wire bonding to the quarter wavelength transmission line as well as an imperfect simulated representation of the experimental device.

**Figure 6.11:** Contact-mode AFM measurements validate the simulated device and depict the absolute displacement of the standing SAW pattern.
6.8 Parametric Analysis of IDT Devices

Without a geometry-sensitive predictive model, optimizing IDT device design requires extensive fabrication and testing, which quickly becomes expensive due to high-frequency devices relying on photolithography fabrication techniques. High-fidelity FEM modeling of device mechanical performance enables design optimization for mechanical resonator and electronic filter IDT devices. A parametric analysis of the experimental IDT device is conducted to study the effects of electrode width and device thickness on various device performance factors, which are otherwise unattainable using common phenomenological methods.

The results of this analysis are depicted in Fig. 6.12, wherein Fig. 6.12 (a) illustrates the general effect of mass loading on $f_0$, which tends to shift to higher frequencies for the higher mass loading of the aluminum electrodes. As discussed earlier, $k_{eff}^2$ describes the relative frequency spacing between the series and parallel resonant frequencies, which is a key figure-of-merit for electromechanical power conversion efficiency. Figure 6.12(b) depicts how $k_{eff}^2$ changes with electrode width and device thickness, which illustrates that a thinner device is preferable for a better coupling coefficient. The quality factor is a key parameter for discerning damping within an oscillating system in mechanical resonators and increases for thicker devices and smaller electrode widths, contrary to the device parameter preferences of higher coupling-coefficient devices.

Figure 6.12 (d) depicts the effects of the electrode width and electrode thickness on the vertical displacement achieved by the standing SAW in the center of the IDT delay line region. Unsurprisingly, the results are similar to Fig. 6.12 (c), as a higher quality
mechanical resonator would produce a stronger acoustic field. Increasing the device thickness from 80 nm to 200 nm increases the vertical displacement response from approximately 4 nm to nearly 7 nm. A stronger acoustic response within the device could benefit many stress-sensitive phenomena.

**Figure 6.12**: Surface plots depict how the IDT electrode width and thickness affect various device variables. A higher (a) series resonant frequency prefers a thicker device and a wider electrode. The (b) effective coupling coefficient is increased for smaller device thickness. The (c) quality factor and (d) anti-node vertical displacement increase with increasing device thicknesses.
6.9 Conclusion

In this study, a surface acoustic wave cavity comprised of opposing IDT structures and distributed acoustic mirrors is fabricated and subsequently modeled using FEM software. Experimental device scattering parameters are measured using a vector network analyzer and compared to the agreeing simulated results. FEM modeling predicts the vertical displacement amplitude achieved by the standing SAW field produced in the delay-line region of the IDT that compares well with AFM measurements of the experimental device. A parametric analysis is completed to study the effects of electrode width and device thickness on key device performance factors for electronic filters and mechanical resonators. In the next chapter, high-temperature measurements of the SAW resonator devices reveal device performance at temperatures as high as 177 °C, which agrees well the high-temperature FEM simulation.
CHAPTER 7: HIGH-TEMPERATURE CHARACTERIZATION OF INTERDIGITATED TRANSDUCERS

7.1 Relevance of High-Temperature Modeling of IDT Devices

As a potential platform to study stress-enhanced phenomena, the temperature response of IDT devices must be well understood. From the perspective of high-temperature semiconductor processes, IDT structures may not be expected to perform at extremely high temperatures. However, the experimental platform should anticipate temperature variations due to a locally heated portion of the device. As discussed in Appendix B, a laser heating system can be used to locally heat the delay line region of the SAW resonator structure. The device is therefore not heated directly by the laser heating setup. However, the device may operate at a higher than optimal temperature due to thermal conduction.

The tuning of an IDT’s mechanical response through optimization of the device geometry is significantly aided by finite element method (FEM) modeling, as device fabrication and characterization can be an extensive and costly process. For elevated temperature modeling, knowledge of the temperature dependence for the relevant material properties is necessary. Gallium arsenide (GaAs) and its tertiary compounds have been used as a micromechanical material for piezoelectric sensors, actuators, and modulators for many decades[158]–[160], and are commonly studied materials for IDT devices[111], [161], [162]. There are a variety of nearly identical material parameters available in material literature, especially over wide temperature ranges.
The piezoelectric and elastic properties of GaAs have been thoroughly investigated for device applications at room temperatures[163]–[166]. Many of the material properties for GaAs, such as the elasticity matrix[167], relative permittivity[168], and thermal expansion coefficient[153] are well understood over an extensive range of temperature values. This study compares scattering parameter measurements from a SAW resonator with an FEM simulation for temperatures ranging from 20 °C to 177 °C. Standing SAW stress analysis is then completed over the range of tested temperatures to demonstrate how IDT devices are a promising platform for investigating high-temperature stress-enhanced phenomena.

7.2 Simulation Description and Scattering Matrix Components

Two-dimensional device simulations are completed using COMSOL Multiphysics 5.6, employing a similar simulation procedure used in Chapter 6 of this dissertation. As discussed in previous chapters, the electrical and mechanical behavior of an IDT is governed by an extension to Hooke's law that couples the mechanical stress and electric displacement of the system[27], [28], [111]. The stress tensor, $T$, and electric displacement, $D$, within a piezoelectric domain are related to the strain tensor, $S$, and the electric field, $E$, by the following mathematical framework[27], [28], [111]:

\[ T_{ij} = c_{ijkl}^{E} S_{kl} - e_{kl}^{E} E_{k} \]  
\[ D_{i} = e_{ijk}^{E} S_{jk} + \varepsilon_{ij} E_{j} \]

where $c_{ijkl}^{E}$ are the components of the elasticity tensor for a constant electric field, $\varepsilon_{ij}$ are the components of the permittivity tensor for constant strain and each demonstrate
temperature dependence. \( e_{ijk} \) are the components of the piezoelectric tensor, however, there is little to suggest a significant temperature dependence that needs to be accounted for in the simulation.

The FEM simulation models the piezoelectric substrate material as GaAs(100) and considers the temperature effects for the density, elasticity matrix, and relative permittivity. The material orientation for GaAs(100) is defined by a general rotation input using the Euler angle (Z-X-Z) orientation of \( (90^\circ - 45^\circ - 90^\circ) \) to match the experimental device orientation. The piezoelectric coefficient, \( e_{14} \), is assumed to be constant for the temperature range studied in this experiment[145], [164]. The device material is modeled after aluminum and considers the temperature effects of density[150], Young's modulus[151], and Poisson's ratio[152]. Thermal expansion coefficients are incorporated for both materials to account for frequency shifts due to thermal expansion of the substrate and metal fingers[153], [154]. Device scattering response coefficients, \( S_{ij} \), are calculated from simulated admittance parameters, described more thoroughly in Chapter 6. Standing SAW stress analysis is then completed to probe temperature effects on IDT mechanical performance and their application as an investigating platform for high-temperature stress-enhanced phenomena is discussed.

7.3 COMSOL Materials and Physics Discussion

The piezoelectric substrate material is modeled after GaAs(100) and considers the temperature effects for the density, elasticity matrix, and relative permittivity. The material orientation for GaAs(100) is defined by a general rotation input in a 'Rotated System' definition using the Euler angle (Z-X-Z) orientation of \( (90^\circ - 45^\circ - 90^\circ) \) to match the
experimental device orientation. The device material is modeled after aluminum and considers the temperature effects of density, Young's modulus, and Poisson's ratio. Thermal expansion coefficients are incorporated for both materials to account for resonant frequency shifts attributed to thermal expansion of the substrate and metal fingers. The material properties for aluminum and gallium arsenide and their respective temperature dependences are detailed in Table 6.1. Customized' component materials' were generated for aluminum and gallium arsenide, which considered the temperature effects by linking the properties to the user-defined 'Device Temperature' input parameter.

7.4 Measured and Simulated Device Temperature Response

Figure 7.1 shows $S_{21}$ responses for device temperatures of 20 °C and 177 °C. The maximum $S_{21}$ frequency, often referred to as the resonant frequency ($f_r$), at 20 °C for the wire-bonded experimental device is measured to be 287.23 MHz and decreases to 284.67 MHz at 177 °C. The dashed lines depict the corresponding simulation results, demonstrating a comparable result to the experimental measurements. The simulated frequencies at the same temperatures are 287.19 MHz and 284.60 MHz. A slight degradation in power transmission is observed with increasing temperature at the maximum $S_{21}$ frequency, while the minimum $S_{21}$ magnitude increases. Additionally, a scattering response phenomenon is observed for frequencies higher than the anti-resonance frequency, suggesting that the IDT device produces additional resonant modes. This effect has been shown to result from SAW reflections within the delay line and multi-transit interference[156], [169] and is discussed more thoroughly in Chapter 6.
Figure 7.2 shows the agreeing experimental and simulated relative shift in resonant frequency from the room temperature value for the tested range of device temperatures. The frequency shift is attributed to various factors, most notably the material's changing elasticity and density. As the temperature increases, the components of the elasticity matrix and the material density decrease, reducing the velocity of the SAW mode. Additionally, the frequency shift can be attributed to the thermally expanded finger spacing of the interdigitated transducer. For instance, the 10-μm finger spacing is calculated to increase
by approximately 8 nm at 177 °C compared to room temperature, which accounts for nearly 230 kHz in the frequency shift.

Figure 7.2: The simulated frequency shift decreases linearly with temperature and matches well with measured results. The shift is primarily attributed to the changing elastic material parameters and the thermal expansion of the piezoelectric domain.

### 7.5 The Effects of Temperature Effects on Acoustic Attenuation

As discussed in Chapter 3 of this dissertation, acoustic attenuation effects associated with thermoelastic dissipation[74], Akhiezer damping\(^{19}\), device fabrication defects, and other contributions to SAW attenuation[143] are approximated using an isotropic loss coefficient, \(\eta_s\). This coefficient modifies the elasticity tensor components to
be complex values and is experimentally determined to be $1.25 \times 10^{-4}$ at 20 °C and $3.00 \times 10^{-4}$ at 177 °C. The elasticity matrix, $c_{ijkl}^E$, then becomes:

$$c_{ijkl}^E = (1 + i\eta_s)c_{ijkl}^E$$

(7.3)

The impact of temperature on the acoustic mechanisms in gallium arsenide are measureable over the studied temperature range, which is made apparent by the dramatic change in the electrical response of the IDT device. The isotropic loss coefficient used in Eq. (7.3) is empirically determined and attempts to approximate the effects of acoustic attenuation on the device's performance. This alludes to an opportunity to improve the current FEM model to study temperature effects on phonon interactions in piezoelectric materials, which helps understand physical phenomena and the nature of a material's properties.

Figure 7.3 depicts the device's measured (solid line) and simulated (dashed line) power loss due to acoustic attenuation and an inefficient mirror assembly. The solid black line represents the experimentally determined power loss at room temperature and shows that power loss is maximum near the resonant frequency of the acoustic wave. The simulated power loss approximately tracks the room temperature measurement and slightly increases for an increased device temperature. While there is a slight increase in the acoustic power loss at higher temperatures, the change is minimal compared to the total power loss. The relatively unchanging peak heights point to the power loss being mostly associated with an inefficient mirror assembly that cannot contain the standing acoustic field.
Utilizing the temperature-dependent GaAs material properties, device simulations are completed to provide insight into the temperature effects on the stress fields produced by an IDT resonator. Due to the dynamic nature of standing SAW fields, the crystal domain undergoes a rapid oscillation corresponding to the frequency of the acoustic wave. The anti-node displacement oscillates between compressive and tensile values every half temporal period. Figure 7.4 shows the non-zero stress field component profiles for the

**Figure 7.3:** A vector network analyzer measures the experimental acoustic power loss (solid line) at room temperatures, which is assumed to be due to inefficient acoustic mirrors and acoustic attenuation. The simulation approximates these phenomena using an isotropic damping coefficient, as described in Eq. (7.3). The simulation also predicts acoustic power loss at 177 °C (red).

### 7.6 Surface Acoustic Wave Simulation and Stress Field Analysis

Utilizing the temperature-dependent GaAs material properties, device simulations are completed to provide insight into the temperature effects on the stress fields produced by an IDT resonator. Due to the dynamic nature of standing SAW fields, the crystal domain undergoes a rapid oscillation corresponding to the frequency of the acoustic wave. The anti-node displacement oscillates between compressive and tensile values every half temporal period. Figure 7.4 shows the non-zero stress field component profiles for the
snapshot of maximum SAW amplitude for an applied power of 20.85 dBm. The stress fields are characteristically contained within a single wavelength from the surface and comply with the stress-free boundary condition. Surface stress is primarily described by the $\sigma_{xx}$ component, which achieves an absolute magnitude of 336 MPa at the standing SAW anti-node. At this same snapshot, the vertical surface displacement of the 10-µm SAW is calculated to be 5.83 nm at 20 °C. Previous studies have demonstrated that comparable displacement values are measured using contact-mode atomic force microscopy for a device of similar design under the same operating conditions[157], [169].

Figure 7.5 demonstrates how the anti-node profiles of these fields change in magnitude for the same applied power when the simulated device temperature increases to 177 °C. As the simulated device temperature increases, the magnitudes decrease for all non-zero stress components, reducing in magnitude by approximately 32%. The maximum vertical surface displacement calculated at the anti-node of the standing SAW decreases to 3.74 nm. Device components such as the gold wire bonds, finger-pair busbars, and device package geometry may contribute parasitic conductance and inductance effects at elevated temperatures, which decrease mechanical performance. Provisions regarding the temperature response of these device component materials need to be considered when fabricating robust IDT devices for high-temperature applications. Furthermore, these parasitic effects can be accounted for within the FEM simulation via an equivalent circuit model[143], which may be necessary for simulating higher frequency devices.
Different behaviors may be observed for stress-dependent surface and bulk phenomena at the anti-nodal and nodal region of the standing SAW[34]–[39]. Due to the relatively high bandgap of GaAs (1.4 eV), device technologies can be optimized for GaAs-based SAW resonators to remain operational up to 300 °C[166]. While these device temperatures are still lower than temperatures at which most interfacial phenomena, like

**Figure 7.4:** The non-zero stress components, (a) $\sigma_{xx}$, (b) $\sigma_{xy}$, (c) $\sigma_{yy}$, and (d) $\sigma_{zz}$ are calculated for a single snapshot at their maximum values, which switches every half temporal period. The stress components demonstrate the mechanical response of the standing SAW is contained to be within a single wavelength (10 μm) of the surface.
atomic diffusion or crystal growth, become prevalent, the surface mobility of atoms may be significant [170], [171].

A more temperature-robust piezoelectric substrate such as aluminum nitride or lithium niobate can be used to study the effects of standing SAWs on stress-sensitive phenomena at even higher temperatures [172], [173]. SAWs can also be injected into a locally heated area within a significantly wider delay region to minimize temperature effects on the device. GaAs poses an additional problem in which arsenic sublimation

Figure 7.5: A slice from the sagittal plane of maximum absolute stress for each of the non-zero stress components. The stress component magnitudes decrease by approximately 32% when the temperature increases from 20 °C (solid line) to 177 °C (dashed line).
becomes ubiquitous for substrate temperatures as low as 370 °C, which would impact the ability to study stress-enhanced phenomena in the bulk domain[174]. Miroshnik et al. demonstrate a thermal processing technique for GaAs that utilizes an encapsulant-and-sacrificial-layer method, which mitigates issues associated with arsenic sublimation and pairs well with localized heating techniques[175].

### 7.7 Conclusion

SAW devices offer a new platform to study the effects of surface and bulk stress on interfacial phenomena such as thermal diffusion and crystal growth and provide an opportunity to develop new device fabrication techniques. Finite element method modeling is used with experimental device measurements to perform high-temperature analysis on the surface acoustic waves generated by a SAW cavity device fabricated on GaAs. Device resonance frequencies decrease linearly with increasing temperature, and the simulated scattering parameter response agrees well with experimental results. SAW analysis reveals substantial room-temperature stress component values, which decrease by approximately 32% when the device temperature increases to 177 °C. Acoustic power loss due to acoustic attenuation seems to be minimally impacted by device temperature and is predominantly associated with an inefficient mirror assembly.

Strain-enhanced semiconductor phenomena may not necessarily require a SAW-generating device to function at high temperatures. However, it is nonetheless essential to understand how device performance behaves with increasing temperature to better design an experimental stage. Future works will explore the effects of SAW-induced stress fields
on surface diffusion in semiconductor systems at elevated temperatures using a localized laser-heating system.
CONCLUSION

Scalably manipulating quantum barriers in highly organized lateral structures has significant technical advantages that directly impact a variety of semiconductor-based technologies. Semiconductor device fabrication standards are approaching angstrom-scale resolutions and require new techniques and materials for next-generation solid-state technologies. The principal outcome of the work contained within this dissertation is the demonstration of an experimental platform for studying stress-enhanced phenomena such as crystal growth and compound semiconductor interdiffusion. The success of this endeavor naturally leads to a scalable technique to form three-dimensional quantum structures in epitaxially grown III-V compound semiconductor layers by applying patterned stress fields at elevated temperatures.

The potential of surface acoustic wave devices has not yet been fully realized, despite their remarkable performance over various applications, as the effects of their acoustic strain fields on surface or near-surface phenomena have not been extensively studied. From this perspective, it is necessary to develop techniques to characterize the stress fields produced by surface acoustic waves. IDT-based devices are fabricated on GaAs(100) using photolithography and electron-beam metal deposition. The fabricated SAW resonators produce powerful standing SAW fields that can potentially enhance stress-sensitive phenomena in semiconductor systems. Vector network analysis measures the device scattering response and determines electrical performance before wire bonding the devices to a quarter wavelength transmission line. The fabricated IDT assemblies are powered using a frequency generator and the standing SAW fields are measured using contact-mode AFM.
An improved understanding of mechanics and quantitative analysis would prove very useful in harnessing the benefits of stress-induced phenomena. Raman microscopy is used to improve our quantitative understanding of the surface stress induced by the interdigitated transducer (IDT) devices. IDTs are often analyzed through electrical characterization, providing limited insight into the mechanical nature of surface acoustic waves. The relationship between the Raman peak broadening and the crystal strain induced by the standing surface acoustic waves is defined, and stress values are acquired using a unique Raman peak fitting scheme. The Raman peak fitting suggests that a higher resolution spectrometer may be necessary to translate Raman peak broadening to the SAW displacement amplitude with greater accuracy. Nevertheless, the Raman stress values agree well with the data collected from the AFM, thus demonstrating the potential of 2D Raman microscopy to characterize SAW fields and devices. This new characterization technique directly measures the mechanical behavior of these SAW-generating devices, enabling more rigorous quantitative analysis necessary to utilize stress-induced phenomena.

Finite element modeling considers the detailed physical description of the entire IDT device geometry and provides the electrical and mechanical response characterization needed to predict more complex device behaviors. With ever-increasing and widely distributed computational resources, FEM modeling is becoming a more and more practical method for IDT device design and optimization. An interdigitated transducer and acoustic mirror assembly form a surface acoustic wave cavity resonator, which is subsequently modeled using COMSOL Multiphysics 5.6. Experimental device scattering parameters are measured using a vector network analyzer, and the measured results compare well to the simulated results. FEM modeling predicts the vertical displacement amplitude achieved by
the standing SAW field produced in the delay-line region of the IDT that compares well with AFM measurements of the experimental device. High-temperature device analysis compares scattering parameter measurements from a SAW resonator with an FEM simulation for temperatures ranging from 20 °C to 177 °C. The study reveals substantial room-temperature stress component values, which decrease by approximately 32% when the device temperature increases to 177 °C. A parametric analysis considers the effects of electrode width and device thickness on key device performance factors for electronic filters and mechanical resonators. The optimization study suggests increasing the electrode thickness to significantly increase the amplitude of the SAW fields produced within the resonator structure.

Exploring novel fabrication techniques is an ongoing engineering endeavor that receives substantial attention from the semiconductor research community. The growing demand for an expanded materials palette and more complex structures requires novel fabrication techniques to advance the limits of present technological capabilities. SAW devices offer an experimental stage to study interfacial phenomena such as surface/bulk atomic diffusion and crystal growth through the introduction of surface strain, which provides an opportunity for new device fabrication techniques.
FUTURE WORK

Future work should include further optimizing the SAW-resonator structures using the FEM simulation to generate more rigorous acoustic fields. At present, the model has shown that increasing the device thickness leads to impressive strain field magnitudes, which is beneficial for studying strain-enhanced semiconductor processes. Other parameters worth exploring are electrode geometries, ambient conditions, and delay-line obstructions. It is also worthwhile to study higher frequency acoustic fields or increase the dimensionality of the IDT structures to accommodate 2-D acoustic fields. In addition, FEM modeling would be a crucial means in exploring different piezoelectric domains to broaden the experimental platform for these devices.

Strain-enhanced semiconductor phenomena may not necessarily require a SAW-generating device to function at high temperatures. However, it is nonetheless essential to understand how device performance behaves with increasing temperature to better design an experimental stage. Building a robust heating system that couples well with SAW-based devices is a necessary step in exploring the possibilities of strain-enhanced phenomena. ‘Appendix B’ of this dissertation discusses the computational results for a laser heating system. This preliminary analysis suggests using a laser heating setup coupled with sufficient sample cooling to locally heat the experiment windows built into the center of the IDT structures while minimally heating the surrounding device.

An immediate opportunity for researching strain-enhanced phenomena in semiconductor systems is to study the effects of a standing SAW field on surface or bulk atomic diffusion. Miroshnik et al. have recently demonstrated a high-temperature GaAs
processing technique that mitigates arsenic sublimation and preserves an atomically smooth surface\cite{175}. The encapsulant-and-sacrificial-layer method would readily couple with a SAW-based device to enable high-temperature atomic diffusion while allowing reasonable control of thermodynamic conditions that may otherwise alter the diffusion mechanism.
APPENDICES

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Appendix A: FIB Slice Parameters for TEM Analysis

Pin on a Pegboard Description

'Buffon's Needle' is a well-known mathematics problem involving geometric probability and can be solved using integral geometry. The original problem was proposed by George-Louis Leclarc, Comte de Buffon in the 18\textsuperscript{th} century[176]:

"Suppose we have a floor made of parallel strips of wood, each the same width, and we drop a needle onto the floor. What is the probability that the needle will lie across a line between two strips?"

![Figure A.1: Buffon’s Needle is a problem which considers the probability that a pin of defined length, $l$, and random orientation will cross the boundary of equally spaced lines of defined gap length, $t$.](image)
Figure A.1 illustrates the problem statement showing grey strips separated by a length 't' and two black lines of length 'l', where line 'a' crosses the strip boundary and line 'b' does not. The solution to this problem is well understood, and the probability function is equal to [176]:

\[
P = \int_{0}^{\frac{\pi}{2}} \int_{0}^{l/t} \frac{4}{t \pi} dx \, d\theta = \frac{2 \, l}{\pi \, t},
\]

where the two integrals consider the probability contributions for a random line angle, \( \theta \), and a random line position, \( x \). While not the original motivation for this question, the problem can be used to design a Monte Carlo setup to approximate \( \pi \).[177]

A similar problem is posed, which considers a 2-D array of holes rather than a 1-D array of strips. This problem is illustrated in Fig. A.2. The relevance of this problem is important in the context of the 'Press and Print' experiment, which aims to use mechanically impose an elastic strain field and promote diffusion in compound semiconductors and is discussed more thoroughly by Ghosh et al.[23]. Analyzing variations in sub-surface quantum well compositions, which are not readily visible beneath an otherwise homogenous surface, often requires a focused ion beam (FIB) to remove a slice from the altered sample for transmission electron microscopy (TEM) analysis. Analyzing a slice of arbitrary angle with respect to the 2-D array can potentially yield unrevealing results as the FIB slice may not intersect a point of interest. Therefore, a strategic approach must be employed to nearly ensure that the FIB slice intersects a point of interest in the periodically altered quantum well.
The "pin" in the 'Pin on a Pegboard' problem is an analog for the FIB slice, while the "pegboard" is analogous to the imposed "Press and Print" pattern. A Monte Carlo approach is used to suggest reasonable FIB-slice lengths for a range of pegboard hole diameters to ensure TEM analysis is performed across an area that would hypothetically have undergone the "Press and Print" diffusion mechanism.

**Figure A.2:** A pegboard is shown with a periodic 2-D array of "holes" which are shown as black dots. The randomly oriented lines either hit (green) or miss (red) a peg hole. This problem is very relevant for the discussion of the FIB slice for TEM analysis in the ‘Press and Print’ experiment.
Figure A.3: The MATLAB procedure summary for generating a pin and testing if it crosses a circle is as follows: (a) a unit pegboard unit cell is generated. (b) a line of defined length and random angle and position is generated and (c) collapsed into the unit cell by simple translation operations. (d) An intersection check algorithm is employed to determine if a peg hole has been crossed over the entire length of each collapsed line segment.

Figure A.3 illustrates the procedure for the 'Pin on a Pegboard' script. Figure A.3(a) depicts a single unit cell that describes the infinitely large pegboard through unit translations. The pitch of the pegboard is described simply as the pegboard's unit-cell
length. A "dropped" pin is simulated by randomly choosing a start pointing (green dot) for
the line within the unit cell and randomly assigning a $\theta_d$ such that the line’s ending point
(red dot) can be assigned, which is illustrated in Fig. A.3(b). The line collapses into the
unit cell by using unit translations whenever the line crosses over the boundaries of the unit
cell, which is shown in Fig. A.3(c). Finally, the intersection points are determined over the
length of the line. In Fig. A.3(d), a single intersection is observed, which is depicted as a
red 'X'.

Simulation Results

The MATLAB script shown at the end of this section is reconstructed as a
MATLAB function to determine the 'miss or hit' probability for a range of 'Pin Lengths'
and 'Hole Radii', depicted in Fig. A.4. Figure A.4 (a)-(d) depict the probability a pin will
cross a pegboard hole for simulations of 10, 100, 1000, and 10000 dropped pins per pixel,
respectively, for a random $\theta_d$. As the number of pins is increased, the resolution of the
image improves. The total pins dropped for Fig. A.4(a) is approximately 20,000 and
increases to 20,000,000 for Fig. A.4(d), which requires a significantly longer computation
time.

Due to the random drop angle, there is always a non-zero chance the pin does not
cross any peg hole, no matter how large the 'Pin Length' to 'Pitch' ratio. However, the green
band observed in Fig. A.4(d) most precisely states the parameter space for which there is a
50% chance the pin crosses a pegboard hole. A radius-to-pitch ratio of 0.25 corresponds to
a length-to-pitch ratio of approximately 1. A radius-to-pitch ratio of 0.1 corresponds to a
length-to-pitch ratio of approximately 3. However, for a radius-to-pitch ratio of less than
0.05, the length-to-pitch ratio may be excessively high, which, depending on the pitch used
in the ‘Press and Print’ experiment, may extend beyond the limitations of the FIB due to the sliced sample breaking.

When using a FIB to prepare a TEM sample, there is often some knowledge of the FIB slice's orientation with respect to the sample, so it is worthwhile to repeat the pin-drop simulation for set of fixed $\theta_d$. Figure A.5 depicts the results of this analysis for a variety of drop angles. For a $\theta_d$ of (a) 0 degrees and (f) 45 degrees, similar probability distributions are observed, but neither orientation achieves a value greater than 72%. This demonstrates that a FIB-slice orientation that coincides with the orientation of the 2-D array results in a very inefficient analysis procedure. However, there are drastically different probability fields for (b) 9, (c) 18, (d) 27, and (e) 36 degrees, which suggest more optimal FIB-slice angles.

Figure A.6 shows the results of the 1000-pin simulation for a random angle between 4 and 14 degrees and (b) 31 and 41 degrees, which both show a considerable improvement compared to the probability distribution depicted for a random angle between 0 and 45 degrees, shown in Fig. A.6 (a) & (d). It should also be noted that there are even combinations of length-to-pitch and radius-to-pitch ratios that guarantee the pin will cross a peg hole. Therefore, when preparing a sample produced during the 'Press and Print' experiment, removing a sample that is oriented 9 degrees or 36 degrees off-axis from the 'Press and Print' array is favorable.
**Figure A.4:** The resolution of the probability field for the Monte Carlo simulation increases with increasing pin drop simulations. For each defined parameter of radius and pin length, the Monte Carlo procedure simulates (a) 10, (b) 100, (c) 1000, and (d) 10000 pin drops per pixel. This procedure was completed for a random $\theta_d$ per pin drop.
Figure A.5: The probability distribution changes dramatically for a specified $\theta_d$.

A large area of 9deg and 18deg offer a 100% certainty that a hold will be crossed, while the 0 and 45 deg angles never exceed 50%. For this reason, it is ideal to choose a $\theta_d$ that will guarantee a hole will be crossed.
Figure A.6: Due to knowledge of the sample’s general orientation with respect to the 2-D ‘Press and Print’ array, the FIB-slice angle can be approximately picked to lie within a specified range. This provides an assurance that the TEM analysis will be able to observe an area of interest.
MATLAB Code for 'Pin on a Pegboard'

%% Configure Figure Settings
% For publishing purposes, the figure settings are precisely defined such that the figure will be ready for importing.

clear; clc; figure(1); clf(1)
% set the units of the measures used through the file
set(gcf, 'Units', 'centimeters');

% set the position and dimension of the figure on the screen
figureDimensions = [10 10 6.5 6.5]; % [pos_x pos_y width_x width_y]
set(gcf, 'Position',figureDimensions); % [left bottom width height]
set(gcf, 'PaperPositionMode', 'auto');

% set the primary plot settings
xTickVal = []; % ticks of x axis
yTickVal = []; % ticks of y axis
xLimVal = [0 1]; % Range for x axis
yLimVal = [0 1]; % Range for y axis
set(gca, ...
    'XGrid', 'off', ..., %[on | {off}]
    'YGrid', 'off', ..., %[on | {off}]
    'XMinorGrid', 'off', ..., %[on | {off}]
    'YMinorGrid', 'off', ..., %[on | {off}]
    'XTick', xTickVal, ..., %ticks of x axis
    'YTick', yTickVal, ..., %ticks of y axis
    'XMinorTick', 'off', ..., [on | {off}]
    'YMinorTick', 'off', ..., [on | {off}]
    'box', 'on', ..., [on | {off}]
    'TickLength', [.0 .0], ..., %length of the ticks
    'XColor', [0 0 0], ..., color of x axis
    'YColor', [0 0 0], ..., %color of y axis
    'XLim', xLimVal, ..., %limits for the x-axis
    'YLim', yLimVal, ..., %limits for the y-axis
    'LineWidth', 1); % width of the line of the axes

%% Generating the Pegboard Unit Cell
% An infinitely large pegboard can be represented as a single unit cell to greatly simplify the problem. The square unit cell also contains a quarter of four pegs positioned at each corner of the cell.

hold on
Unit_Cell_a = 1;
Circle_Radius = Unit_Cell_a/4;
x1 = linspace(0,Circle_Radius,250);
xr = linspace(Unit_Cell_a - Circle_Radius, Unit_Cell_a, 250);

Square_X = [0, Unit_Cell_a, Unit_Cell_a, 0, 0];
Square_Y = [0, 0, Unit_Cell_a, Unit_Cell_a, 0];

ybl = @(x) real(sqrt(Circle_Radius.^2 - (x).^2));
ybr = @(x) real(sqrt(Circle_Radius.^2 - (x - Unit_Cell_a).^2));
ytl = @(x) -real(sqrt(Circle_Radius.^2 - (x).^2)) + Unit_Cell_a;
ytr = @(x) -real(sqrt(Circle_Radius.^2 - (x - Unit_Cell_a).^2)) + Unit_Cell_a;

plot(xl, ybl(xl), 'k', 'LineWidth', 1.5)
plot(xr, ybr(xr), 'k', 'LineWidth', 1.5)
plot(xl, ytl(xl), 'k', 'LineWidth', 1.5)
plot(xr, ytr(xr), 'k', 'LineWidth', 1.5)

%% Define Line
% A line of defined length is generated to represent an arbitrary slice removed from the sample using a focused ion beam (FIB). The FIB slice is assumed to be infinitesimally thin to simplify the problem significantly. A starting point for the line is generated within the unit cell at a random location and is extended in a random direction. The axis limits are increased to demonstrate the extent of the generated line.

Line_Length = 2;
X_Start = rand(1)*Unit_Cell_a;
Y_Start = rand(1)*Unit_Cell_a;
Theta = rand(1)*360;

X_End = X_Start + cosd(Theta)*Line_Length;
Y_End = Y_Start + sind(Theta)*Line_Length;

Segment_X_Start = X_Start;
Segment_Y_Start = Y_Start;

Remaining_Length = Line_Length;
plot([X_Start, X_End], [Y_Start, Y_End], 'b', 'LineWidth', 2.)
scatter(X_Start, Y_Start, 25, 'g', 'filled')
scatter(X_End, Y_End, 25, 'r', 'filled')
axis([-1.25 2.25 -1.25 2.25])

%% Confine Line to Unit Cell
% Making use of the properties of a unit cell, the line is collapsed into the cell by making simple translations when the line crosses the cell boundary. The line can then be defined as a series of line segments, with lengths that combine to equal the original line length.
axis([0 1 0 1])
i = 1;
while Remaining_Length > 0
    Line_X_End = Segment_X_Start(i) +
cosd(Theta)*Remaining_Length;
    Line_Y_End = Segment_Y_Start(i) +
sind(Theta)*Remaining_Length;
    Segment_Check_X = [Segment_X_Start(i), Line_X_End];
    Segment_Check_Y = [Segment_Y_Start(i), Line_Y_End];

    [X_Int,Y_Int] = intersections(Segment_Check_X,
    Segment_Check_Y, Square_X, Square_Y, 'robust');
    X_Int(X_Int == Segment_X_Start(i)) = [];
    Y_Int(Y_Int == Segment_Y_Start(i)) = [];

    if numel(X_Int) == 0
        Segment_X_End(i) = Line_X_End;
        Segment_Y_End(i) = Line_Y_End;
    end

    plot([Segment_X_Start(i),Segment_X_End(i)],
    [Segment_Y_Start(i),Segment_Y_End(i)],'b','LineWidth',2.)
    Remaining_Length = 0;

    scatter(Segment_X_End(i),Segment_Y_End(i),25,'r','filled')
    continue
else
    Segment_X_End(i) = X_Int;
    Segment_Y_End(i) = Y_Int;
end

    Remaining_Length = Remaining_Length - ((Segment_X_End(i) -
    Segment_X_Start(i))^2 + (Segment_Y_End(i) -
    Segment_Y_Start(i))^2)^(1/2);

    plot([Segment_X_Start(i),Segment_X_End(i)],
    [Segment_Y_Start(i),Segment_Y_End(i)],'b','LineWidth',2.)

    if X_Int(end) == 0
        Segment_X_Start(i+1) = X_Int + Unit_Cell_a;
        Segment_Y_Start(i+1) = Y_Int;
        i = i+1;
        continue
    elseif X_Int(end) == 1
        Segment_X_Start(i+1) = X_Int - Unit_Cell_a;
        Segment_Y_Start(i+1) = Y_Int;
        i = i+1;
        continue
    elseif Y_Int(end) == 0
        Segment_X_Start(i+1) = X_Int;
        Segment_Y_Start(i+1) = Y_Int + Unit_Cell_a;
    end
\[ i = i+1; \]
\[ \text{continue} \]
\[ \text{elseif } Y_{\text{Int}}(\text{end}) == 1 \]
\[ \text{Segment}_X_{\text{Start}}(i+1) = X_{\text{Int}}; \]
\[ \text{Segment}_Y_{\text{Start}}(i+1) = Y_{\text{Int}} - \text{Unit Cell}_a; \]
\[ i = i+1; \]
\[ \text{continue} \]
\[ \text{end} \]
\[ \text{end} \]
\[ \text{Segment}_X = [\text{Segment}_X_{\text{Start}}',\text{Segment}_X_{\text{End}}']; \]
\[ \text{Segment}_Y = [\text{Segment}_Y_{\text{Start}}',\text{Segment}_Y_{\text{End}}']; \]

%% Check for Intersections
% The represented FIB slice is inspected for intersections with any of the four quarter-circle boundaries. Intersections are represented as red and bolded 'X' markers. Intersections are checked using the 'intersections' function, which is a MATLAB-provided function. If the line does not cross the quarter-circle boundary, this would be a case when the pin does not cross a pegboard opening.

\[ \text{Circle}_X = []; \]
\[ \text{Circle}_Y = []; \]

\[ \text{for } i = 1: \text{numel} (\text{Segment}_X(:,1)) \]
\[ [\text{TESTX}1,\text{TESTY}1] = \text{intersections} (\text{Segment}_X(i,:), \text{Segment}_Y(i,:), \text{xl}, \text{ybl(xl)}, '\text{robust}'); \]
\[ [\text{TESTX}2,\text{TESTY}2] = \text{intersections} (\text{Segment}_X(i,:), \text{Segment}_Y(i,:), \text{xr}, \text{ybr(xr)}, '\text{robust}'); \]
\[ [\text{TESTX}3,\text{TESTY}3] = \text{intersections} (\text{Segment}_X(i,:), \text{Segment}_Y(i,:), \text{xl}, \text{ytl(xl)}, '\text{robust}'); \]
\[ [\text{TESTX}4,\text{TESTY}4] = \text{intersections} (\text{Segment}_X(i,:), \text{Segment}_Y(i,:), \text{xr}, \text{ybr(xr)}, '\text{robust}'); \]
\[ \text{Circle}_X = [\text{Circle}_X;\text{TESTX}1;\text{TESTX}2;\text{TESTX}3;\text{TESTX}4]; \]
\[ \text{Circle}_Y = [\text{Circle}_Y;\text{TESTY}1;\text{TESTY}2;\text{TESTY}3;\text{TESTY}4]; \]
\[ \text{end} \]
\[ \text{scatter} (\text{Circle}_X,\text{Circle}_Y,200,'rx','\text{MarkerEdgeColor}',[.9 .15 .1], '\text{LineWidth}', 1.5) \]
Appendix B: Preliminary Laser Heating Simulation

Laser Heating Setup Description

Reliable microscale heating within a standing wave resonator device is necessary for studying the impacts of strain fields on compound semiconductor interdiffusion. Laser heating is popular and efficient for microscale localized heating applications and is a readily applicable technique for the SAW-enhanced diffusion experiment. A simplistic diagram of a potential setup is illustrated in Fig. B.1.

Figure B.1: A simplified diagram illustrates an IDT device (grey) attached to a cooled surface (light blue), with a window open in the device’s center (dark blue). A laser can be focused onto the center of the device surface for localized heating.
The heating capabilities of the laser heating setup can be approximated using COMSOL Multiphysics and requires a relatively simple model description to extract important apparatus parameters. Figure B.2. depicts the COMSOL structure utilized in this analysis, which is separated into three domains: (1) the substrate, (2) the device domain area, and (3) the center window. All three of these domains are gallium arsenide and utilize material properties identical to the properties used in SECTION ## of this dissertation. A visible laser is likely to be used for this setup as a visible light is much easier to position with the naked eye. The emissivity for gallium arsenide is relatively low (around 0.2) and is not ideal for this setup, so a thin silicon nitride window domain is placed at the surface of the ‘center window’ domain. The emissivity for silicon nitride lies between 0.8 and 0.9 depending on the wavelength of light and film content and growth quality[178]. The emissivity is chosen to be 0.85 in the simulation.

The physics module used in the time-dependent study is the ‘Heat Transfer in Solids’. The laser heating was approximated using a ‘Heat Flux’ node and the general inward heat flux profile, $q_0$, is defined as:

$$q_0 = \epsilon \phi$$  \hspace{1cm} (1)

where $\epsilon$ is the emissivity for silicon nitride and $\phi$ is a gaussian heat-flux profile. A ‘Surface-to-Ambient Radiation’ node is applied to all exposed boundaries to account for blackbody radiation effects. Finally, a ‘Heat Flux’ node is applied to the unexposed backside of the device to account for the cooling of the device. The cooling mechanism is assumed to be convective heat transfer and follows Newton’s Law of Cooling:

$$q_c = h(T - T_{\text{ext}}),$$  \hspace{1cm} (2)
which relies on a heat transfer coefficient, \( h \). The ambient temperature \( (T_{\text{ext}}) \) is defined to be room temperature (293 K). The heat transfer coefficient is an unknown parameter and is tested over a range of values which is discussed thoroughly in the results of this section.

An important model output parameter analyzed in this study is the average device temperature, which is described by the integral average of the device domain area temperature. This parameter suggests the operating temperature of the IDT device, which ultimately determines the maximum acoustic amplitude achieved within the SAW cavity. The domain from which the average device temperature is extracted is highlighted in Fig. B.2. Two other output parameters analyzed in this study are the maximum device

**Figure B.2:** The domain analyzed in this COMSOL study is split into three subdomains. The substrate domain (dark grey), the device domain (light grey) and the window domain (blue). Temperature analysis is completed for each domain to provide key insight into the laser apparatus.
temperature and spot size temperature. The maximum device temperature is essential to consider as deviations from the device operating temperature decreases device efficiency. The relative domain positions from which these values are extracted are depicted in Fig. B.3. The maximum spot temperature describes the effectiveness of the laser heating setup. It is ideal to increase the maximum spot size while keeping a relatively low maximum device temperature. This balance can be adjusted by altering the device geometry.

Figure B.3: The domain below the silicon nitride window is the region of interest for the SAW-enhanced diffusion experiment. From this region, the maximum spot size temperature is extracted. The maximum device temperature is also noted to provide important information regarding the efficiency of the IDT device.
COMSOL Simulation Results

Figure B.4 depicts a snapshot of the temperature profile of the y-z plane below the silicon nitride window. The heat profile is considerably developed after 43 milliseconds. The heating step for the considered laser setup is significantly faster than a typical rapid thermal annealing setup, which requires heating times on the order of seconds to minutes. Additionally, the experimental window sees most of the temperature increase, which indicates the temperature profile can be local and kept far from the IDT device.

![Temperature Profile](image)

*Figure B.4: The temperature profile induced by a 5W and 100 µm spot size laser beam is effective in locally heating the gallium arsenide substrate after 43 milliseconds. For a sufficiently large experimental window, the IDT device would also see minimal heating.*
The applied power and the laser beam spot size dramatically alter the resulting maximum temperature of the spot size, as shown in Fig. B.5. The backside-cooling heat transfer coefficient is chosen to be 10,000 W/m²°C for this analysis, which is a reasonably practical value for a sufficiently cooled system. Figure B.5(a) depicts the temperature achieved for a fixed diameter and variable applied power, which varies between approximately 400 °C for 3W and 900 °C for 7W. Figure B.5(b) shows the maximum temperature achieved for a fixed power and variable laser diameter, which varies by similar quantities for diameters ranging from 70 µm to 130 µm. This analysis demonstrates why precise control of the laser’s power and focus is necessary for repeatable experiments.

![Figure B.5](image)

**Figure B.5:** A parametric study of the (a) applied laser power and the (b) spot-size radius of the gaussian beam demonstrates how substrate temperature widely varies. The backside cooling heat transfer coefficient is chosen to be 10,000 W/m²°C.

Figure B.6 depicts key temperature parameters for a variety of cooling scenarios, each defined by different heat transfer coefficients, thus demonstrating the experimental setup’s ability to function over longer time scales. For a fixed laser spot size of 100 µm and an applied power of 5W, all three cooling scenarios reach a temperature of 600 °C almost immediately, as shown in Fig. B.6(a). However, for the inefficiently cooled sample
(h = 1,000 W/m²°C) the steady-state temperature is not achieved for several seconds, while the efficiently cooled sample (h = 100,000 W/m²°C) achieves a steady-state temperature almost immediately. Figure B.6(b) illustrates the effects of the heat transfer coefficient on overall device performance, described by the maximum device temperature (solid line) and the average device temperature (dashed line). The maximally cooled setup achieves both a low average temperature and a low maximum temperature, while the minimally cooled setup is unable to cool the system at all and would lead to a non-functioning IDT device.

Figure B.6: The backside cooling setup has an essential role to play in ensuring an efficient IDT device. For small heat transfer coefficients, the spot size takes an excessively long time to reach a steady state temperature, and the IDT device quickly reaches an impractical temperature.

While this parameterized study does not precisely describe an actual laser heating setup, the results still point to many variables requiring attention to achieve a repeatable and robust experiment. Controlling laser power and gaussian profile is necessary for repeatable temperature profiles, while a rigorous cooling setup would ensure an efficiently performing IDT device. With an appropriately designed laser heating setup paired with a thorough sample cooling system, samples that undergo the SAW-enhanced diffusion experiment can be precisely characterized.
Appendix C – Silver Paste Viscosity Measurements

Osazda Energy’s unique technology offers an innovative, cost-effective product to improve resistance to cell crack performance degradation and promotes a self-healing property in solar cell metallization. The MetZilla Paste Technology requires a unique formulation of silver particles, organic binder, glass frit, and solvent to compliment the crack-resistant technology promised by this product. Osazda Energy is moving to produce a baseline silver paste made almost entirely in-house to transition to a more self-dependent paste production process.

Silver Particles

Silver (Ag) constitutes most of the silver paste, often making up 80-90 wt% of the paste product. The appropriate selection of silver particle topology can lead to more optimal solar cell efficiencies through improved sintering behaviors[179] and sheet resistivity[180]. The most important factors considered for silver powders are the particle shape and size distribution. Silver particles used in silver paste products for solar cell applications are most often produced by reducing silver nitrate (AgNO\textsubscript{3}). Other processes to produce silver powders have been proposed, such as water atomization.[181] In the reduction process outlined by N. Moudir, et al., silver nitrate is mixed into aqueous solutions of ammonium hydroxide (NH\textsubscript{4}OH) or sodium hydroxide (NaOH) to form silver oxides (Ag\textsubscript{2}O). The solution is reduced by formaldehyde to obtain a silver powder. The mixture is heated to 45°C and continuously stirred until the reaction is completed.[182] A careful choice of reducing agent and using additional additives(#) can determine specific parameters such as surface roughness or particle size. After the silver particles are formed,
the silver powder is separated from the acid solution and is typically washed with DI water. The final particle size is tuned to the desired size distribution, and the water is removed with filtration and subsequent drying.

**Glass Frit**

Glass frit plays a vital role in the silver paste and needs to be perfectly tuned to suit the applications of the MetZilla product. This component will require a large amount of testing to ensure the paste functions at optimal performance. The mechanisms of glass frit are as follows:[183]–[185]:

1. Reduction of the anti-reflection coating and allowing metal contact with the silicon surface.

2. The post-fired glass layer acts as a medium for electron transport.

3. Alteration of the metal powder sintering kinetics

Glass frit is often made up of lead (Pb) containing glass systems,[183], [184], [186], though lead-free compositions can be used[180], [187]. PbO serves to reduce the SiNx anti-reflection coating layer on the surface of the solar cell. This process’s mechanism is generally understood as a redox reaction, leaving behind Pb precipitates in the glass matrix that aid in the electron transport[185]. Lead precipitates can be recycled during the firing process. The suspended particles can be re-oxidized and undergo the reduction process again; this requires the firing to be done in an oxygen-containing environment[185].

Other components of glass frit, aside from PbO, may include B$_2$O$_3$, TeO$_2$, SiO$_2$, Al$_2$O$_3$, CdO, BaO, ZnO, Na$_2$O, Li$_2$O, ZrO$_2$. While these components may reduce SiNx, the
current assumption in the Osazda laboratory is that these are widely used to reduce the
glass transition temperature. The glass transition temperature of glass frit may be in the
range of 425°C to 800°C and is often determined by differential thermal analysis
(DTA)[188]. We are currently only working with PbO and TeO$_2$ as these are two
ubiquitous ingredients that result in a glass with a suitably high transition point when mixed
in 1:1 wt% portions. The transition temperature should correspond with the firing time and
temperature of the silver paste. Zheng et al. discuss the effects of too high or too low of a
glass transition temperature. With too high a transition temperature, not enough glass frit
will melt and trickle through the silver particles and collect at the SiN$_x$ surface. The ARC
etching reaction is incomplete and results in poor silver contact. If the transition
temperature is too low, the SiN$_x$ is etched away with ease, but too much glass collects at
the surface and hinder electron transport.

The glass materials are mixed and deposited into an Al$_2$O$_3$ crucible. The glass
mixture and crucible are heated in a muffle furnace between 1000°C and 1100°C to form
molten glass. The molten glass is poured directly into DI water and milled to form the glass
frit. There are currently efforts to obtain a suitable graphite crucible, as any remaining
molten glass does not adhere to the crucible upon cooling. A graphite crucible still poses a
problem as carbon contamination is introduced into the frit as graphite dissolves into the
glass mixture at temperatures higher than 600°C.

**Organic Vehicle**

The organic vehicle may be an organic solvent or an organic solvent mixture, or
even an organic polymer solution in organic solvents. The organic polymer does seem to
be the most critical ingredient to control the paste’s various rheological properties. The
solvent mixture is a heavily guarded secret for large paste manufacturing companies. The benefits of including an organic vehicle are as follows: stable dispersion of insoluble solids, appropriate viscosity and thixotropy for applications of screen printing, appropriate wettability, enhanced drying rate, and good firing properties. The polymer present in the organic vehicle is in the range of, as an example, .2 to 5 wt-% based on total silver paste composition. Examples of organic polymers include ethyl cellulose, ethyl hydroxyethyl cellulose, wood rosin, phenolic resins, and poly(meth)acrylates of lower alcohols.

A few examples of organic solvents include ester alcohols, terpenes, or mixtures of solvents such as kerosene, dibutyl phthalate, diethylene glycol butyl ether, diethylene glycol butyl acetate, hexylene glycol, and high boiling alcohols. More volatile organic solvents can sometimes be included to promote rapid hardening after the application of the silver paste. One solvent identified (from the SDS for PV20A) is Butoxyethoxyethyl acetate.

**Paste Viscosity Description**

Paste viscosity is essential for screen printing silver pastes in solar cell manufacturing. For now, a viscometer measures the viscosity response of the silver paste for different shear rates. Initial paste viscosity tests reveal that the shear-stress is approximated well as a 'power-law fluid,' which is generally described in the following form:

\[ \tau = K \left( \frac{\partial u}{\partial y} \right)^n \]
where $K$ is the flow consistency index, $n$ is the flow behavior index, and $\frac{\partial u}{\partial y}$ is the shear rate (or velocity gradient perpendicular to the shear plane). It is common to calculate the value of the effective viscosity, $\mu_{\text{eff}}$, as a function of shear rate:

$$\mu_{\text{eff}} = K \left( \frac{\partial u}{\partial y} \right)^{n-1}$$

**Paste Measurements and Viscosity Results**

The values of the flow behavior index, $n$, determine the type of fluid, which can be described as *pseudoplastic* for $n < 1$, *Newtonian* for $n = 1$, and *dilatant* for $n > 1$. We have prepared samples to understand better the relationship between solvent wt% and the viscosity of the paste. Sample measurements reveal a pseudoplastic fluid, otherwise known as shear-thinning fluids. These fluids are often solutions of large, polymeric molecules in a solvent with smaller molecules. At lower velocities, the large molecular chains move at random and hinder large volumes of the fluid. However, at greater velocities, these chains align in the direction of shear and produce less resistance. This paste property is essential for rigid and uniform silver gridlines. Higher viscosities mean a lower rate of flow after the paste has been printed. If the viscosity is high enough, the paste remains rigid moments after printing. A higher shear rate instigates a lower viscosity during the printing process, meaning the paste will more easily flow. Substantial shear-thinning properties are necessary for high-quality printing.

The solvent and cellulose ratios are adjusted to study their effects on the thixotropic properties of the paste. We neglect to use butyl cellosolve as it is likely to be used simply as a vehicle for CNTs and a paste thinner. The samples were almost exclusively prepared
with Diethylene Glycol Monoethyl Ether Acetate (DGMEA) as we expect this to be a principal ingredient in the paste, and its low vapor pressure ensures less solvent loss throughout the various fabrication steps of the paste. We recorded the viscosity measurements at a paste temperature of 15°C. The initial viscosity goals for the silver paste viscosity response are 200,000 cP at lower shear rates and 100,000 cP at higher shear rates. This response is referred to as the viscosity standard. An ideal viscosity curve widens this window to 280,000 cP at lower shear rates and 50,000 cP at higher shear rates.

We theorized that for a higher wt% of cellulose, the viscosity of the paste would increase for lower shear rates, but a dramatic drop-off in viscosity with higher shear rates would still be present. This effect has been demonstrated in Fig. 3, shown below. Increasing the cellulose wt% from x% in 'Sample C' to y% in 'Sample B' increased the viscosity of the silver paste at low shear rates by 1438%, while the viscosity only increased by 537% at higher shear rates. This dramatic increase in viscosity at low shear rates but not at high shear rates demonstrates the potential for cellulose to control the shear-thinning properties of the silver paste.

'Sample B' was adequately close to the Osazda standard. 'Sample D' has a similar composition to 'Sample B' but uses DGBE as the primary solvent. DGBE produced a slightly superior viscosity curve as the paste achieved a higher low shear rate viscosity while keeping the viscosity below 100,000 cP at higher shear rates. The drawback to using DGBE is the higher vapor pressure and lower molecular weight of the solvent, which might negatively affect the paste's shelf life or temperature response during paste firing.
The solvent content found in Samples A, B, & C is around 11.40 wt-% which is slightly higher than desired compared to competing paste products. The sample-set 'Sample D' was ordered to reduce the solvent content of the silver paste to 10 wt% while still achieving the Osazda standard. With less solvent within the paste, the solar cell needs to spend less time in the RTA. This goal was achieved at the cost of sacrificing a substantial amount of the shear-thinning capabilities of the paste.

**Figure C.1:** Cellulose affects the shear-thinning properties of the silver paste. The three silver pastes contain nearly identical proportions of solvent but vary in their cellulose content. 'Sample A' contains x wt% cellulose, 'Sample C' contains y wt% cellulose, and 'Sample B' contains z wt% cellulose.
'Sample D' contains a solvent content of 10.04 wt% and produces a viscosity curve very similar to 'Sample B'. However, the viscosity for high shear rates is too high for the viscometer to get an accurate reading. Achieving a similar viscosity curve to 'Sample B' required an adjustment to the cellulose content. The cellulose content is reduced from z-wt% to x-wt%. The reduction in cellulose instigated a loss of the shear-thinning properties of the paste as the flow behavior index increased. A better-performing paste should see a significantly lower flow behavior index. We have begun testing hydroxyethyl cellulose (HE-cellulose) as a polymer binder for its shear thinning properties. The current expectations of the HE-cellulose are a significant improvement in the paste's shear-thinning ability but a drastic reduction in the flow consistency index. For this reason, we suspect a combination of the two polymer binders is necessary.

Figure C.2 depicts the trends between the power-law coefficients and the different component relationships of the silver paste. Figure C.2(a) illustrates the exponential relationship between the flow consistency index, K, and the cellulose/solvent ratio. The flow behavior index, n, is plotted against the cellulose wt% to demonstrate its linear relationship, as shown in Fig. C.2(b). We assume that the unchanging components (silver, glass, and CNTs) do not play a substantial role in the cellulose and solvent interactions. At this point, there are no adequate reasons why exponential and linear relationships are used for these trends other than their $R^2$ values.
Figure C.2: (a) The flow consistency index, $K$, is plotted against the Cellulose/Solvent ratio to show an exponential trend. (b) The flow behavior index, $n$, is plotted against the cellulose wt% to demonstrate the linear trend. The red data points are taken from incomplete data sets where only four points were collected instead of the preferred five.
Appendix D: Crack Propagation Analysis in CNT-Silver Paste

Silver Paste Crack Propagation

A key ingredient in Osazda’s silver paste is the carbon nanotube additive, which aims to mitigate gridline cracking damage by electrically bridging gaps that would otherwise sever the gridline’s electrical connection. Figure D.1 depicts a silver-CNT matrix that contains an evenly dispersed quantity of randomly oriented carbon nanotubes. The efficiency of the silver paste’s ability to electrically bridge cracks and gaps is a function of the CNT intersections. In this study, a simplistic model for gap bridging capability is analyzed as a function of CNT concentration, gap distance, and CNT orientation.

Figure D.1: A crack (red line) that propagates through the evenly dispersed silver-CNT matrix will intersect (blue circles) with randomly oriented carbon nanotubes. The CNT gap bridging efficiency is a function of the number of CNT intersections.
CNT Intersections Results and Discussion

The incorporation of carbon nanotubes within the silver matrix introduces a mechanism for electrically bridging gaps in the silver gridline. These gaps are produced by cracks generated within the silver paste. MATLAB is used to outline a portion of the silver gridline geometry and generate an array of randomly oriented and dispersed carbon nanotubes. Figure D.2 shows the effects of an increasing CNT wt% on the number of intersections between the randomly dispersed and oriented CNTs and a randomly generated crack. As the CNT wt% increases, the number of carbon nanotube intersections increases linearly. However, as CNT wt% increases, the material properties of the silver paste can change mechanically, and the fabrication process can become more tedious due to CNT agglomerations that further hinder the mechanical durability of the paste.

![Graph showing the relationship between CNT wt% and CNT intersections](image)

**Figure D.2:** Carbon nanotube intersections as a function of weight percentage increases linearly, however the intersections are not a function of CNT length.
The orientation of the carbon nanotubes is an interesting parameter to consider as carbon nanotubes that are aligned in the direction of the silver gridline can increase the number of CNT intersections. Figure D.3 illustrates this effect, as the CNT’s intersection quantity for the dispersion with an orientation of -90° to 90° (black line) were nearly an order of magnitude less than the dispersion with an orientation that was in line with the silver gridline (0° - purple line). Implementing a preferential orientation into the silver gridline matrix is challenging as the CNT’s are randomly dispersed inside the pre-printed silver paste. However, during the printing process, there may be a fluid-flow mechanism that could orient the carbon nanotubes in the direction of silver paste flow. For now, however, no such mechanism has been explored.

*Figure D.3:* Carbon nanotube connections (or intersections) are a function of CNT orientation with respect to the gridline. As the CNT’s become more oriented with the direction of the gridline (90° to 0° deg), the number of intersections increases.
The gap distance of the generated crack is an important parameter to consider, as the larger the gap, the less likely a carbon nanotube will be long enough to bridge the gap electrically. As a result, the chosen carbon nanotube length likely needs to reflect the average gap distance observed in typical solar cell applications. Figure D.4 depicts the results of this analysis.

![Graph showing the relationship between gap distance and number of bridged connections](image)

**Figure D.4:** As the gap of the generated crack increases, the number of bridged connections decreases. There is a wide standard deviation for small gap distances, however the standard deviation decreases with increasing gap distance.

**MATLAB Code for ‘CNT Intersections’**

```matlab
%% Defining the Figure Settings
% For publishing purposes, the figure settings are precisely defined such that the figure will be ready for importing.

clear; clc; figure(1); clf(1)
hold on
%set the units of the measures used through the file
set(gcf, 'Units', 'centimeters');

%set the position and dimension of the figure on the screen
figureDimensions = [10 10 10 10]; % [pos_x pos_y width_x width_y]
```
set(gcf, 'Position',figureDimensions); % [left bottom width height]
set(gcf, 'PaperPositionMode', 'auto');

% set the primary plot settings
Paste_Width = 50; % micrometers
Paste_Height = 100; % micrometers

xTickVal = [0, Paste_Width/2, Paste_Width]; % ticks of x axis
yTickVal = [0, Paste_Height/2, Paste_Height]; % ticks of y axis
xLimVal = [-Paste_Width/4, 5*Paste_Width/4]; % Range for x axis
yLimVal = [0, Paste_Height]; % Range for y axis

set(gca, ...
  'XGrid', 'off', ... [%on | {off}]
  'YGrid', 'off', ... [%on | {off}]
  'XMinorGrid', 'off', ... [%on | {off}]
  'YMinorGrid', 'off', ... [%on | {off}]
  'XTick', xTickVal, ... % ticks of x axis
  'YTick', yTickVal, ... % ticks of y axis
  'XMinorTick', 'off', ... [%on | {off}]
  'YMinorTick', 'off', ... [%on | {off}]
  'box', 'on', ... [%on | {off}]
  'TickLength', [.0 .0], ... % length of the ticks
  'XColor', [0 0 0], ... % color of x axis
  'YColor', [0 0 0], ... % color of y axis
  'XLim', xLimVal, ... % limits for the x-axis
  'YLim', yLimVal, ... % limits for the y-axis
  'LineWidth', 1); % width of the line of the axes

%% Generate Paste and CNT Nodes
% The carbon nanotubes are generated for a set CNT length and a defined
quantity of CNT's in total. For a known CNT density, these values can
be used to determine CNT weight percentage. Additionally, the CNTs are
generated in such a way that both their start point and ending point
are contained within the silver gridline, rather than have points
sticking out of the paste.

CNT_Length = 2.5; % micrometers
Num_CNT = 500;

plot([0,Paste_Width],[Paste_Height,Paste_Height],'k')
plot([0,Paste_Width],[0,0],'k')
plot([0,0],[0,Paste_Height],'k')
plot([Paste_Width,Paste_Width],[0,Paste_Height],'k')

Theta_Deviation = 90; % deviation in degrees of CNT orientation from
being completely vertical
Phi_Deviation = Theta_Deviation;

for i = 1:Num_CNT
  CNT_X(i,1) = Paste_Width*rand(1);
CNT_Y(i,1) = Paste_Height*rand(1);

test_1 = 0;

while test_1 == 0
    test_array = [0,0,0,0];
    theta(i) = (2*rand(1)-1)*Theta_Deviation*pi/180+randsample([-1,1],1)*pi/2;
    phi(i) = (2*rand(1)-1)*(Phi_Deviation*pi/180);
    CNT_Length_Sample(i) = CNT_Length*cos(phi(i));
    CNT_X(i,2) = CNT_X(i,1) + CNT_Length_Sample(i)*cos(theta(i));
    CNT_Y(i,2) = CNT_Y(i,1) + CNT_Length_Sample(i)*sin(theta(i));

    if CNT_X(i,2) > 0
        test_array(1) = 1;
    end
    if CNT_X(i,2) < Paste_Width
        test_array(2) = 1;
    end
    if CNT_Y(i,2) > 0
        test_array(3) = 1;
    end
    if CNT_Y(i,2) < Paste_Height
        test_array(4) = 1;
    end
    if sum(test_array) == 4
        test_1 = 1;
    end
end

for i = 1:Num_CNT
    plot(CNT_X(i,:),CNT_Y(i,:),'g')
end

%% Generate Random Crack and Test for Intersections
% A random crack is generated by defining two random points along the sides of the gridline. Using the polyxpoly function, each CNT is individually tested to determine if the crack intersects with the CNT.

Crack_Y(1) = Paste_Height*rand(1);
Crack_Y(2) = Paste_Height*rand(1);

for i = 1:Num_CNT
    [X,Y] = polyxpoly(CNT_X(i,:),CNT_Y(i,:),[0,Paste_Width],[0,Paste_Height],Crack_Y(:)');
    if X > -1
        X_Intersect(i) = X;
        Y_Intersect(i) = Y;
CNT_Termination_Distance_Top(i) = CNT_Y(i,1) - Y_Intersect(i);
CNT_Termination_Distance_Bottom(i) = CNT_Y(i,2) - Y_Intersect(i);
end
end
X_Intersect(X_Intersect == 0) = [];
Y_Intersect(Y_Intersect == 0) = [];
CNT_Termination_Distance_Top(CNT_Termination_Distance_Top == 0) = [];
CNT_Termination_Distance_Bottom(CNT_Termination_Distance_Bottom == 0) = [];

for i = 1:numel(X_Intersect)
    if rand(1) > .5
        CNT_Termination_Point(i) = CNT_Termination_Distance_Top(i)/CNT_Length;
    else
        CNT_Termination_Point(i) = CNT_Termination_Distance_Bottom(i)/CNT_Length;
    end
end

Gap_Distance = (0:.1:1);
for i = 1:numel(Gap_Distance)
    Gap_Connection_Count(i) = sum(CNT_Termination_Point>Gap_Distance(i));
end

scatter(X_Intersect,Y_Intersect)
plot([0, Paste_Width],[Crack_Y(1),Crack_Y(2)])
nnumel(Y_Intersect)
xlabel('Gridline Width (\mum)')
ylabel('Gridline Length (\mum)')
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