Design, Manufacture, Modelling and Testing of Surface Acoustic Wave Strain Sensors

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A dissertation submitted to the University of Dublin in partial fulfilment of the requirements for the degree of Doctor of Philosophy

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2008
Declaration

I declare that the work described in this dissertation is, unless otherwise stated, entirely my own work and has not been submitted as an exercise for a degree at this or any other University. I agree that Trinity College Library may lend or copy this dissertation upon request.

Signature of author:________________________________________

Brian Mc Cormack
February 2008
Abstract

There is an increasing demand for multi-sensor strain measurement systems, particularly those which incorporate wireless sensors. A possible application of such a system is the Real-Time Weigh-In-Motion (RTWIM) of heavy goods vehicles. Surface Acoustic Wave (SAW) strain sensors have been proposed for this application as they offer both wireless interrogation and passive operation, but considerable development work is required before they can be successfully deployed.

This thesis details the design, manufacture, modelling and testing of SAW strain sensors for the RTWIM application. Following a discussion of surface wave theory and devices, the design and manufacture of the prototype sensors is detailed. This is achieved through a new system which integrates the design and manufacturing processes from initial sensor specifications to finished devices, thus yielding significant improvements over existing schemes. Sensor modelling is achieved through new modifications to the coupling-of-modes (COM) SAW model, which allows both the complete frequency responses of the devices, and their sensitivity to biases, to be simulated. The prototype sensors are then tested in both unstrained and strained states, thus enabling the evaluation of both the device fabrication and the COM modelling.

Although issues were encountered with each of the research strands, this work successfully extends and improves the development of SAW strain sensors. It is hoped that the research can facilitate the deployment of these innovative sensors in a range of applications.
List of Publications


Acknowledgements

It is a pleasure to thank just some of the many people who made this work possible. I would like to express my gratitude to my supervisor, Mr. Dermot Geraghty, for his steadfast support and guidance throughout the project. His enthusiasm and trust in the work, even in difficult times, was instrumental to its success. Special thanks are also extended to Prof. Margaret O’Mahony for financial support, patience in the face of problems and kind words of encouragement along the way. Funding from the Higher Education Authority’s Programme for Research in Third-Level Institutes (Cycle 3), through the Centre for Transportation Research and Innovation for People (TRIP) in TCD, and from Enterprise Ireland’s Proof of Concept fund, is gratefully acknowledged.

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# Nomenclature

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<tr>
<td>α</td>
<td>SAW decay into crystal</td>
<td>–</td>
</tr>
<tr>
<td>α_s</td>
<td>COM transduction coefficient</td>
<td>1/(\sqrt{Ω_m})</td>
</tr>
<tr>
<td>α_T</td>
<td>Temperature coefficient of delay</td>
<td>ppm/°C</td>
</tr>
<tr>
<td>β</td>
<td>SAW wavenumber</td>
<td>m⁻¹</td>
</tr>
<tr>
<td>β_i</td>
<td>SAW eigenvectors</td>
<td>–</td>
</tr>
<tr>
<td>δ</td>
<td>COM detuning parameter</td>
<td>m⁻¹</td>
</tr>
<tr>
<td>ε_ij</td>
<td>Non-linear strain component</td>
<td>–</td>
</tr>
<tr>
<td>ε_0</td>
<td>Permittivity of free space</td>
<td>F/m</td>
</tr>
<tr>
<td>ε_s</td>
<td>Effective permittivity</td>
<td>F/m</td>
</tr>
<tr>
<td>ε_ij</td>
<td>Dielectric tensor component</td>
<td>F/m</td>
</tr>
<tr>
<td>η</td>
<td>Metallisation ratio</td>
<td>–</td>
</tr>
<tr>
<td>κ</td>
<td>COM electrode reflectivity</td>
<td>m⁻¹</td>
</tr>
<tr>
<td>λ</td>
<td>SAW wavelength</td>
<td>m</td>
</tr>
<tr>
<td>λ_r</td>
<td>Wavelength of UV light</td>
<td>m</td>
</tr>
<tr>
<td>ν</td>
<td>Poisson’s ratio</td>
<td>–</td>
</tr>
<tr>
<td>ρ</td>
<td>Material mass density</td>
<td>kg/m³</td>
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<tr>
<td>σ_ij</td>
<td>Stress component (non-piezoelectric)</td>
<td>Pa</td>
</tr>
<tr>
<td>τ</td>
<td>SAW delay time</td>
<td>s</td>
</tr>
<tr>
<td>φ</td>
<td>Electrical potential</td>
<td>V</td>
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<tr>
<td>ω</td>
<td>Angular wave frequency</td>
<td>rad/s</td>
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<thead>
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<th>Unit</th>
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<tr>
<td>$\psi$</td>
<td>Normalised SAW power</td>
<td>$\sqrt{\text{W}}$</td>
</tr>
<tr>
<td>$a$</td>
<td>Crack length</td>
<td>m</td>
</tr>
<tr>
<td>$a$</td>
<td>Electrode linewidth</td>
<td>m</td>
</tr>
<tr>
<td>$A$</td>
<td>Direction cosine matrix</td>
<td>–</td>
</tr>
<tr>
<td>$B$</td>
<td>Partial field amplitude</td>
<td>–</td>
</tr>
<tr>
<td>$B$</td>
<td>Susceptance</td>
<td>$\Omega^{-1}$</td>
</tr>
<tr>
<td>$c_{ijkl}$</td>
<td>Elastic stiffness constant (2&lt;sup&gt;nd&lt;/sup&gt; order)</td>
<td>Pa</td>
</tr>
<tr>
<td>$c_{ijklmn}$</td>
<td>Elastic stiffness constant (3&lt;sup&gt;rd&lt;/sup&gt; order)</td>
<td>Pa</td>
</tr>
<tr>
<td>$C$</td>
<td>Capacitance</td>
<td>F</td>
</tr>
<tr>
<td>$C_n$</td>
<td>Capacitance/finger pair/aperture</td>
<td>F/m</td>
</tr>
<tr>
<td>$d_{ijkl}$</td>
<td>Piezoelectric tensor component</td>
<td>C/N</td>
</tr>
<tr>
<td>$D_i$</td>
<td>Electrical displacement component</td>
<td>C/m&lt;sup&gt;2&lt;/sup&gt;</td>
</tr>
<tr>
<td>$e_{ijkl}$</td>
<td>Piezoelectric constant</td>
<td>C/m&lt;sup&gt;2&lt;/sup&gt;</td>
</tr>
<tr>
<td>$E$</td>
<td>Young’s Modulus</td>
<td>Pa</td>
</tr>
<tr>
<td>$E_k$</td>
<td>Electrical field component</td>
<td>V/m</td>
</tr>
<tr>
<td>$f$</td>
<td>SAW frequency</td>
<td>Hz</td>
</tr>
<tr>
<td>$F$</td>
<td>Applied force</td>
<td>N</td>
</tr>
<tr>
<td>$g$</td>
<td>IDT-reflector spacing</td>
<td>m</td>
</tr>
<tr>
<td>$h$</td>
<td>Electrode height</td>
<td>m</td>
</tr>
<tr>
<td>$G$</td>
<td>Conductance</td>
<td>$\Omega^{-1}$</td>
</tr>
<tr>
<td>$G_c$</td>
<td>Toughness</td>
<td>Jm&lt;sup&gt;−2&lt;/sup&gt;</td>
</tr>
<tr>
<td>$I$</td>
<td>Current</td>
<td>A</td>
</tr>
<tr>
<td>$I_i$</td>
<td>2&lt;sup&gt;nd&lt;/sup&gt; moment of area about axis $i$</td>
<td>m&lt;sup&gt;4&lt;/sup&gt;</td>
</tr>
<tr>
<td>$K^2$</td>
<td>Electromechanical coupling coefficient</td>
<td>–</td>
</tr>
<tr>
<td>$K_c$</td>
<td>Fracture toughness</td>
<td>Nm&lt;sup&gt;−1.5&lt;/sup&gt;</td>
</tr>
<tr>
<td>$L$</td>
<td>SAW structure length</td>
<td>m</td>
</tr>
<tr>
<td>$M_i$</td>
<td>Moment about axis $i$</td>
<td>Nm</td>
</tr>
<tr>
<td>$N$</td>
<td>Number of electrodes</td>
<td>–</td>
</tr>
<tr>
<td>$p$</td>
<td>Electrode periodicity</td>
<td>m</td>
</tr>
<tr>
<td>$P$</td>
<td>SAW power flow</td>
<td>W</td>
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<thead>
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<th>Unit</th>
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<tr>
<td>$P$</td>
<td>Total applied load</td>
<td>N</td>
</tr>
<tr>
<td>$q$</td>
<td>SAW wavenumber deviation</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$Q$</td>
<td>Quality factor</td>
<td>–</td>
</tr>
<tr>
<td>$Q_F$</td>
<td>IDT element factor</td>
<td>F/m</td>
</tr>
<tr>
<td>$r$</td>
<td>Mechanical displacement vector</td>
<td>m</td>
</tr>
<tr>
<td>$R$</td>
<td>Resistance</td>
<td>Ω</td>
</tr>
<tr>
<td>$R$</td>
<td>COM wave component</td>
<td>√W</td>
</tr>
<tr>
<td>$S$</td>
<td>COM wave component</td>
<td>√W</td>
</tr>
<tr>
<td>$S_{ij}$</td>
<td>Linear strain component</td>
<td>–</td>
</tr>
<tr>
<td>$S_{ij}$</td>
<td>S-parameter</td>
<td>–</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
<td>°K</td>
</tr>
<tr>
<td>$T_{ij}$</td>
<td>Stress component</td>
<td>Pa</td>
</tr>
<tr>
<td>$u_i$</td>
<td>Component of mechanical displacement</td>
<td>m</td>
</tr>
<tr>
<td>$U$</td>
<td>Strain energy density</td>
<td>J/m$^3$</td>
</tr>
<tr>
<td>$v$</td>
<td>SAW phase velocity</td>
<td>m/s</td>
</tr>
<tr>
<td>$V$</td>
<td>Signal voltage</td>
<td>V</td>
</tr>
<tr>
<td>$w_i$</td>
<td>Static displacement component</td>
<td>m</td>
</tr>
<tr>
<td>$W$</td>
<td>Electrode aperture</td>
<td>m</td>
</tr>
<tr>
<td>$Y$</td>
<td>Admittance</td>
<td>Ω$^{-1}$</td>
</tr>
<tr>
<td>$Z$</td>
<td>Impedance</td>
<td>Ω</td>
</tr>
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**Naming and symbol conventions**

Wherever possible, symbols and quantities were chosen to be compatible with those already in use. Constants are shown in upright type (e.g., the imaginary operators ‘i’ and ‘j’), while variables are shown in italics (e.g. $S_{ij}$). The number of indices on a variable denotes its type: scalars have no indices (e.g., the density $\rho$), vectors have one index (e.g., the material displacement $u_i$) while tensors of second rank and higher (see Section 2.1.1 and below) have two or more indices.
(e.g., the stress \( T_{ij} \)).

**Tensor summation**

Tensor summation (also known as Einstein summation) has been frequently used to reduce the size of equations and provide more clarity. All tensors in this work are Cartesian, and thus an \( n^{th} \)-rank tensor has \( 3^n \) components. The summation convention states that where one or more indices are repeated on the right-hand side of an equation, the attendant quantities should be summed over the range of the indices. For example, \( \sigma_{11} \) from equation (2.13) equates to:

\[
\sigma_{11} = c_{1111} S_{11} + c_{1112} S_{12} + c_{1113} S_{13} + c_{1121} S_{21} + c_{1122} S_{22} + \cdots + c_{1133} S_{33}
\]

Unless otherwise stated, all indices (whether summed or not) cover the range 1-3. The choice of letters used in the indices is unimportant provided that the summation (if required) is unambiguous. An index (e.g., \( j \)) preceded by a comma denotes differentiation with respect to the space coordinate \( x_j \), e.g.:

\[
u_{i,j} = \frac{\partial u_i}{\partial x_j}
\]

The dot notation (e.g., \( \dot{u}_j \)) denotes differentiation with respect to time.
Chapter 1

Introduction

This chapter outlines the project’s background, exploring how strain may be measured and the limitations of current sensors. A novel application of strain sensing is introduced, along with a potential sensor solution. The project objectives are then outlined, along with a guide to this thesis.

1.1 Strain sensing

Strain is often defined as the elongation of a body per unit length [1]. Such a general definition masks an extremely broad subject, for the effect is integral to all physical systems. The measurement of strain is of fundamental importance for all branches of engineering, and has been investigated for hundreds of years.

The history of strain is closely connected with studies into the strength of materials. Building on Galileo’s initial work on elastic bodies, pioneers such as Hooke, Euler, Navier, Cauchy and Poisson developed the theory of elasticity as a link between mathematical modelling and actual engineering behaviour. A comprehensive history of their work may be found in [2] and [3].

Today the dominant technology used to measure strain is the bonded electrical resistance strain gauge [4]. The operation of these sensors is based on the piezoresistive effect first described by Lord Kelvin [5]. This is the change in resistance of a material due to an applied stress. Early resistance strain gauges were wires stretched between supports mounted on the strained surface, which were
susceptible to error. Bonded wire gauges, where the resistive element is attached directly to the component, were introduced in the late 1930s. The present bonded foil resistive strain gauges were made available in the early 1950s, and have been the dominant measurement device ever since [6]. Other devices available include semiconductor, capacitive and vibrating wire strain gauges [7]; these are typically used in specialist applications.

While modern strain sensors offer adequate performance as measurement devices, they are hampered by the physical connections required for interrogation and power. Foil resistive strain gauges, for example, require wiring to connect each sensor to a voltage source or Wheatstone bridge. There are two major disadvantages with such physical connections:

- **Measurement of moving components**: difficulties can arise if the component to be measured is moving relative to the interrogation system. For example, strain gauges connected to robotic arms for load sensing require cable harnesses to ensure that the wiring does not tangle as the arm moves. Similarly, torque measurement on rotating shafts requires slip rings or other connections to maintain electrical contact between sensor and interrogation system.

- **Networking of multiple sensors**: if a number of sensors are to be connected in a network, a physical link must be established between each sensor and the interrogation device. This means that the interrogation hardware must have enough ports or access points for all sensors, and if more nodes are needed then an expensive upgrade is often required.

The obvious solution is to use wireless connections; witness the stunning success of wireless telephony in recent times. Most of the available wireless sensor systems incorporate an existing strain sensor with a wireless communications interface. A typical example of this is MicroStrain’s SG-Link [8]: a sensor module is shown in Figure 1.1. This product connects to a conventional strain gauge, and can acquire, process and wirelessly transmit strain information to a base station. Although the system has excellent measurement capabilities, each sensor node requires its own battery which must be changed or charged on a regular basis.
1.1. STRAIN SENSING

In addition to the cost of replacement batteries, the component under strain may need to be taken out of service; in the case of the robot arm mentioned above, this could have serious production consequences. Batteries are also known to perform poorly at low and high temperatures [9], which could restrict the applications of such wireless devices.

The provision of power remains a major issue for modern sensor systems. Renewable energy sources which work effectively on a large scale (e.g., wind and solar power) are difficult to scale down for microelectronic use, in particular when the working environment of the sensors may vary. An alternative approach is to use power harvesting, which is the process of acquiring the energy surrounding a system and turning it into useful electrical energy [10]. While this may develop into a practical solution, the power outputs are currently too low for most sensor systems.

With the above in mind, it is clear that a strain sensor combining passive operation and wireless interrogation would be useful. In the next section a target application for such a sensor is outlined, and it is clear that such a device could act as an enabling technology for future measurement systems.
1.2 Real-Time Weigh-in-Motion

The development of passive, wireless strain sensing in this project was driven by a novel application: Real-Time Weigh-In-Motion (RTWIM). Weigh-In-Motion is the calculation of static axle loads (or gross vehicle weights) of heavy vehicles travelling at highway speeds [11], and possible applications areas include:

1. Vehicle taxation: the German and Swiss governments have recently introduced road taxes for HGVs based on a ‘polluter pays’ principle. An on-board unit monitors the distance travelled, and also stores information on the vehicle’s maximum gross weight and exhaust emission class. The operator is then charged per kilometre travelled. It should be noted that only the maximum permitted gross weight of the vehicle is stored: no actual weighing takes place.

2. Regulatory enforcement / public safety: the damage inflicted by a vehicle on a road surface is proportional to the fourth power of its static weight [12]. Therefore, overloaded vehicles (HGVs in particular) can cause accelerated damage to road surfaces. In Ireland, roads with a 20 year design life typically require rehabilitation after 16 years, and this can be traced to the large number (c. 30%) of overloaded HGVs using them. Public safety may be put at risk due to brake failure, tyre blowout etc. of overloaded vehicles.

3. Fleet management: the management of a large haulage fleet could be improved by a detailed knowledge of loads carried by any vehicle at any time. This would allow combined deliveries of complementary loads, real-time scheduling, reduced fleet requirements etc.

4. Vehicle condition monitoring: basic maintenance protocols could be implemented by analysing the dynamic response of a vehicle to road conditions. For example, this could be used to diagnose impending faults in the suspension system.

5. Point of delivery weighing and billing: for bulk loads, the vehicle itself could act as an automatic weighing and billing system, removing the need for dedicated weigh stations.
1.2. REAL-TIME WEIGH-IN-MOTION

Current WIM systems can be divided into road-based and vehicle-based solutions. Road-based systems include bending plates, piezoelectric strips, load cells, capacitive mats etc.: an example is shown in Figure 1.2. In all cases, the sensor is embedded in, or laid on, the road surface, and the vehicle is weighed as it drives over. The technology is simple and well established, but only offers point measurements; as the sensors are fixed on the road surface, only weight measurements at a single location can be performed. An effective road-based system would require a large number of measurement points, which would need excessive capital expenditure. Road-based systems can only provide static load information as just point measurements are taken: a statistical measurement history is required to get dynamic load data (mean load, standard deviation etc.) [11].

Vehicle-based systems allow true real-time measurements to be made, as all of the instrumentation is mounted on the vehicle. Examples of this type of technology include pressure sensors (for vehicles with air suspension, see Figure 1.3) and shear beams. These systems are more flexible than the road-based options (and can provide dynamic load data), but include expensive force transducers and involve long installation times.

It is clear that neither system type is ideal. Following an analysis of existing technologies, it was concluded that a practical RTWIM system should be vehicle-based, utilising cheap transducers and simple installation processes. This project proposes that passive, wireless sensors be used to measure strain on the vehicle axles, which can be correlated to the gross weight of the vehicle. Due to their
wireless nature, each device must act as a combined sensor and ID tag, i.e., transmitting both measurement and identification information, in order to link a particular sensor measurement with its location. No such devices are commercially available at present. The interrogation system for the sensors is to be integrated with a commercial ‘off-the-shelf’ (COTS) unit that provides GPS capability and is interfaced to a Geographical Information System (GIS) to provide road positioning. A system diagram is shown in Figure 1.4.

1.3 Proposed sensor solution

It is proposed that Surface Acoustic Wave (SAW) devices be used as strain sensors in the RTWIM system. SAW devices have the following advantages:

1. *Wireless, passive operation*: SAW devices can be operated passively and interrogated wirelessly, as RF signals can be used for both device excitation and communication [14]. The operation of these devices as sensors has already been demonstrated (see Chapter 3), but much work remains to be done: the research targets for this project will be discussed in Section 1.4.
is proposed that the sensor function can be seamlessly integrated with these two natural device advantages.

2. *Measurement flexibility relative to strain gauge systems:* RTWIM could conceivably be performed by mounting conventional strain gauges onto the HGVs’ axles, and using these to calculate weight. However, this would require long wired links to a central interrogation unit, which would be vulnerable to road damage and would be difficult to install. Alternatively, data acquisition and processing could be performed at each sensor point using the wireless strain gauge systems described previously. The RTWIM project, however, requires many sensors nodes and this would make the system extremely expensive. SAW sensors are increasingly being used in vehicular applications where physical communications links and device pow-
Current technologies include non-contact torque measurement on driveshafts \[15\] and tyre pressure monitoring systems \[16\] (see Section \[3.1.1\]). For this project, it is envisaged that the sensors will be attached to the axles in a similar fashion to conventional strain gauges, but without the long and difficult wiring process.

3. **Cheap transducers**: SAW sensors should be cheaper than an equivalent strain gauge, given that a conventional SAW filter device retails for about €2 (as opposed to several Euro for a basic strain gauge). Although weldable strain gauges are available, which could be directly attached to an axle, their high cost (about €25 each) precludes their use in a multi-sensor environment. All of the signal processing, data acquisition etc. for the SAW sensors is performed by the central interrogation system, and this component represents the bulk of the system cost. This means that a large network of sensors can be deployed in a measurement network (e.g., over a number of axles), with little effect on overall system cost.

4. **Proven communications system**: in addition to the applications cited above, SAW devices are used in remote keyless entry (increasingly used on modern vehicles) and in low-power RF networks. The success of such systems indicates that wireless, low-power SAW networking is viable for the project. An added advantage is that the sensors can be designed to operate within the European Industrial, Scientific and Medical (ISM) frequency band (see Chapter \[3\]) which allows for licence-free communication between low-power devices. Wireless interrogation of passive sensors remains a challenge, however, particularly where multiple devices are used: this will be discussed in Chapter \[3\].

5. **Robustness under extreme environmental conditions**: the lack of on-board power and wired links are major advantages in the extreme environmental conditions experienced by HGVs. In contrast to battery-powered devices, SAW sensors can operate normally in a very wide temperature range \[17\].
1.4 Project objectives

My research is based on the characterisation of SAW strain sensors. The key aims of my research are to as follows:

- **Design, manufacture and testing of SAW strain sensors**: a central part of the project involves the design, manufacture and experimental testing of physical SAW devices as strain sensors (see Chapter 3 and 5).

- **Modelling and simulation of SAW strain sensors**: development of models to predict and explain device behaviour (see Chapter 4 and 5).

While the RTWIM system is considered as a target application for the sensors, it should be stressed that only the SAW sensors themselves will be considered in this work. The wider RTWIM project is a collaboration between the Department of Mechanical and Manufacturing Engineering and the Department of Civil, Structural and Environmental Engineering in Trinity College Dublin. Other research areas in the project include:

- Sensor interrogation and vehicle networking
- Axle modelling and vehicle dynamics

1.5 Layout of thesis

The subsequent chapters of this document show how the research aims were defined, evaluated and accomplished. Chapter 2 describes the nature of surface waves and SAW devices, which is essential to the understanding of their operation as sensors. The process of designing and manufacturing a SAW sensor is detailed in Chapter 3 where an integrated design and manufacturing process for sensors is introduced. Chapter 4 outlines how the strain effects on a SAW sensor may be modelled and simulated using a new extension to an existing SAW design tool. In Chapter 5 the results for both the experimental and theoretical approaches are presented, while in Chapter 6 the results set and future work are discussed.
Chapter 2

Surface Acoustic Waves: Theory and Devices

The field of SAW devices brings together elements of piezoelectricity and surface wave propagation. In this chapter, the elastic behaviour of materials is reviewed, followed by a discussion of piezoelectric effects. The motion of elastic waves along the surface of a piezoelectric material is then explained. Common elements of modern SAW devices are introduced, and finally their use in complete components is discussed.

The aim of this chapter is to present a unified treatment of surface waves and SAW devices, which is often omitted in literature on SAW device design. Surface wave devices used in signal processing applications (the dominant market for these devices, see Section 2.5) are usually unstrained, and thus the devices are typically treated as electrical transfer functions with constant coefficients. However, as will be discussed in Chapter 3, the effects of loads on SAW devices can markedly change their performance, thus enabling their use as sensors. Therefore it is crucial that the fundamental operation of SAW devices be understood before sensor effects are considered.
2.1 Theory of elasticity

Most engineering analyses presume that the relevant material properties are isotropic. For example, linear elastic problems commonly presume that the stiffness of a material is determined by its Young’s Modulus $E$ and Poisson’s ratio $\nu$. However, the substrates used for SAW devices are inherently anisotropic (see Section 2.2), and normally have to be treated as such. Anisotropic analyses of small-scale deformations are performed using the theory of elasticity, which examines stress and strain in a more fundamental manner.

The theory of elasticity is designed to treat explicitly the linear or nonlinear elastic response of materials to applied forces [18]. This project mainly deals with the linear theory of elasticity, where the relationship between the stress and the deformation is linear: extensions for nonlinear behaviour will be presented in Section 4.5.3.

2.1.1 Strain

The elongation of an infinitesimal line element $ds$ is fundamental in the theory of deformation [18], and will be used to derive strain expressions. Figure 2.1 shows an undeformed line element $ds$ which has been deformed into element $ds^*$ in a continuous, dense, homogeneous material. Both elements are referenced to the same Cartesian coordinate system $(X_1,X_2,X_3)$, where $(i,j,k)$ are unit vectors along the positive axes, and we may also presume that the deformation is proper and admissible [18], i.e., that the deformation is physically possible. The displacement vector $r$ of any point on the element during deformation is given by:

$$ r = iu_1 + ju_2 + ku_3 $$

(2.1)

where $(u_1,u_2,u_3)$ are the components of displacement along the $(X_1,X_2,X_3)$ axes:

$$ u_1 = y_1 - x_1 $$
$$ u_2 = y_2 - x_2 $$
$$ u_3 = y_3 - x_3 $$

(2.2)
2.1. THEORY OF ELASTICITY

The length of the line element before deformation is given by:

\[ ds^2 = dx_1^2 + dx_2^2 + dx_3^2 \]  \hspace{1cm} (2.3)

while after deformation the element length is:

\[ ds^{*2} = dy_1^2 + dy_2^2 + dy_3^2 \]  \hspace{1cm} (2.4)

The dimensions of the deformed element \( dy_i \) can be expresses in terms of the original dimensions \( dx_i \) using partial derivatives [19]:

Figure 2.1: Extension of infinitesimal line element
\[ dy_1 = y_{1,1}dx_1 + y_{1,2}dx_2 + y_{1,3}dx_3 \]
\[ dy_2 = y_{2,1}dx_1 + y_{2,2}dx_2 + y_{2,3}dx_3 \]
\[ dy_3 = y_{3,1}dx_1 + y_{3,2}dx_2 + y_{3,3}dx_3 \]

(2.5)

Substituting equation (2.2) into (2.5) produces:

\[ dy_1 = (1 + u_{1,1})dx_1 + u_{1,2}dx_2 + u_{1,3}dx_3 \]
\[ dy_2 = u_{2,1}dx_1 + (1 + u_{2,2})dx_2 + u_{2,3}dx_3 \]
\[ dy_3 = u_{3,1}dx_1 + u_{3,2}dx_2 + (1 + u_{3,3})dx_3 \]

(2.6)

Combining equations (2.3), (2.4) and (2.6) produces:

\[ 0.5(ds^2 - dx^2) = \varepsilon_{11}dx_1^2 + \varepsilon_{22}dx_2^2 + \varepsilon_{33}dx_3^2 + 2\varepsilon_{12}dx_1dx_2 + 2\varepsilon_{13}dx_1dx_3 + 2\varepsilon_{23}dx_2dx_3 \]

(2.7)

The coefficients of the above expression are given by:

\[ \varepsilon_{11} = u_{1,1} + 0.5(u_{1,1}^2 + u_{2,1}^2 + u_{3,1}^2) \]
\[ \varepsilon_{22} = u_{2,2} + 0.5(u_{1,2}^2 + u_{2,2}^2 + u_{3,2}^2) \]
\[ \varepsilon_{33} = u_{3,3} + 0.5(u_{1,3}^2 + u_{2,3}^2 + u_{3,3}^2) \]

\[ 2\varepsilon_{12} = u_{2,1} + u_{1,2} + u_{1,1}u_{1,2} + u_{2,1}u_{2,2} + u_{3,1}u_{3,2} \]
\[ 2\varepsilon_{13} = u_{3,1} + u_{1,3} + u_{1,1}u_{1,3} + u_{2,1}u_{2,3} + u_{3,1}u_{3,3} \]
\[ 2\varepsilon_{23} = u_{3,2} + u_{2,3} + u_{1,2}u_{1,3} + u_{2,2}u_{2,3} + u_{3,2}u_{3,3} \]

(2.8)

The \(\varepsilon_{ij}\) above are exact expressions of the deformation state at a particular material point, and are clearly symmetrical \((\varepsilon_{ij} = \varepsilon_{ji})\). They are also components of a second-rank tensor (the Green-Saint-Venant strain tensor \([18]\)). Tensors are
2.1. THEORY OF ELASTICITY

mathematical structures whose components transform according to rules defined by their ranks [20],[21]. For example, a vector is an example of a first-rank tensor because its components transform as \( c_i^* = a_{ij}c_j \) (see Section A.3). Tensors are extremely useful in the theory of elasticity for describing the properties of a system which are independent of a coordinate system, e.g., the strain state at a particular point. Although the individual components of the tensor may change, the resultant remains constant.

If we consider only small strains (\( \ll 1 \)) and small angles of rotation relative to the strains, the strain tensor \( \bar{\varepsilon} \) is given by:

\[
\begin{bmatrix}
S_{11} &= u_{1,1} \\
S_{12} &= u_{2,1} \\
S_{13} &= u_{3,1} \\
S_{22} &= u_{2,2} \\
S_{23} &= u_{3,2} \\
S_{33} &= u_{3,3}
\end{bmatrix}
\]  
(2.9)

or in index notation:

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) = \frac{1}{2} (u_{i,j} + u_{j,i})
\]  
(2.10)

This definition matches the engineering definition of strain, i.e., the elongation of a line element relative to its original length [1]. Note that strain is now denoted by \( S_{ij} \) as this is the standard symbol used in surface wave work. It may be shown that the above equations obey the conditions of strain compatibility, i.e., the six independent \( S_{ij} \) components are determined completely by the three displacement components \( u_i \): the procedure is outlined in [22].

Some observations should be made at this point regarding the suitability of this theory to SAW strain sensors. Equations (2.9) and (2.10) form the basis of classical small-displacement theory, giving the normal and shear strain components at a point in a material. The presumption that the strains and rotations are small appears to be applicable to this project, given that the strain sensors are substrate-limited to maximum strains of \(< 0.002 \) (see Section 3.3.2). The theory is less suitable for flexible plates and rods, but given the rigid fixation planned for the sensors, the treatment appears to be valid.
2.1.2 Stress

Next we must consider the stresses in a body. Consider an infinitesimal cubic element with dimensions dx, dy, dz under applied stresses as shown in Figure 2.2. Each stress is denoted by $\sigma_{ij}$, where $i$ denotes the direction of the normal to the surface under consideration and $j$ the direction of the force; positive orientations are shown on the positive faces of the element. Body forces and couples (caused by gravity, magnetism, inertial effects etc.) have been ignored; piezoelectric effects will be treated in Section 2.2. This is because the body forces reduce as the cube of the linear dimensions (being based on volume) of the differential element, whereas the surface forces only reduce with the square of the dimension \[22\]. Taking moments about point $O$:
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\[ M_x = (\sigma_{23} dx dz) dy - (\sigma_{32} dx dy) dz = 0 \]  
\[ (2.11a) \]

\[ M_y = (\sigma_{31} dx dy) dz - (\sigma_{13} dy dz) dx = 0 \]  
\[ (2.11b) \]

\[ M_z = (\sigma_{12} dy dz) dx - (\sigma_{21} dx dz) dy = 0 \]  
\[ (2.11c) \]

Hence \( \sigma_{ij} = \sigma_{ji} \) and the stress array is symmetrical, so only six components are required to completely specify the stress state:

\[ \sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} \end{bmatrix} \]  
\[ (2.12) \]

It can further be shown that the stress array is a symmetrical second-rank tensor, similar in character to \( S \).

2.1.3 Elasticity

The theory of elasticity can be used to link the concepts introduced in the previous two sections, i.e., the strains in a body and the applied stresses that caused them. We may assume that the stress at every point \( P \) in a body depends at all times solely on the simultaneous deformation in the immediate neighbourhood of \( P \). This allows the stress and strain at a point to be related. Any previous history of loading (heat treatment, residual stresses from fabrication etc.) is ignored. We also assume that the material instantly returns to its original size and shape after the load has been removed, i.e., perfect elasticity. For small deformations these are usually valid assumptions. Temperature conditions should also be specified: here they are assumed to be adiabatic.

The problem of equilibrium of a deformed solid body remains indeterminate until the relationships between components of the displacement vector and those of the stress tensor are established. In general, the linear elastic behaviour of arbitrary anisotropic materials may be expressed by the generalised Hooke’s law:

\[ \sigma_{ij} = c_{ijkl} S_{kl} \]  
\[ (2.13) \]
where \( c_{ijkl} \) is the second-order elastic stiffness of the material. This is a fourth-rank tensor structure with \( 3^4 \) elements in a Cartesian system. While it can be derived from the strain energy density \( U \) \( [18] \), in practice it is usually found from experimental measurements of materials, e.g., a simple stress-strain test for isotropic materials. The complexity of this tensor can be reduced by considering the symmetries of the stress and strain tensors. As \( \sigma_{ij} = \sigma_{ji} \) it follows that \( c_{ijkl} = c_{jikl} \), and from the symmetry of the strain tensor \( c_{ijkl} = c_{ijlk} \). Expressing \( U \) in terms of the strain components, it can also be shown that \( c_{ijkl} = c_{klij} \), i.e., that the first and second pairs of indices are symmetrical. Thus a general anisotropic material has at most 21 independent second-order stiffnesses, and in practice most have considerably less: quartz, for example, only has 6 (see Section A.1).

Given the reduction in independent elements in all of the tensors, it is useful to define a contracted notation so that relationships are more easily shown. Voigt notation is commonly used to remove unnecessary indices, for example changing the stress tensor \( \sigma_{ij} \) (with two indices) to a simplified vector of independent stresses \( \sigma_\alpha \) (with a single index) by the following rule \( [23] \):

\[
\sigma_\alpha = \begin{cases} 
  i & \text{if } i = j, \\
  9 - i - j & \text{if } i \neq j.
\end{cases}
\]  

(2.14)

It should be noted here that \( \alpha = 1 - 6 \) whereas \( i, j = 1 - 3 \). Similar transformation rules apply for higher-rank tensors, usually treating the indices in pairs as above. Care should be exercised in transforming certain tensors (e.g., \( S_{ij} \)), however, as symmetry must be preserved (see the discussions in \( [23] \) and \( [24] \)), and the transformed quantities are no longer tensors. As an example of the contracted notation, equation \( (2.13) \) for an isotropic material can be expressed as:
The coefficients in the stiffness matrix above are:

\[ c_{11} = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)} \]  
(2.16)

\[ c_{12} = \frac{\nu E}{(1+\nu)(1-2\nu)} \]  
(2.17)

From the above, it is clear that the linear elastic behaviour of an isotropic solid can be completely described by \( E \) and \( \nu \).

### 2.2 Piezoelectricity

All modern surface wave devices use piezoelectric substrates, and an understanding of piezoelectric effects is important in all SAW work. Piezoelectricity (from the Greek ‘piezein’, meaning ‘to press’) describes the linear coupling between electrical and mechanical fields in a material. This is a linearised version of electroelasticity (general electromechanical coupling), which will be discussed in Section 4.5.3. The direct piezoelectric effect, where an electrical polarisation is produced by a mechanical strain, was discovered in 1880 by Pierre and Jacques Curie [25]; the converse effect (where an electrical field causes mechanical strain) was demonstrated a short time later. The phenomenon remained a curiosity until Voigt [26] developed the crystal physics theory necessary to model piezoelectric materials. In the 1920s and 30s, piezoelectric oscillators became available with far higher stabilities than the commonly-used vacuum tubes, and their application in sonar equipment became practical [27]. Piezoelectric ceramics (formed
from sintered metallic oxide powders) were introduced in the late 1940s, offering larger piezoelectric and dielectric effects than natural quartz crystals. They also allowed the piezoelectric material to be tailored to a specific application [28]. In parallel with the advances in materials, piezoelectric transducers were developed: a thorough review of early developments is given by Mason [29]. The development of sensors based on bulk piezoelectric effects is an active field [30], while transducers and actuators for ‘smart’ structures often use piezoelectric elements [31].

The piezoelectric effect is caused by the displacement of charge centres in a material. Positive and negative charges form electrical dipoles, which are initially symmetrically distributed in the material, making it electrically neutral. However, applied strain causes the charge centres to displace, polarising the crystal. Similarly, an applied electrical field will cause the material to deform. This coupling between strain and electrical polarisation is the key feature of piezoelectric media. Piezoelectricity can only occur in materials lacking a centre of inversion symmetry, and thus all piezoelectric single crystals are anisotropic. A review of material classes suitable for piezoelectricity may be found in [32] and [33].

As with the elasticity section, in this project we are mainly concerned with the linear theory of piezoelectricity; nonlinear effects will be introduced in Section 4.5.3. From conservation of energy and enthalpy arguments [34], it can be shown that the stress in a piezoelectric material is given by [33]:

\[ T_{ij} = c_{ijkl}^{E} S_{lk} - e_{ki}^{E} E_{k} \]

(2.18)

where \( e_{ki}^{E} \) are constants related to the third-rank piezoelectric tensor \( d_{ki} \) which couples the electrical and mechanical fields, and \( E_{k} \) is the applied electrical field. While \( e_{ki}^{E} \) is usually used in SAW analysis, transformations of coordinate systems are performed using \( d_{ki} \) (see Section A.3). Note that stress is now denoted by \( T_{ij} \) as this is the standard symbol used in surface wave work. The \( E \) superscript in \( c_{ijkl}^{E} \) denotes that the stiffnesses were measured at constant electric field: this can be assumed in the project and the superscript will be removed for clarity. When compared to equation (2.13), it is clear that (2.18) includes both the mechanical and electrical behaviour of the material, demonstrating the converse piezoelectric
effect. The electrical displacement $D_i$, which is the charge induced per unit area in an insulator by an electric field [35], is given by:

$$D_i = e_{ikl}S_{lk} + e_{ij}^S E_j$$  \hspace{1cm} (2.19)

where $e_{ij}^S$ is the second-rank dielectric tensor of the material. The $S$ superscript denotes that the values were measured at constant strain; again, this will be omitted in future work. This equation shows how the same $e_{klj}$ coupling causes the direct piezoelectric effect.

The symmetry conditions and contracted notation used in the elasticity section may also be employed here. Equations (2.18) and (2.19) are thus given by:

$$\begin{bmatrix}
T_1 \\
T_2 \\
T_3 \\
T_4 \\
T_5 \\
T_6 \\
\end{bmatrix} = \begin{bmatrix}
c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\
c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\
c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} \\
c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} \\
c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} \\
c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} \\
\end{bmatrix} \begin{bmatrix}
S_1 \\
S_2 \\
S_3 \\
S_4 \\
S_5 \\
S_6 \\
\end{bmatrix} + \begin{bmatrix}
e_{11} & e_{21} & e_{31} \\
e_{12} & e_{22} & e_{32} \\
e_{13} & e_{23} & e_{33} \\
e_{14} & e_{24} & e_{34} \\
e_{15} & e_{25} & e_{35} \\
e_{16} & e_{26} & e_{36} \\
\end{bmatrix} \begin{bmatrix}
E_1 \\
E_2 \\
E_3 \\
\end{bmatrix} $$  \hspace{1cm} (2.20)

$$\begin{bmatrix}
D_1 \\
D_2 \\
D_3 \\
\end{bmatrix} = \begin{bmatrix}
e_{11} & e_{12} & e_{13} & e_{14} & e_{15} & e_{16} \\
e_{21} & e_{22} & e_{23} & e_{24} & e_{25} & e_{26} \\
e_{31} & e_{32} & e_{33} & e_{34} & e_{35} & e_{36} \\
\end{bmatrix} \begin{bmatrix}
S_1 \\
S_2 \\
S_3 \\
S_4 \\
S_5 \\
S_6 \\
\end{bmatrix} + \begin{bmatrix}
e_{11} & e_{12} & e_{13} \\
e_{21} & e_{22} & e_{23} \\
e_{31} & e_{32} & e_{33} \\
\end{bmatrix} \begin{bmatrix}
E_1 \\
E_2 \\
E_3 \\
\end{bmatrix} $$  \hspace{1cm} (2.21)

### 2.3 Surface acoustic waves

The term ‘surface acoustic wave’ is given to a wide variety of wave types in media where the wave energy is concentrated close to a material surface. Many different types of wave exist depending on the medium, boundary conditions, propagating layers etc. The existence of surface acoustic waves in isotropic materials was first
proposed by Lord Rayleigh in his seminal paper of 1885 [36]. He began with the following:

*It is proposed to investigate the behaviour of waves upon a plane free surface of an infinite homogeneous isotropic elastic solid, their character being such that the disturbance is confined to a superficial region, of thickness comparable with the wave-length.*

Rayleigh’s work describes the motion of waves propagating along the plane surface of an infinite half-space, with particle motion in the sagittal plane \((x_1,x_2)\) (see Figure 2.3) and amplitude decreasing with depth into the substrate [37]. These waves are presumed to be straight-crested, i.e., without variation in the \(x_3\) direction. It should be noted that only the propagation of waves was treated, not their generation or reception. The prime interest at this time was in earthquake modelling, and further work by Love [38] and Sezawa [39] examined surface waves in layered media and higher-order modes. Modern SAW devices use a variety of surface wave types (see Section 2.3.1) depending on device requirements [40]; the characteristics of these waves can be found in texts such as [41] and [42]. A useful review of early work on anisotropic surface waves may be found in [43].

### 2.3.1 SAW velocity calculation

An instructive method of examining the properties of surface waves is to determine the SAW velocity \(v\) (i.e., the phase velocity of the wave) for a particular propagation direction in a material. As will be shown in Chapter 3, \(v\) is a key design parameter for SAW devices, especially those deployed as sensors. The method of velocity determination detailed below (known as the superposition of partial waves [41]) was proposed by Campbell and Jones in 1968 for surface waves [44], while a more detailed explanation is given in [45]; the axis system used here is explained in Section A.3.

Acoustic wave propagation in an arbitrary anisotropic piezoelectric medium is described by a set of linear equations, which are solved for a given set of propagation and boundary conditions. Fig 2.3 shows the geometry under consideration,
with an infinite half-space representing the piezoelectric substrate. The equations of motion in the piezoelectric medium are given by \[46\]:

\[
T_{ij,i} = \rho \ddot{u}_j
\]  
(2.22)

where \(\rho\) is the mass density of the material. Electromagnetic waves (described by Maxwell’s equations) also propagate through the piezoelectric substrate, but here these fields are presumed to be quasi-static. This is because the solutions of interest are predominately mechanical, where the wave velocity is approximately \(10^5\) times slower than that of free-space electromagnetic waves. Under the quasi-static assumption the electric field \(E_i\) is given by the gradient of the potential \(\varphi\):

\[
E_i = -\varphi_j
\]  
(2.23)

The substrate is an insulator, and thus \(D_i\) is given by the charge equation of electrostatics:

\[
D_{i,j} = 0
\]  
(2.24)
For \( x_2 \geq 0 \) the potential is described by Laplace’s equation:

\[
\nabla^2 \varphi = 0 
\]  

(2.25)

In the absence of rotations, equations (2.22) to (2.25) may be combined with (2.10), (2.18) and (2.19) to form:

\[
e_{ijk,l} u_{l,ki} + e_{kij} \varphi_{,ki} = \rho \ddot{u}_j 
\]  

(2.26)

\[
e_{iki} u_{l,ki} - e_{ik} \varphi_{,ki} = 0 
\]  

(2.27)

The solutions to these equations (\( u_i \) and \( \varphi \)) are assumed to be complex travelling waves:

\[
u_i = \beta_i e^{\alpha \omega x_2 / v} e^{j \omega (t - x_1 / v)} 
\]  

(2.28)

\[
\varphi = \beta_4 e^{\alpha \omega x_2 / v} e^{j \omega (t - x_1 / v)} 
\]  

(2.29)

where \( \beta_i \) are unknowns of the linear system and \( \alpha \) is the wave decay into the crystal. An estimated value of \( v \) is assumed at this stage: the aim of the procedure is to find the true value. Substituting equations (2.28) and (2.29) into (2.26) and (2.27) yields a linear homogeneous system in \( \beta_i \). Although full tensor quantities are required to calculate \( v \) when the substrate is biased (see Section 4.5.3), contracted notation will be used here for brevity. The linear system is thus given by:
Another type of ‘pseudo’ wave form occurs due to the separation of variables. In a wide variety of new wave types; a good introduction to the field is given in [47].

Attenuation may be minimised for certain propagation directions, opening up a face waves in that some energy is radiated into the substrate during propagation.

of ‘pseudo’ surface wave behaviour can be investigated. These are not ‘true’ surface waves in that some energy is radiated into the substrate during propagation; such solutions may be real or complex. These particular roots represent waves with amplitudes decreasing with depth (see equation 2.28), fulfilling the surface wave condition; in general four such roots can be found. The admissible eigenvalues \( \alpha \) can then be used to determine the eigenvectors \( \beta \) to a constant factor.

If one or more of the roots with a negative real part is retained, the existence of ‘pseudo’ surface wave behaviour can be investigated. These are not ‘true’ surface waves in that some energy is radiated into the substrate during propagation, leading to attenuation of the surface wave power with distance. However, this attenuation may be minimised for certain propagation directions, opening up a wide variety of new wave types; a good introduction to the field is given in [47].

Another type of ‘pseudo’ wave form occurs due to the separation of variables. In

\[
C \beta = \begin{bmatrix}
  c_{66} \alpha^2 - 2c_{16}j\alpha & c_{62} \alpha^2 - c_{16} & c_{64} \alpha^2 - c_{15} & e_{26} \alpha^2 - e_{11} \\
  -c_{11} + \rho v^2 & -[c_{66} + c_{12}]j\alpha & -[c_{65} + c_{14}]j\alpha & -[e_{16} + e_{21}]j\alpha \\
  c_{26} \alpha^2 - c_{61} & c_{22} \alpha^2 - 2c_{26}j\alpha & c_{24} \alpha^2 - c_{64} & e_{22} \alpha^2 - e_{16} \\
  -[c_{21} + c_{66}]j\alpha & -c_{66} + \rho v^2 & -[c_{25} + c_{64}]j\alpha & -[e_{12} + e_{26}]j\alpha \\
  c_{46} \alpha^2 - c_{51} & c_{42} \alpha^2 - c_{56} & c_{44} \alpha^2 - 2c_{45}j\alpha & e_{44} \alpha^2 - e_{15} \\
  -[c_{41} + c_{56}]j\alpha & -[c_{46} + c_{52}]j\alpha & -c_{55} + \rho v^2 & -[e_{14} + e_{25}]j\alpha \\
  e_{26} \alpha^2 - e_{11} & e_{22} \alpha^2 - e_{16} & e_{24} \alpha^2 - e_{15} & -e_{22} \alpha^2 + 2\varepsilon_{12}j\alpha + \varepsilon_{11} \\
  -[e_{21} + e_{16}]j\alpha & -[e_{26} + e_{12}]j\alpha & -[e_{25} + e_{14}]j\alpha &
\end{bmatrix} \begin{bmatrix}
  \beta_1 \\
  \beta_2 \\
  \beta_3 \\
  \beta_4
\end{bmatrix} = 0
\]

(2.30)

Each element in the \( 4 \times 4 \) coefficient matrix \( C \) is a polynomial in \( \alpha \). The determinant of this matrix must be zero for a non-trivial solution to exist. For the above system the characteristic equation is given by:

\[
A_8 \alpha^8 + jA_7 \alpha^7 + A_6 \alpha^6 + jA_5 \alpha^5 + A_4 \alpha^4 + jA_3 \alpha^3 + A_2 \alpha^2 + jA_1 \alpha + A_0 = 0
\]

(2.31)

where \( A_i \) are real coefficients composed of the material tensor components. In all but the simplest cases these coefficients must be calculated numerically: the procedure will be discussed in Section \[2.3.4\]. Although the equation has eight roots, only those solutions with non-negative real parts are physically admissible for Rayleigh waves; such solutions may be real or complex. These particular roots represent waves with amplitudes decreasing with depth (see equation 2.28), fulfilling the surface wave condition; in general four such roots can be found.
general, all of the elements of $C$ in equation (2.30) are non-zero, thus $u_i$ and $\varphi$ are coupled together. However, for particular propagation directions (e.g., normal to a two-fold axis of symmetry, see Section A.1), the entries in the upper-right and lower left quadrants of $C$ may be zero. This means that $u_1$ and $u_2$ are decoupled from $u_3$ and $\varphi$. The determinant of $C$ is thus given by:

$$
|C| = \begin{vmatrix}
  c_{66}\alpha^2 - 2c_{16}\jmath\alpha & c_{62}\alpha^2 - c_{16} & c_{44}\alpha^2 - 2c_{45}\jmath\alpha & e_{24}\alpha^2 - e_{15} \\
  -c_{11} + \rho \nu^2 & -(c_{66} + c_{12})\jmath\alpha & -c_{55} + \rho \nu^2 & -[e_{14} + e_{25}]\jmath\alpha \\
  c_{26}\alpha^2 - c_{61} & c_{22}\alpha^2 - 2c_{26}\jmath\alpha & e_{24}\alpha^2 - e_{15} & -e_{22}\alpha^2 + 2e_{12}\jmath\alpha \\
  -[c_{21} + c_{66}]\jmath\alpha & -c_{66} + \rho \nu^2 & -[e_{25} + e_{14}]\jmath\alpha & +e_{11}
\end{vmatrix} 
$$

Setting the first sub-determinant to zero to satisfy equation (2.30) produces a Rayleigh wave solution with displacements in the sagittal plane only, and no piezoelectric coupling. By contrast, the second sub-determinant produces a piezoelectrically coupled wave with displacements in $x_3$ only. This is known as a shear-horizontal (or SH) wave, which is analogous to a shear bulk wave in an infinite substrate. Unguided SH waves are known as surface-skimming bulk waves (SSBW) \[48\], and for practical usage some form of energy trapping is necessary to confine the wave energy to the substrate surface. Mass loading using thick layers may be used to produce Love waves \[38\], while the surface of strongly-piezoelectric materials may be shorted in order to produce Bleustein-Gulyaev waves \[49\],[50\]. Yet another method is to use grating structures to produce surface transverse waves (STW) \[51\],[52\], which has become popular for surface wave devices in recent years. An introduction to all of these SH waves types may be found in [40].

For Rayleigh waves, the total mechanical and electrical fields may be expressed as linear combinations of the components described in equations (2.28) and (2.29) with the admissible $\alpha$ values and boundary conditions:

$$
u_i = \sum_{l=1}^{4} B^{(l)} \beta_i^{(l)} e^{\alpha^{(l)} \omega x_3 / \nu} e^{j\omega(t - x_1 / \nu)} \quad (2.33)$$
\[ \varphi = \sum_{l=1}^{4} B_l^{(l)} \beta_4^{(l)} e^{i\alpha_l \omega x_1 / v} e^{j\omega (t - x_1 / v)} \]  

(2.34)

The \( B_l^{(l)} \) terms are scalars known as the partial field amplitudes, and determine the relative ‘weight’ of each wave component in the final wave mode. Analogous equations may be found for ‘pseudo’ SAW.

### 2.3.2 Application of boundary conditions

As the substrate is piezoelectric, both mechanical and electrical boundary conditions must be considered. The substrate surface is assumed to be stress free (i.e., \( T_{2j} = 0 \) at \( x_2 = 0 \)), and thus equation (2.18) reduces to:

\[ T_{2j} = c_{2jkl} u_{l,k} + e_{k2j} \varphi \]  

(2.35)

One of two electrical boundary conditions may be specified, depending on whether a conducting layer is present on the substrate surface. The potential \( \varphi \) must be continuous at the surface in either case, and satisfy equation (2.25) for \( x_2 \geq 0 \). In the absence of a conducting layer, no free charges are present, and \( \varphi \) for \( x_2 \geq 0 \) may be given by [42]:

\[ \varphi = \beta_4 e^{-i \omega / v x_1} e^{j\omega (t - x_1 / v)} \]  

(2.36)

This is known as the free surface electrical boundary condition. In addition, the normal component of electrical displacement (i.e., \( D_2 \)) must be continuous at \( x_2 = 0 \). The displacement within the substrate is described by equation (2.19), while for \( x_2 \geq 0 \) it is a function of the permittivity of free space \( \varepsilon_0 \):

\[ D_2 = -\varepsilon_0 \varphi_2 = \varepsilon_0 \omega / v \varphi \]  

(2.37)

If a conducting layer is present on the substrate surface, the potential is simply given by \( \varphi(x_2 = 0) = 0 \): this is the conducting or metallised boundary condition.

Substitution of equations (2.33) and (2.34) into (2.35) allows the stress boundary conditions to be evaluated. The normal component of electrical displacement in the substrate is given by equations (2.19), (2.33) and (2.34), while the same
quantity for \( x_2 \geq 0 \) is given by equations (2.37) and (2.36): \( D_2 \) is then equated at \( x_2 = 0 \). A set of homogeneous equations for the free surface condition can thus be formed in \( B^{(l)} \):

\[
\begin{bmatrix}
A_1^{(1)} & A_1^{(2)} & A_1^{(3)} & A_1^{(4)} \\
A_2^{(1)} & A_2^{(2)} & A_2^{(3)} & A_2^{(4)} \\
A_3^{(1)} & A_3^{(2)} & A_3^{(3)} & A_3^{(4)} \\
A_4^{(1)} & A_4^{(2)} & A_4^{(3)} & A_4^{(4)}
\end{bmatrix}
\begin{bmatrix}
B^{(1)} \\
B^{(2)} \\
B^{(3)} \\
B^{(4)}
\end{bmatrix} = 0 \tag{2.38}
\]

where the \( i^{th} \) column in the coefficient matrix is given by:

\[
\begin{bmatrix}
A_1^{(i)} \\
A_2^{(i)} \\
A_3^{(i)} \\
A_4^{(i)}
\end{bmatrix} =
\begin{bmatrix}
-je_{61} + \alpha^{(i)} c_{66} & -je_{66} + \alpha^{(i)} c_{62} & -jc_{65} + \alpha^{(i)} c_{64} & -je_{16} + \alpha^{(i)} e_{26} \\
-je_{21} + \alpha^{(i)} c_{26} & -je_{26} + \alpha^{(i)} c_{22} & -jc_{25} + \alpha^{(i)} c_{24} & -je_{12} + \alpha^{(i)} e_{22} \\
-je_{41} + \alpha^{(i)} c_{46} & -je_{46} + \alpha^{(i)} c_{42} & -jc_{45} + \alpha^{(i)} c_{44} & -je_{14} + \alpha^{(i)} e_{44} \\
-je_{21} + \alpha^{(i)} e_{26} & -je_{26} + \alpha^{(i)} e_{22} & -je_{25} + \alpha^{(i)} e_{24} & -e_0
\end{bmatrix}
\begin{bmatrix}
\beta_1^{(i)} \\
\beta_2^{(i)} \\
\beta_3^{(i)} \\
\beta_4^{(i)}
\end{bmatrix} \tag{2.39}
\]

The conducting boundary condition is evaluated using \( A_4^{(i)} = \beta_4^{(i)} \). As before, the determinant of the coefficient matrix in equation (2.38) is determined: this will be minimised by the correct surface wave velocity \( v \) for a given set of \( \alpha^{(i)} \) and boundary conditions. The partial field amplitudes may then be evaluated to a constant factor, forming the complete solution.

If the electrical boundary conditions are not specified, the effective permittivity \( \varepsilon_s \) of a particular substrate orientation may be evaluated [53]. This gives the electrical behaviour at the \( x_2 = 0 \) interface, usually as a function of \( 1/v \). The procedure for calculating \( \varepsilon_s \) is similar to that presented above for \( v \). Although \( \varepsilon_s \) may be used to calculate \( v \), its main value is that all piezoelectrically-coupled waves for a particular orientation which satisfy the mechanical boundary conditions are included in its definition [42], rather than just the Rayleigh modes. This is useful where the wave type (or types) for a particular orientation need to be determined. In addition, \( \varepsilon_s \) is frequently used in the modelling parameters for SAW devices: these are discussed in Section 4.5.
2.3. SURFACE ACOUSTIC WAVES

2.3.3 Displacement and velocity profiles

Given the complexity of the method, and the size of the tensors involved, calculation of \( v \) is usually performed numerically. The procedure outlined above was implemented using MATLAB 6.5 [54] and Mathematica 5.0 [55] software using the following program flow:

1. The initial elastic, dielectric and piezoelectric matrices from published data (see Section A.2) were expanded to their tensor form and rotated to the propagation direction of the SAW (see Section A.3).

2. The coefficients in equation (2.31) were evaluated symbolically using Mathematica before porting to MATLAB. Substituting the rotated tensor values (and an estimated \( v \) value) allowed the admissible \( \alpha^{(l)} \) and corresponding \( \beta^{(l)} \) values to be found.

3. The determinant of the coefficient matrix in equation (2.38) was then evaluated: the magnitude of this should be minimised in order to find the correct SAW velocity [43]. A combination of golden section and parabolic optimisation was used in MATLAB to converge on the correct value of \( v \). The golden section method presumes that the function to be optimised is unimodal (i.e., has a single minimum) within the optimisation interval (i.e., the range of \( v \) values to be checked) [56], and thus the interval size must be carefully chosen. An initial interval was selected based on a known \( v \) for the orientation in question, and the velocity was then calculated for the given material properties. Intervals for subsequent orientations were based on determinant values for velocities about the previous value. This method was found to be robust for small orientation changes. It should be noted that small variations in \( v \) may appear between sources depending on the particular material constant set(s) used (see Section A.2). For certain propagation directions (e.g., where the wave type changes or several wave types exist) there may be many local minima. This problem was solved by quadratically fitting the velocity at these particular angles to surrounding values.

The method not only converges on a value for \( v \) but also gives \( u_i \) and \( \varphi \). Figure 2.4 shows \( |u_i| \) for ST-X quartz (see Section A.3) as functions of depth into
the substrate, which is calculated from equation (2.33). Free surface boundary conditions were assumed, with the $|u_i|$ arbitrarily normalised by $|u_1|$ at $x_2 = 0$, while $t = x_1 = 0$ for simplicity. The substrate penetration is scaled by the SAW wavelength $\lambda$:

$$\lambda = \frac{v}{f}$$

(2.40)

Several important points may be made about the nature of the wave:

- All of the displacement components decrease rapidly with depth into the substrate, demonstrating the surface wave nature. The bulk of the wave energy is concentrated within about a wavelength of the free surface. As will be shown in Section 2.4 this allows for easy access to the wave for
2.3. **SURFACE ACOUSTIC WAVES**

transduction, reflection etc. using a wide variety of electrode structures. By contrast, bulk or volume acoustic wave devices (where waves travel through the entire substrate) are limited to electrodes at just the ends of the propagation path. Figure 2.5 gives a profile of $|\varphi|$ near the free substrate surface, normalised to $|\varphi|$ at $x_2 = 0$, which shows similar surface behaviour.

- The particle trajectory is elliptical, with the major axis in the $x_2$ direction; both $u_2$ and $u_3$ are $\pm \pi/2$ out of phase with $u_1$ at the surface. The $u_1$ component shows interesting behaviour, changing sign near $x_2/\lambda = 0.3$. For a SAW propagating left-to-right, this corresponds to a change in particle trajectory from anti-clockwise to clockwise. The wave motion is probably best explained using animation: some excellent examples are given in [57].

- As mentioned above, there are in general three coupled SAW displacements for a given propagation direction. Some analyses disregard $u_3$, however, as it is usually small relative to the other displacements.

- The magnitudes of the displacement components are related to the wave power. In most SAW devices these components are exceptionally small, typically about six orders of magnitude smaller than the SAW wavelength.

The velocity calculation program can easily be adapted to find $v$ over a range of angles, e.g., to map the velocities for a particular wafer cut. Figure 2.6 shows the velocity of the ST quartz cut as a function of propagation angle; the profile is symmetrical about $180^\circ$ (see Section A.1). Velocities for both the free surface ($v_f$) and conducting ($v_c$) boundary conditions are shown. The plot demonstrates the considerable variation in the SAW velocity with propagation direction. This information is crucial for SAW device design as it can determine the operating frequency of the device (see equation (2.40)). Experimental measurements with evaporated metal films show excellent agreement with the theoretical approach [58], provided that accurate material constants are available.

The crystal structure of the substrate determines not only the SAW velocity but also the direction of the power flow vector. In isotropic materials, the velocity and power flow vectors are parallel, i.e., the wave power propagates in the same direction as the phase velocity. For anisotropic materials, however, the power flow
vector can be rotated towards a symmetry direction of the substrate, a condition known as beam steering [59],[42]. The power flow angle (the angle between the phase velocity and power flow vectors) is given by the slope of the velocity curve. A related effect is the beam diffraction, whereby the SAW wavefront spreads and distorts as it propagates. There is a tradeoff between beam steering and diffraction [60], the implications of which will be discussed in Section 3.3.5.

Another key feature of note is the difference between $v_f$ and $v_c$. The electromechanical coupling coefficient for SAW propagation ($K^2$) is estimated by [40]:

$$K^2 \approx \frac{2(v_f - v_c)}{v_f}$$  \hspace{1cm} (2.41)
2.4. **SAW DEVICE ELEMENTS**

The sections above describe only the propagation of SAW on a free surface, without any reference to how they are generated or received. This section describes the ‘building blocks’ used in SAW devices to harness the useful properties of the waves. Key tasks include wave generation, manipulation for a given signal and is plotted in Figure 2.6. This coefficient determines the magnitude of the piezoelectric coupling in a propagating SAW; other definitions are used for other piezoelectric applications [32]. The ST-cut of quartz demonstrates maximum coupling at 0° and c. 35°, and is classed as a weakly-piezoelectric material due to its small coupling. An analysis of different material types in terms of device performance will be given in Section 3.3.2.

**2.4 SAW device elements**

Figure 2.6: SAW velocity as function of propagation angle

SAW Velocity Profile for ST Quartz

![Graph showing SAW Velocity Profile for ST Quartz](image_url)
processing or sensor application and transduction to an output form. Although
many different types of SAW device element exist, this section only covers the
two most common ones: the interdigital transducer and reflector structures. Ba-
sic modelling concepts will be introduced to outline their operation, with more
detailed coverage in Chapter 4.

\subsection{Interdigital transducer}

The most important element in almost every modern SAW device is the interdi-
gital transducer (IDT). It is the main structure used both to generate and receive
surface waves, and in many cases is integral to the signal processing behaviour
of the device. Many different types of structure may be used to generate surface
waves, and a review of early developments may be found in [37]. However, the in-
introduction of the IDT by White and Voltmer in 1965 [61] allowed practical devices to become a reality, combining efficiency, flexibility and easy planar fabrication.

Fig. 2.8 shows a single-electrode IDT used to generate surface waves [42]. The structure consists of two sets of thin-film electrodes deposited onto the piezoelectric substrate and connected alternately to busbars. The electrodes have a physical periodicity $p$ and an aperture (SAW beam width) $W$. The metallisation ratio $\eta$ (the fraction of $p$ which is metallised) in this case is 0.5, i.e., lines and spaces in the IDT are of equal width; this is the most common layout found in SAW devices. A basic simulation method known as the delta-function model [62] is used here to demonstrate how the device operates. Several assumptions are made in this model:

- The electrodes are massless and do not perturb the transmission of surface waves.
- Gaps between the electrodes are treated as localised, independent sources
or receivers.

- The wave amplitude is proportional to the SAW potential $\phi$.

In the upper part of the figure, the IDT is shown in generation mode, with an alternating voltage $V$ applied between the busbars. The electrical field between adjacent electrodes expands and contracts the substrate surface by the converse piezoelectric effect, thus launching surface waves (shown as broken and solid lines). This IDT is a bidirectional device, and thus waves are launched in both directions. Summing the contributions from each wave source, it may be shown that the magnitude of the frequency response of a device with $M$ sources is proportional to:

$$|A(\omega)| = \left| \frac{\sin M\theta/2}{\sin \theta/2} \right|$$

(2.42)

where $\theta = \omega p/v - \pi$. Defining $\omega_c$ as the centre frequency at which $2p = \lambda$ produces $\omega_c = \pi v/p$ (from equation (2.40)) and thus $\theta = \pi(\omega - \omega_c)/\omega_c$. Figure 2.9 plots this frequency response, with peaks occurring at the fundamental $\omega_c$ and odd harmonics. This is a key finding, as it shows that the maximum frequency response is directly related to the periodicity of the electrodes, i.e., $f_c = v/2p$, in the absence of reflections and other perturbations. Multiple electrodes, rather than a few highly-powered ones, are used to minimise the generation of bulk acoustic waves and to determine the bandwidth of the structure.

In the reception mode (the lower part of Figure 2.8), surface waves are incident on the structure. The IDT sections are now taken to be shorted, acting as generators to convert the mechanical wave energy into current $I$ by the direct piezoelectric effect. Using the same arguments as the generation case, it may be shown that the magnitude of the frequency response (i.e., the magnitude of $I$ as a function of frequency) is of the same form as equation (2.42). Thus the device can act both as a generator and a receiver, giving it great flexibility for signal processing tasks.

In light of their importance in SAW devices, IDTs have been developed in a multitude of different forms. Apodised structures [62] were developed whereby the electrode overlap in the IDT (i.e., $W$) varies with position (see Figure 2.10).
2.4. SAW DEVICE ELEMENTS

Figure 2.9: Frequency response of interdigital transducer with M=10

Figure 2.10: Example of an apodised IDT showing the change in SAW aperture W with position
This uses the fact that the frequency response of the device is given by the Fourier transform of its time response, which in turn is given by the electrode layout. The desired frequency response can thus be transformed and directly implemented in the electrode design. Multi-finger IDTs, where several electrodes are used per wavelength, may be used for diffraction compensation, reflection minimisation and for utilising harmonic modes\cite{40}. Unidirectional IDTs, where the SAW propagates from one side of the device only, are increasingly common in modern filter devices: the most common of these is the single-phase unidirectional transducer (SPUDT)\cite{63}. Several other variations exist, including devices with weighted, slanted and multi-layer electrodes. Apart from SAW work, IDTs are used in many different types of sensors and transducers; a review may be found in\cite{64}.

### 2.4.2 Reflectors

In the previous section it was presumed that the electrodes were effectively ideal probes on the substrate surface, electrically but not mechanically loading the material. Real electrodes, by contrast, have finite mass and conductivity. These properties create discontinuities on the substrate surface, leading to reflected waves and dispersive behaviour. Four main reflection mechanisms may be considered\cite{40}:

1. **Piezoelectric shorting**: as shown in Figure 2.6 shorting the SAW’s electrical field reduces the wave velocity, and this discontinuity leads to reflections.

2. **Geometric discontinuity**: in common with bulk acoustic waves, geometric changes in the propagation path lead to SAW reflections. Such changes include deposited electrodes, conducting layers, substrate grooves etc.

3. **Electrical regeneration**: surface waves incident on an electrode structure can induce time-varying voltages across the electrodes, causing regenerated SAW to propagate back towards the incident waves.

4. **Mass loading**: the different densities and elastic properties of the deposited electrodes can cause SAW propagation discontinuities.
2.4. SAW DEVICE ELEMENTS

Figure 2.11: Reflector elements consisting of grooves (top), open metal strips (middle) and shorted metal strips (bottom)

The relative magnitude and phase of each mechanism depends on the substrate and material cut: this will be explored in Section 4.5.4. Reflections may occur in IDTs (which may be a positive or negative effect depending on the device) or in structures specifically designed as reflectors, where the aim is to maximise the in-phase reflection of the incident waves. Figure 2.11 depicts some typical reflector structures: designs for several others may be found in [65]. As with the IDT, reflectors use multiple elements (up to several hundred in a single reflective grating) to minimise scattering into bulk waves and to set the structure’s bandwidth. Most reflectors to date have used linear electrodes or grooves, though reflective dots have also been investigated [66].
CHAPTER 2. SURFACE ACOUSTIC WAVES: THEORY AND DEVICES

2.5 Types of SAW device

Before detailing two typical types of SAW device, it is instructive to look at their place in the electronics market. Over the past 30 years the dominant market for SAW devices has been in communications, primarily in filter, oscillator and delay line modules. In recent times, the explosion of mobile and wireless communications has fuelled production, with industry revenues of $1.35 billion in 2001 and predicted revenues of $2.1 billion in 2007 [67]. This equates to the production of several hundred million SAW devices per year [40]. There are a number of reasons why these devices are so widespread:

- **One-chip filtering**: a SAW device can perform complex filtering tasks using a single substrate and an appropriate electrode layout, and thus can be packaged as a single component. For example, a typical Epcos mobile phone 2-in-1 filter (for dualband operation over different networks) has a footprint of 2.5x2mm [68], far smaller than equivalent solutions using discrete components.

- **Outstanding frequency response and stability**: SAW filters can have responses equivalent to LC circuits with several hundred inductors and capacitors. Insertion loss (i.e., the decrease in transmitted power relative to the input power caused by the filter) in the passband is typically low: the Epcos device mentioned above has less than 3dB loss. They also display excellent ageing characteristics, allowing their use in demanding applications like satellite communications.

- **Rugged packaging**: SAW devices can be designed with low temperature dependencies, and use rugged packages for mobile phones and other wireless devices.

- **Low cost**: existing semiconductor fabrication techniques can be used (see Chapter 3), typically with less than four layers, and thus production costs are minimised.

In terms of device structure, the elements described in the previous section can be combined in many different ways to build complete components. The
2.5. TYPES OF SAW DEVICE

following sections detail the two most common types: delay lines and resonators.

2.5.1 Delay line

Delay lines are probably the simplest form of SAW device, consisting of at least one IDT and a relatively long propagation path. White and Voltmer [61] detailed the original design whereby an input signal $V_{in}$ was applied to one IDT, transduced to a SAW and then re-transduced to an output signal $V_{out}$ by an identical IDT displaced by $x = v \tau$ along the propagation path (see Figure 2.12). The device filters signals outside of the IDT bandwidth, and delays the signal by $\tau$. As mentioned previously, different types of IDT (most notably those using apodisation) can perform more complex signal processing tasks. Unidirectional IDTs are very useful in these devices as all of the wave power can be utilised. In most of these designs the IDTs are designed to be nonreflective, as reflected waves give rise to spurious responses.

Another delay line type uses a single IDT and several reflective strips (see Figure 2.13). A burst signal of short duration is applied to the IDT, causing a SAW to propagate. The wave is then reflected by reflectors placed at arbitrary positions along the propagation path. These reflected SAW are then converted back to electrical signals in the IDT, giving a ‘train’ of pulses corresponding to each reflector position. Such designs can be used in radio frequency identification (RFID) and sensor applications, where the reflector layout identifies the device and the time delay changes with the measurand: this will be discussed in Section 3.2.1.
Many other delay line variations exist, including dispersive or chirped devices \[69\] which can be used for pulse compression, and multiple delay lines where several devices are connected in series or parallel.

### 2.5.2 Resonator

SAW resonators (SAWRs) use reflective structures to contain the wave energy within a resonance cavity. While delay lines use propagating SAW, resonators use standing waves to maximise energy storage at a particular range of frequencies. The first work in this field was performed by Ash in 1970 \[70\], and a review of early work can be found in \[71\]. One or more IDTs are used to generate surface waves, which are then reflected back to the source. In contrast to the reflective delay line mentioned above, the SAW resonator uses strongly reflective structures: typically over 95% of the incident wave energy is reflected. Figure 2.14 depicts a one-port SAW resonator, where one IDT is used for both input and output. Resonators are widely used in oscillator components and as filters.

As with delay lines, a vast range of resonator designs exist for different ap-
2.6. CONCLUSION

In this chapter, the basics of surface wave theory and devices were examined. It is clear that SAW devices incorporate work from many different fields (elasticity, piezoelectricity, wave propagation etc.), and a unified treatment of these areas was presented. The variety of effects found in SAW devices makes them a rich research topic, particularly those devices implemented as sensors.

In the next chapter, the ideas introduced in this chapter will be expanded to the design and manufacture of SAW strain sensors.

applications: a short overview is given in [72]. Modern devices often use cascaded resonators as impedance elements, which can offer improved performance over single devices. A more detailed analysis of their use as sensors will be given in Section 3.2.1.
Chapter 3

Design and Manufacture of SAW Sensors

A key aspect of the project is the design and manufacture of prototype sensors for experimental testing. In this chapter, possible sources for SAW sensors are first evaluated. The sensor specifications are then outlined, along with the desired device characteristics. Implementation of surface wave devices as strain sensors is then introduced, followed by a new integrated design and manufacturing process for SAW sensors. The various steps in the integrated process are then outlined, along with the fabrication procedure and physical characteristics of the finished devices.

3.1 Sources of SAW devices

The most obvious issue at the start of this project was the sourcing of SAW devices for testing as strain sensors. This project is a new venture, and thus no previously-fabricated SAW devices were available for test. Similarly, no design expertise could be called upon within the research group. With this in mind, it was decided to evaluate the sources of ‘ready made’ SAW devices for their suitability in this project. The next two sections detail two such possible sources.
3.1.1 SAW sensor systems

Although SAW sensors are an emerging area, very few ‘off the shelf’ measurement systems are available. To the author’s knowledge, no dedicated SAW strain sensors are commercially available. Two related measurement areas have active commercial work:

- **Torque**: a torque measurement system called TorqSense is now available for torque sensing on shafts [73]. Figure 3.1 shows a typical system layout, with a SAW sensor placed in each of the principal strain directions. When a torque is applied to the shaft, one sensor is strained by $S_{11}$ while the other is strained by $-S_{11}$. RF couplers are used to wirelessly interrogate the sensors, and the signal is processed to give a torque measurement. This is a good demonstration of passive, wireless SAW sensing, and the technology allows torque measurement to be performed in a production environment. Similar devices have been developed by Transense Technologies [74],[15] (see Figure 3.2).

- **Pressure**: another SAW sensor application is the measurement of pressure, particularly in vehicle tyres. Safety concerns due to incorrectly inflated tyres have led to the development of wireless pressure sensors which can be installed in each tyre [75]. SAW sensors are emerging as an excellent solution to this problem. Figure 3.3 shows a tyre pressure measurement system, again developed by Transense Technologies, which can be integrated into a tyre valve. The top of the sensor package acts as a membrane, and as this deflects with pressure the simply-supported SAW devices underneath also deflect. This strains the SAW propagation surface, thus enabling pressure readings to be taken. As the figure shows, three devices are utilised in each sensor: this is used for temperature compensation.

The examples above use technology based on proprietary information, and thus many of the design and implementation details are unavailable. This is undesirable in a research project, as it merely allows the evaluation of existing technology rather than an understanding of the fundamental processes involved. The systems are also designed to be application-specific, e.g., the signal processing
algorithms used in the TorqSense system are designed for measuring torque rather than strain. While they provide some excellent information on sensor design, it was felt that neither of the above systems were suitable for this project.

3.1.2 Adaptation of SAW communications devices

As dedicated SAW sensor systems were unsuitable for this project, another option was to use adaptations of existing SAW communications devices. As will be discussed in Section 3.2.1, SAW strain sensors are fundamentally the same as SAW filter devices, and thus ‘reverse engineering’ of existing devices was considered. Figure 3.4 shows the die area of a typical 1-port SAW resonator after the package cover was removed. The bright areas are the electrode structures, which have a protective layer over the active SAW portions. While the device has the strong advantage of a proven design, there are a number of serious disadvantages. A key
CHAPTER 3. DESIGN AND MANUFACTURE OF SAW SENSORS

Figure 3.2: Transense torque measurement system with (inset) torque sensor (adapted from [74])

Figure 3.3: Transense pressure measurement system with (inset) pressure sensor (adapted from [74])
3.1. SOURCES OF SAW DEVICES

Problem to applying these devices as prototype sensors is their very advantage as filters – their small size. The die in the figure is approximately $2.8 \times 1.7$ mm, which is too small for practical manual handling. In an experimental testing scenario, the small size of the bond pads (the wiring connection areas) would make it extremely difficult to connect the device to an external circuit, especially in the absence of wire bonding machines. Validation as a strain sensor would also be difficult, with significant mounting errors (e.g., alignment errors, poor adhesion control etc.) due to the small substrate area. The die is mounted on a flexible carrier material to minimise die loading, and removing this without damaging the die would be challenging. A final disadvantage is the same barrier to proprietary information found in SAW sensor systems.

An alternative sourcing route is to have a custom-designed SAW sensor manufactured by a SAW device manufacturer. Traditionally, a client who requires a custom-designed SAW device (e.g. for a new communications application) specifies a number of important parameters (e.g. operating frequency, stopband rejection etc.) required of the device to the SAW manufacturer, who then produces a
prototype wafer of devices. These experimental devices are usually adapted from existing designs, and are tested to select the best candidate for production. While successful for mainstream SAW devices (which are produced in bulk and used for electronic applications), there are two major disadvantages for SAW sensor research:

1. *Cost of development*: the cost of a design run, which may have to be iterated as specifications change, is prohibitive for a university research project. The development approach is optimised for high volume, low diversity commercial products rather than the low volume, high diversity devices required for testing. Prototyping costs are excessive given the small production volumes used for research purposes.

2. *Separation of design and manufacture*: for research purposes it is essential that each stage of the project is ‘visible’, i.e., that the processes used can be easily examined. This is especially true of this project, as both the electrical and mechanical characteristics of the SAW sensors need to be considered. Mainstream SAW manufacturers use different proprietary techniques to fine-tune device performance, effectively separating the design and manufacturing processes.

In light of these disadvantages, it was decided to design and manufacture the sensors within a university environment: this will be documented in Section 3.3. Before any design or manufacture was performed, however, the specifications of the final sensors were required.

### 3.2 Specification of sensors

In specifying the SAW sensor, the major objective is to describe a device which will fulfil the strain sensing aspect of the RTWIM system, i.e., a device which will act as a module of a cohesive system. A successful SAW sensor must act both as a wireless, passive device (conforming to industry standards, existing equipment etc.) and as a strain sensor (with comparable performance to conventional strain gauges). This modular approach means that, for example, possible interrogation
systems for the sensors need to be considered even though they are not part of this project. The following sections detail how SAW devices can be implemented as strain sensors, and the desirable characteristics of such devices.

### 3.2.1 SAW devices as strain sensors

In most electronics applications, the SAW device is enclosed in a protective package, so that only the desired electrical signals can affect SAW propagation. Figure 3.5 shows a modern SAW package which is designed to protect and isolate the device from environmental effects [76]. However, if the substrate is exposed to external influences (e.g., mechanical, chemical etc.), the SAW device can act as a sensor. The application of SAW devices as sensors began in the early 1970s, prompted by the need to identify sources of device instability; early developments are reviewed in [77]. Pressure sensors based on SAW oscillators were first discussed in 1974 [78], [79], and chemical sensors were also introduced [80]. In the following years, SAW chemical sensors developed relatively quickly as commercial products (especially for laboratory environments) and are now used in a variety of applications [81]. By contrast, research on mechanical SAW sensors was limited during the 1980s and early 1990s, with just a few papers dealing with propagation effects. A probable reason for this is that many chemical applications require the high resolution provided by SAW sensors (e.g., to detect concentrations in the parts per billion range) while conventional mechanical sensors were sufficient for most applications. The emergence of wireless devices brought SAW sensors to the forefront again, especially those that could be operated passively. A recent development has been the reduction in cost of interrogation equipment [82], which should make the technology more attractive for mainstream applications.

As the examples in the previous sections demonstrate, SAW mechanical sensors do not appear to be displacing existing sensor types but are instead opening up new measurement applications.

In this project, it is envisaged that the SAW device will be strain-sensitive. As the propagation path of the SAW deforms due to the applied strain on the substrate, the properties of the device (e.g., operating frequency, time delay, phase, amplitude etc.) will be altered. Comparing the altered wave with a nominal reference state
allows the device strain to be inferred. The treatment here presumes that the SAW devices are passive and wireless, but the same techniques apply to wired sensors.

The SAW delay line introduced in Section 2.5.1 can be implemented as a strain sensor. Figure 3.6 shows such a reflective DL with its interrogation and response signals [83]. The device is the same as that shown in Figure 2.13 except that an antenna rather than a voltage supply is connected to the IDT. An RF burst interrogation signal is transmitted from an interrogation unit: the bandwidth of this signal is centred on the nominal centre frequency of the IDT. The signal is transduced to a SAW which reflects from the isolated reflectors in the usual manner. These reflected SAW are transduced to RF signals in the IDT and broadcast by the antenna. The device response thus consists of attenuated, time-delayed versions of the interrogation signal. If a uniaxial strain state $S_{11}$ (for simplicity) is applied in the direction of SAW propagation, both the dimensions of the electrode structures and the propagation properties of the substrate will change. For example, a tensile strain will widen the electrodes, thus lowering the centre frequency of the IDT and increasing the delay between the reflected SAW pulses; the SAW velocity will also change (see Section 4.5.3). Usually only the change in the delay times from a reference state are used for measurements, though frequency domain
3.2. **SPECIFICATION OF SENSORS**

Methods may also be used [84]. The number, nominal position and nominal delay associated with each reflector must be known to reference the measurements and to identify each device.

An alternative technique is to use a conventional resistive strain sensor with the simple delay line shown in Figure 2.12. These impedance-loaded delay lines [85] have the conventional sensor connected to the output IDT, and may be interrogated in the same way as reflective delay line sensors. Changes in the sensor’s impedance change the reflectivity of the output IDT, and thus the effect of the measurand can be indirectly sensed. This type of sensor is more flexible than ‘pure’ delay lines as a wide variety of impedance-based sensors can be used [86].
particularly those using capacitive effects, but its sensitivity is generally lower.

The SAW resonator structure introduced in Section 2.5.2 can also be used as a strain sensor (see Figure 3.7). An interrogation signal is emitted by the interrogation unit, with the frequency sweep centred on the nominal resonant frequency of the device. The signal is received by the antenna on the IDT, and transduced to surface waves. Although all interrogation frequencies are received by the device, the sensor only resonates at a narrow range of frequencies corresponding to the electrode configuration and the propagation properties of the substrate [40]. Once the interrogation signal is switched off, the energy stored as standing SAW is reconverted to RF signals which are transmitted by the antenna. If the device is submitted to a uniaxial strain as above, the resonant frequency will shift, and by comparing the new resonant frequency with a nominal reference state the strain can be inferred.

The relative merits of each SAW sensor type for this project will be discussed in Section 3.3.1.

3.2.2 Desired device characteristics

The correct choice of SAW device is crucial to the success of the RTWIM project. The chosen device should provide a ‘best-fit’ to the project requirements as will be outlined in Section 3.3.1. Similarly, the detail design of the sensor device should ensure that the desirable attributes are maximised, while possible disadvantages are minimised.

It is envisaged that the ideal SAW device will be passive, wireless, uniquely identifiable and strain-sensitive. Desirable characteristics of a general strain sensor are [3]:

1. Precise measurement of strain under static and dynamic conditions.
2. Small size (for use in confined spaces and high stress gradients) and weight (to reduce inertial effects).
3. Remote observation and recording.
4. Independence from temperature.
Figure 3.7: Sketch of resonator interrogation and response signals
5. Easy installation.


7. Linear response to strain.

8. Low cost.

9. Reliability.

10. Single or multiple sensors using one interrogation system.

In addition, the RTWIM sensors have additional constraints which must be considered:

- The devices are passive, and thus they must operate efficiently in order to return the maximum signal power. A link budget is given in [14] which shows how the SNR degrades in a wireless SAW application through different loss mechanisms. The SAW device insertion loss is a major factor (20dB attenuation in this particular case), and should be minimised wherever possible. It should be noted that the insertion loss is dependent on the antenna-sensor matching as well as the performance of the sensor itself, and both need to be considered in a wireless application.

- The sensors must operate within a defined bandwidth. Strain sensitivity must be such that the measurand can be detected over the operating range, without interfering with the responses from other sensors.

- The RF channel is guaranteed to be noisy, with interference from the vehicle and from other devices in the frequency band. This could lead to problems with the discrimination of individual sensors, even if each has a defined bandwidth, as noise sources could be interpreted as sensor responses.

- The multiple sensors will be distributed around the vehicle, and thus will have different signal paths, lines-of-sight etc. The position of the sensor should not affect the resolution of the measurement.
Therefore, the chosen device type for the project will have the best combination of:

- High efficiency
- Narrow operating bandwidth for use in a multi-sensor environment
- Clearly defined signal response to reduce channel problems caused by noise or sensor positioning

3.2.3 Sensor packaging

The packaging of a sensor can have a major impact on its performance. There are two major packaging issues with SAW strain sensors:

1. For device-sized packaging (where the package is approximately the same size as the substrate), no package connection to the back face of the substrate is desirable, and thus standard packages (see Figure 3.5) cannot be used. This is because the back face should be directly bonded to the component under test. Conventional foil resistive strain gauges have a plastic film between the electrode pattern and the component, but this requires than the whole device be encased. For SAW devices, this causes additional problems, as will be described below. SAW pressure sensors are easier to package as the substrates usually fit inside a membrane structure, and can be sealed like a normal SAW device. It is interesting to note that the torque measurement solutions (see Figure 3.2) use packages which are much larger than the substrate, even though this may distort the strain field around the device.

2. The wave propagation surface of the sensor should be protected from dirt and foreign matter. Any dirt deposited on the surface will attenuate the SAW, and larger particles may cause spurious reflections. The most serious issue, however, is that a conducting particle could short the IDT and stop the sensor from operating. This problem is compounded by the fact that the surface should be mechanically free so that surface waves can propagate. Deposited layers on the propagating face can change the surface wave
mode (see Section 2.3) or lead to excessive attenuation due to mass loading effects. Some passivation processes have been introduced to make SAW devices more resilient to surface contamination. The substrate in Figures 3.4 and 3.5 has a polymer ‘hood’ defined during the fabrication process which protects the propagation area [76]: this technology is proprietary, however. Other schemes have involved the deposition of Al₂O₃ layers to improve yield during manufacturing [87]. However, it appears that the natural oxidation of Al SAW electrodes can introduce a ‘natural’ passivation, effective even when iron filings are deposited on the device [88].

For this project it was decided to test only ‘bare’ die, i.e., unpackaged substrates. In the longer term, using directly-bonded wafers (probably with micromachined cavities) looks to be a promising packaging solution [89], but developing such a package is a research project in itself. Passivation layers are not part of the core manufacturing process, but can be applied at a later stage if required.

### 3.3 Integrated design and manufacture

In light of the disadvantages of existing SAW measurement systems, it was decided to implement a new integrated design and manufacturing system for this project [90], which will allow the devices to be fabricated in a university research environment. Figure 3.8 shows a flowchart for the system. At each stage of the process, the different (and sometimes conflicting) requirements of design and manufacturing must be considered. This coordinated approach is designed to reduce production problems, as the sensors have effectively been ‘designed for manufacture’. Production costs are significantly reduced as the devices can be produced in small microelectronics laboratories, and at every stage the effect of design decisions on production can be examined.

The process is designed to transform SAW sensor specifications into production equipment for device manufacture. Surprisingly little information is available in the literature on the design process used for SAW devices, i.e., a framework for the design of successful components. Some production-related projects are outlined in [91] and [92], but these concentrate on improving device yield rather than
3.3. INTEGRATED DESIGN AND MANUFACTURE

**SAW Sensor Specifications**

- *Literature review*
- *Existing devices*
- *Interrogation systems*

- *Surface wave type*
- *Piezoelectric coupling*
- *Temp. dependence*

- *No. of individual sensors*
- *Frequency separation*

- *Electrode layout*
  - *Die sizes*
  - *Multiple designs*

- *Variable parameters*
  - *Large results set*

**Design**

- SAW device type selection

**Manufacturing**

- Selection of substrate (material and cut)

- *Available wafers*
- *Cost per wafer*

- *Available frequency bands*
- *Photomask resolution*

- *Sized for handling*
- *Dicing considerations*

- *No. of samples per design*
- *Alignment tolerance*

- Photomask design and production

- Device fabrication (photolithography, sputtering and dicing)

- SAW Sensors for Testing

*Literature review*
*Existing devices*
*Interrogation systems*
*Surface wave type*
*Piezoelectric coupling*
*Temp. dependence*
*No. of individual sensors*
*Frequency separation*
*Electrode layout*
*Die sizes*
*Multiple designs*
*Variable parameters*
*Large results set*
*Equipment availability*
*Production feasibility*
*Available wafers*
*Cost per wafer*
*Available frequency bands*
*Photomask resolution*
*Sized for handling*
*Dicing considerations*
*No. of samples per design*
*Alignment tolerance*

Figure 3.8: Flowchart for integrated design and manufacturing process
design. As noted in [81], SAW device design is a complex task, and often relies on commercial software using proprietary techniques. General books on SAW devices such as [42], [40] and [93] all give excellent information on the general operation of the devices, but case studies using actual design decisions are very rare. This is compounded by the ‘Catch 22’ situation where device parameters for design are based on experimental measurements, which require tested components. In addition, no in-house fabrication expertise was available for devices of this scale. The integrated system is designed to address all of these issues, providing a methodical framework for design and manufacture. Advanced IC design now commonly integrates design and manufacture to improve performance and yield, where previously most of the design would be finalised before the fabrication was considered. While the driver in IC components is reliable performance and increased yield using small feature sizes, the same integrated approach can be used to improve research projects.

The following sections detail each part of the integrated process.

### 3.3.1 Selection of SAW device

The first task is to choose the most suitable SAW device type for sensor development. It was decided to use a ‘pure’ SAW sensor rather than combine a SAW device with a conventional sensor (as mentioned in Section 3.2.1): this is to maximise the sensitivity of the final device. The choice was therefore between delay line and resonator solutions.

There appears to be only one paper that directly compares SAW resonators and delay lines for sensor applications [94]. This deals with gas sensors, and uses SAW devices in active, wired oscillator circuits rather than in a passive, wireless system as is proposed here. The basic findings indicate that a resonant sensor has a lower attenuation and higher sensitivity than an equivalent delay line, but the limited results make it difficult to demonstrate this conclusively. Seifert et al., [95] qualitatively compare the different types of wireless SAW sensors from a number of independent studies, but their paper does not include experimental results. However, they note that SAWRs have lower insertion losses than ordinary delay lines, confirming the results in [94].
Both types of SAW device fulfil most of the criteria for a general strain sensor outlined in Section 3.2.2. Strain resolution is c. 1% of full scale [86], while typical device footprints are <10mm². Wireless interrogation ensures remote observation and relatively easy installation. Most of the other requirements can be achieved through careful choice of substrate materials, or by using dummy devices to remove RF channel and temperature effects.

There are a wide variety of papers which describe applications of passive, wireless SAW sensors, but the results cannot in general be compared across studies. For example, little or no information is given about the RF channel (i.e. sensor-interrogator distance, noise sources, line-of-sight etc.), and thus details of sensor responses only characterise the particular sensors in the system, rather than the measurement method as a whole. Some useful work has, however, been performed on the modelling and testing of various interrogation approaches. An overview of methods for different sensor types is given in [96], while the accuracy of wireless SAW temperature sensors using different signal models is evaluated in [97]. The performance of differential phase measurement is detailed in [98], while receiver noise issues are discussed in [99].

The desired device characteristics from Section 3.2.2 were analysed, and the following factors were deemed to be the most important in the selection process:

- **Interrogation of multiple sensors**: for multi-sensor wireless systems it is essential that each sensor be uniquely identifiable. For delay line devices the layout of the isolated reflectors gives the sensor’s signature. A huge number of devices may be discriminated: modern designs for SAW RFID tags provide for 256 bit identifiers [100], and similar capabilities could be expected of sensors. Resonators rely on different electrode widths to provide different resonance frequencies. This requires close control of electrode dimensions, which is challenging for high frequency devices. In both cases, providing a unique response from a passive device requires a physically unique layout.

- **Narrowband operation**: the operating frequencies of the SAW sensors are constrained by the available fabrication equipment and by European frequency regulations (e.g. [101]). Wireless SAW sensor systems are treated as low power devices (LPDs) because although the sensors themselves may be
passive, a broadcasting unit is required for interrogation. In order to avoid problems with licensing bandwidth, it is useful to use unlicensed parts of the spectrum. In Europe, two suitable unlicensed bands (the Industrial, Medical and Scientific (ISM) bands) are available, starting at 433MHz and 2.4GHz. The upper band is popular with low power wireless networks (Bluetooth, IEEE 802.11 (WiFi) etc.) and has a relatively wide bandwidth of 83MHz. For SAW devices on quartz this equates to electrode linewidths of about 330nm. However, the main piece of fabrication equipment available (a Karl Süss MJB3 UV400 mask aligner, see Section 3.4.3) can nominally only resolve features down to 600nm \[102\]: in practice the working resolution is over 1\(\mu\)m. Therefore, the lower ISM band of 433.05-434.79MHz was selected for the sensors, which commonly requires linewidths in the 1.8\(\mu\)m range. All of the sensors should be interrogable within a 1.74MHz bandwidth, which is very narrow when many sensors are to be considered. SAW resonators are preferable in this respect as they use a much narrower bandwidth than delay lines. An added advantage is that SAWR devices can use narrowband receivers, which pick up less noise than the broadband receivers used with delay lines \[15\].

- **Low attenuation**: delay line systems typically have an extra insertion loss of 10-20dB compared to resonator systems \[15\]. This means that SAWR systems return more of the applied interrogation signal power to the receiver, allowing for lower interrogation power, reduced receiver sensitivity, or both.

- **Cheap interrogation system**: delay line solutions typically require interrogation systems with fast sampling rates and powerful signal processing. While these are readily available in laboratories, the high cost of the systems precludes their use in RTWIM. By contrast, resonator-based solutions can utilise slower frequency sweeps and sampling rates systems with slower sampling rates, or alternative solutions like gated phase-locked loops \[103\]. While ordinary PLL systems can only lock to a single reference, software-synthesised PLL systems allow multiple references to be set \[104\], possibly enabling the interrogation of multiple sensors.
• **Smaller die size:** the quality factor of a SAW device, $Q$, may be defined as the ratio of stored energy in the device to the energy dissipated per cycle [40]. This quantity is an important measure of the stability of the device, and should be maximised for sensors. For a comparable quality factor, a delay line must be several time longer than a resonator, thus increasing die size and cost [15]. Although delay lines are flexible in that the wave paths can be overlapped, the smaller size of the resonator makes this advantage marginal at best.

• **Previous successful implementations:** applications of SAW devices to measure strain [105] and torque [15] have both used SAWR systems. The success of these projects, both closely related to the RTWIM concept, indicated that a resonator solution would be preferable.

From a manufacturing perspective, both delay lines and resonators use the same fabrication technology, and linewidth control in both is of paramount importance.

The proposed delay line and resonator solutions were compared under the above headings, and it was decided to design the sensors as SAW resonators. As was shown above, SAW resonators are well suited to the RTWIM application, in most cases providing superior performance to delay line solutions. It should be stressed, however, that the choice of sensor strongly depends on the application, and delay lines may be preferable for other wireless sensing systems. Although 2-port SAWR have been successfully used as strain sensors in the past [105],[106], a 1-port design was selected to reduce the interrogation requirements [15] and to provide a simpler design.

### 3.3.2 Substrate selection

The piezoelectric substrate has a key role in the performance of the sensor. From the discussion in Section 2.2 it would appear that piezoelectric ceramics would offer a good solution, given that their performance can be optimised for a particular application. Deposited thin-film piezoelectric films (e.g. ZnO and AIN) have been used to implement SAW devices on non-piezoelectric substrates [107].
CHAPTER 3. DESIGN AND MANUFACTURE OF SAW SENSORS

<table>
<thead>
<tr>
<th>Material</th>
<th>Cut</th>
<th>SAW Axis</th>
<th>$v$</th>
<th>$K^2$ (%)</th>
<th>$\alpha_T$</th>
</tr>
</thead>
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<td>X</td>
<td>3159</td>
<td>0.18</td>
<td>-24</td>
</tr>
<tr>
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<td>75</td>
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<td>Z'</td>
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<td>0.72</td>
<td>35</td>
</tr>
</tbody>
</table>

Table 3.1: Properties of piezoelectric substrate materials

but their use has been restricted to comparatively low frequencies (up to about 100MHz). This is because acoustic propagation losses in these materials become large at high frequencies, mainly due to wave scattering at grain boundaries [41], which is a problem for passive, wireless sensors. Therefore piezoelectric single crystals must be used.

Many different substrates have been used in experimental SAW devices, but relatively few materials are used in commercial components. The choice of material and cut is firstly determined by the required type of surface wave. Classical Rayleigh waves, rather than the ‘pseudo’ SAW types mentioned in Section 2.3.1 were chosen in this study as they have been widely analysed and provide a good basis for the study of strain effects. Table 3.1 lists the main materials in common use for surface wave devices [40],[42] along with some relevant propagation properties: more detailed information may be found in [32]. The first column gives the type of single crystal: data for quartz, lithium niobate (LiNbO$_3$) and lithium tantalate (LiTaO$_3$) are given. As described in Appendix A and Section 2.3.3 the SAW properties for a substrate can be tailored (to a certain extent) by the crystal cut and propagation direction chosen. Velocity and coupling values are also given for each propagation direction. The variation in SAW delay time $\tau$ with temperature $T$ is given by [42]:

$$\alpha_T = \frac{1}{\tau} \frac{d\tau}{dT}$$

(3.1)

where the difference in delay is measured from an arbitrary reference (usually room temperature). The properties of the materials are given below:

- **Quartz**: the crystalline form of SiO$_2$ is one of the oldest piezoelectric ma-
3.3. INTEGRATED DESIGN AND MANUFACTURE

Quartz is known as a weakly coupled piezoelectric as its coupling coefficient is very low: this gives inherently narrowband behaviour with relatively high insertion losses. The ST-cut (see Section A.3) is actually a family of orientations designed to give almost zero $\alpha_T$ at room temperatures \cite{108}: this is extremely useful for strain sensing as cross sensitivities with temperature are minimised. Quartz is often used in precision oscillators where temperature stability is important, and in a variety of narrowband devices. It is relatively cheap and is available in a wide variety of substrate forms.

- $\text{LiNbO}_3$: lithium niobate has much higher coupling than quartz, making it suitable for wideband, low loss devices like IF filters. Its major disadvantage is the large $\alpha_T$ which can cause frequency drift with temperature changes. This is used advantageously, however, in SAW temperature sensors where high sensitivities can be achieved \cite{109}. The Y+128° cut provides a higher velocity and coupling coefficient while reducing $\alpha_T$ and coupling to spurious bulk waves. Lithium niobate wafers are several times more expensive than quartz.

- $\text{LiTaO}_3$: lithium taltanate represents a compromise between the properties of quartz and $\text{LiNbO}_3$, providing moderate coupling and temperature delay. The cut shown in the table demonstrates very little diffraction, which can be useful for devices with long delay paths. $\text{LiTaO}_3$ wafers are also several times more expensive than quartz.

Other materials such as langasite ($\text{La}_3\text{Ga}_5\text{SiO}_{14}$) and gallium orthophosphate ($\text{GaPO}_4$) have been investigated for SAW sensor devices \cite{110}, but these materials are not generally available yet and are very expensive. Both of these substrates can operate at higher temperatures than conventional SAW materials (above 400°C), and in the case of $\text{GaPO}_4$ combine the narrowband performance of quartz with increased piezoelectric coupling.

As the substrates will be strained as sensors, their failure behaviour is of interest. All of the materials are brittle in nature due to their crystalline structure, and while the theoretical fracture mechanics of piezoelectric ceramics has been
studied in detail \[111\], studies of single crystal materials are usually experimental. This may be because piezoelectric ceramics are usually transversely isotropic, which simplifies the analysis. Single crystals, by contrast, have lower symmetry and thus need more rigorous approaches or purely experimental treatments. The fracture toughness $K_c$ of a material is a measure of whether fast fracture (the probable mode of failure for these materials) will occur. In the simplest case of an isotropic material under fixed uniaxial loading, $K_c$ is given by \[112\]:

$$K_c \propto \sqrt{E G_c} \propto \sigma_{11} \sqrt{\pi a}$$

(3.2)

where $G_c$ is the toughness and $a$ is the crack length. $G_c$ (and naturally $E$) are material constants, and thus the fracture toughness of the material is dependent both on the applied stress and the crack size. $K_c$ values for quartz in various crystallographic planes were measured in \[113\], which suggested that the toughness was almost isotropic and similar to that of glass. A study of quartz wafers reported that polished specimens were almost three times as tough as unpolished specimens \[114\]: the polishing reduces the length of cracks on the substrate surface, thus improving the toughness. Equation 3.2 demonstrates that crack lengths should be minimised in order to maximise the allowable stress on the material, therefore increasing the strain range of the sensor. The largest cracks on SAW substrates are found not on the propagating surface but at the die edges: Figure 3.4 demonstrates a typical chipped perimeter. Possible methods of improving die edge quality will be discussed in Section 3.3.4.

The failure behaviour of lithium niobate is reported in \[115\]. Although testing was performed at elevated temperatures, the brittle nature of the material was emphasised. Similar behaviour may be expected of LiTaO$_3$ given that it has the same fundamental structure \[32\]. While small differences in fracture toughness exist between materials and cuts, all of the substrates fail at strains below $< 0.002$ and thus the surface wave rather than mechanical properties are more important for material selection.

After an evaluation of the different material options, ST-cut quartz was selected as the sensor substrate. The narrowband performance is an advantage in this application, as this allows more SAWR responses to be evaluated in the available
bandwidth. Its low temperature dependence, particularly for ST-X SAW propagation, is also useful given that the sensors could operate in a variety of weather conditions. The low piezoelectric coupling is partly mitigated by the fact that a resonator structure will be used, which acts to store energy and reduce insertion loss. 3” diameter wafers were chosen as this is the maximum allowable substrate size on the MJB3 mask aligner (see Section 5.3.1). A standard wafer thickness of 0.5mm was also selected.

3.3.3 Multiple sensors

A multi-sensor measurement system is required for the RTWIM project, where each device can be uniquely identified and interrogated. As the SAW resonator was chosen for development, Frequency Division Multiple Access (FDMA) [84] may be used for interrogation of multiple devices. This approach allocates each sensor a particular sub-band in the interrogation bandwidth, such that any response from the sub-band is assumed to come from a particular sensor. The width of the sub-band should be sufficient to accommodate the shift in resonant frequency as the sensor is strained. As mentioned in Section 3.2.2, this is constrained by the fact that sensor responses should not overlap. At the design stage the sensor sensitivities (i.e., the shifts in resonant frequency with applied strain) were unknown, and thus it was decided to allocate as many sub-bands as possible within the interrogation bandwidth. While this may introduce some interference effects in a multi-sensor system, it will allow the evaluation of many different device designs.

The operating frequency of any SAW device is mainly determined by the frequency response of the IDT. As shown in Section 2.4.1 the optimum (or centre) frequency of an IDT occurs at \( f_c = v/2p \), in the absence of reflections or other perturbations. Although the SAWR sensors rely heavily on reflection effects, these are not considered at this stage for simplicity and because experimental measurements of reflectivity are required (see Section 4.3). As the velocity is effectively constant for a particular propagation direction, only the electrode periodicity \( p \) may be altered, where the electrode linewidths are \( p/2 \). For an operating frequency of about 433.5MHz on ST-X quartz \( (v = 3158\text{m/s}) \), this equates to linewidths of about 1.82\( \mu \)m. To determine the exact linewidths, a brief discussion
of some fabrication equipment is required.

The sensor designs were implemented on a photomask (see Section 3.3.6), effectively a stencil for light, which is used to define the device layouts. The MJB3 uses a 4” square mask on which the layout is nominally the same size as the finished devices, i.e., 1:1 scale. Following consultations with the photomask manufacturer, an Etec Systems Alta3000 mask writing tool was selected as it offered the smallest address size available (8.33nm) for a 4” mask. The address size is the length between adjacent vertices on the mask writer’s design grid: all device dimensions are rounded (‘snapped’) to this grid before the mask is created. Thus the address size determines the maximum resolution of the mask features, and by knowing the dimensions of the design grid, the dimensions of the sensor layouts can be optimised to minimise rounding and distortion. Like any production equipment, the mask writer is subject to tolerances: ±0.05µm is the highest achievable tolerance on this machine over critical dimensions (CDs). Although the linewidths of the finished devices will show much larger tolerances due to the interaction of different production equipment, process variations etc., the choice of machine-matched dimensions was designed to show the effect of data conversion and machine tolerance on mask dimensions.

With the 8.33nm address size in mind, three linewidths (1.82427, 1.81594 and 1.80761µm) were chosen, which give nominal device frequencies on ST-X quartz of 432.78, 434.76 and 436.76MHz. Although only the middle frequency lies within the ISM band, this spread of frequencies was chosen to allow a wider study of the parameters affecting SAW strain sensors (see Section 3.3.5).

### 3.3.4 Wafer layout

As detailed in Section 3.1.2, die for communications devices are generally too small to be used as strain sensors. A standard die size of 6 × 6mm was chosen for manual handling and ease of attachment to components. The size is compatible with existing strain gauges and provides space for different electrode configurations. Bond pads (for connections to antennas and external circuits) were given a nominal size of 2 × 2mm, which roughly equates to the size of solder tabs on strain gauges. Larger die (7.5 × 7.5mm) were also defined for more experimental
configurations requiring additional SAW elements.

Figure 3.9 shows the layout of the die on a 3” wafer. 48 standard die (blue) and 18 large die (red) are provided. Streets on the wafer (the distance between die) are 1mm wide to allow adequate clearance for quartz dicing saws. The layout is designed for easy dicing in two stages: a vertical cut to separate standard and large die, followed by dicing along the streets of each part. High quality dicing (i.e., cutting with minimum chipping) is much more important in SAW strain sensors than in SAW communications devices. Careful examination of Figure 3.4 shows numerous chips around the perimeter of the die caused by dicing. While this is of little consequence for filters, these chips could act as failure sites for devices under strain (see Section 3.3.2). As mentioned above, the quartz substrate is brittle, and thus any chips or cracks should be avoided wherever possible. An interesting option would be to use the laser excision techniques pioneered by Xsil [117]. Lasers rather than circular saws are used for dicing, giving much improved edge quality.
and the capability to dice virtually any shape. Unfortunately the technology was not available for quartz dicing at the time, and so conventional dicing was used for the sensors.

### 3.3.5 Die details

With many die available per wafer, there was scope for designing a large number of sensor configurations. An early decision was made to have only two examples of each unique design on each wafer. To get statistically meaningful results on a per wafer basis would require many examples of the same design on each wafer, but this would severely limit the number of possible device variations. Given the desire to investigate various sensor parameters, and the uncertainties inherent in prototype design, it was more prudent to produce many different device variations. Wafers are much cheaper than photomasks, and so if many examples of a single design are required it is more economic to fabricate them over multiple wafers.

Each of the standard die were designed with a single resonant element. Most complete SAW sensors use a number of SAW elements within the device (e.g., see Figure 3.3) for temperature compensation, increased overall sensitivity etc., but to reduce complexity and risk only the large die in this work use more than one resonator. It should be noted that practical SAW strain sensors would almost certainly require multiple elements, given the uncertainties in the operating environment [88].

Many device variations are available in the design stage, the most important involving:

- SAW propagation direction
- Device centre frequency (nominal)
- Resonator type
- Number of finger pairs in the IDT
- Number of reflectors
- SAW aperture
3.3. INTEGRATED DESIGN AND MANUFACTURE

- Use of multiple resonators per die

The propagation direction on the wafer is a key parameter as it determines the operating frequency for a particular electrode pitch; the resonance properties are also significantly affected (see Section 4.5). As introduced in Section 2.3.3 beam steering and diffraction can be significant in piezoelectric materials, and needs to be considered during device design. An ideal propagation direction should provide:

1. Pure mode propagation to avoid beam steering, or an appropriate direction to minimise diffraction
2. High piezoelectric coupling
3. Low $\alpha_T$
4. Small power flow angles (if a pure mode is unavailable or undesirable)
5. Good reflectivity behaviour

In most materials there is a tradeoff between beam steering and diffraction [60], [40], and the choice of propagation direction is often related to the type of SAW device used. Resonators use reflectors in the near-field (Fresnel) region of propagation where diffraction is minimal, and thus the design has been optimised for minimum beam steering. Examining Figure 2.6 a propagation angle of 0° (relative to the X axis on the local XZ plane) is an obvious choice being a pure mode direction and offering relatively high coupling with $\alpha_T = 0$ (see Table 3.1). Similarly, 35° is another good choice as it is also a pure mode direction. The coupling and phase velocity are higher than at 0°, though $\alpha_T \neq 0$. Given that 0° is a pure mode direction, it would be very useful if 90° could also be used as this would allow strain sensing on orthogonal axes. However, examining Figure 2.7 shows that $K^2 = 0$ at that direction, i.e., it is a non-piezoelectric solution for Rayleigh waves (see Section 2.3.1), though ‘pseudo’ SAW solutions may exist. Therefore 0° and 35° were chosen as the main propagation directions. A number of die were designated with different propagation directions to investigate the effect of beam...
steering and diffraction (see below), even though this will produce sub-optimal performance in these devices.

During the design stage, the reflectivity behaviour of different propagation directions was unknown and therefore did not influence the design decisions. This was subsequently investigated as part of the device modelling work (see Section 4.5.4). For resonant SAW devices, the reflectivity behaviour is crucial to device operation and should be considered in future design work. A discussion on the reflectivity effects in the prototype sensors is given in Section 5.1.5.2.

Implementing the different propagation directions on the mask’s die layout posed a number of problems. If both 0° and 35° devices are implemented in the same layout, the rotated devices are subject to the same design grid problems as encountered with the linewidths. This could cause deformed designs as rotated elements are snapped to the nearest grid intersection. Given the small dimensions involved, this is unlikely to be a major problem, but it is one that can be avoided. More significantly, implementing both propagation directions on the same layout would reduce the other design variations available. A more elegant solution was found by utilising the MJB3’s vacuum wafer chuck. This can precisely translate and rotate a wafer below a static mask for alignment, and is usually used when multiple device layers are required. For the SAW sensor mask, all of the layouts are orientated in the same direction (with the exception of the sub-optimal devices), and alignment marks corresponding to 0° and 35° propagation were provided on the mask to align with the wafer below. The marks are designed to match with the recognisable parts of the wafer, i.e., the flat and the perimeter: this was to ensure relatively good alignment control. Although an auxiliary flat must be cut on the 35° wafers before dicing (as the original flat is now at 35° to the devices), this is not a major obstacle. Given that the same linewidths are now used for both directions, the nominal frequencies of the rotated devices rise to 448.81, 450.87 and 452.95MHz as \( v \approx 3275\text{m/s} \). These frequencies are well outside the ISM band, but as previously mentioned they allow the study of more device parameters.

As 48 standard die are available, 24 unique designs were implemented. The possible variations were divided in the following order:
3.3. **INTEGRATED DESIGN AND MANUFACTURE**

1. **Device frequencies:** each design is fabricated using each of the three selected linewidths, i.e., three frequencies variations of each design are provided. This leaves eight other parameters that can be varied.

2. **Resonator type:** the placement of the reflectors either side of the IDT is crucial to device performance. This is especially true in resonators, as the standing wave pattern can be degraded or even destroyed by poor element alignment. Two different types of 1-port SAWR were chosen for this project (optimal [40] and synchronous [72]), both of which will be discussed in Section 4.4.3. In general, optimal designs provide better resonant performance but synchronous designs are easier to manufacture. Given the moderate frequencies involved (by SAW device standards), either type of resonator should be feasible for the sensors, and thus each design was implemented both in an optimal and a synchronous configuration for comparison. This leaves four other parameters that may be varied.

3. **IDT finger pairs:** the number of finger pairs in the IDT determines both its bandwidth (see Section 2.4.1) and its radiation conductance, which may be related to the device impedance [40]. Commercial SAW components usually have a nominal impedance of 50Ω at their operating frequencies, which is designed to match the characteristic impedance of most RF devices. In this project, however, uncertainties in the actual performance of the SAW structures meant that such matching was not possible. After an examination of successful SAW devices in the literature, two variations in finger pairs (40 and 60 pairs) were chosen as reasonable values. This left two other unique designs.

4. **Reflector lengths:** the final design choices were used to vary the reflector lengths. Efficient reflectors are very important in resonators, with the aim of reflecting all of the incident wave energy back to the source without distortion. This could be achieved by simply having as many reflective elements as possible, thus achieving a high $Q$ factor. However, spurious propagation modes must also be accounted for. Long resonant cavities may induce longitudinal modes which degrade the frequency response [118], but these are
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more important in 2-port resonators where the cavities are generally long. Transverse modes, though, are an issue for all types of resonator. The SAW diffracts as it propagates through a grating structure of finite length, eventually reflecting from the reflector ends in long gratings. This leads to transverse modes caused by waveguiding in the reflector structures [119], [120], which are manifested as spurious frequency responses close to the resonant peak. Although design methodologies are available to analyse transverse mode effects [93], these were not implemented in this project. One reason for this is the lack of design information from experimental work, which is common to many of the other design choices. Another reason is that for wireless sensors the power of the response signal was considered to be more important than its absolute purity, i.e., it is better to have a slightly distorted signal rather than a pure signal too weak to be detected. In either case, long reflectors can be made acoustically shorter by applying an acoustic absorber (e.g., silicon gel or rubber) over the unwanted grating portions after fabrication. Reflectors using 550 and 650 elements per gratings were selected to evaluate how reflector size affects sensor performance.

As all of the design choices had been exhausted, the SAW aperture must be constant across all of the layouts. An aperture of $45\lambda$ was chosen as a balance between minimising diffraction in the structures [42] and keeping the electrodes to a manageable length for fabrication (see Section 3.4).

As many variables are involved in the sensor design, some preliminary modelling was performed using an equivalent circuit [40]; more complex model types are detailed in Section 4.2. Such circuits use lumped electrical elements to describe the general frequency response, though typically the detailed resonance behaviour is not simulated. Commercial SAW devices are frequently provided with parameters for these circuits: Figure 3.10 shows the typical shunted RLC layout used for 1-port SAWR [121]. This preliminary modelling was not designed to predict final device performance, but rather to examine the effects of changing design variables. Figure 3.11 shows a typical impedance magnitude and phase response of a 1-port SAWR around its centre frequency. The following conclusions were drawn:
3.3. INTEGRATED DESIGN AND MANUFACTURE

Figure 3.10: Equivalent circuit of an Epcos R820 1-port SAWR [121]. R=14Ω, L=63.16µH, C₁=2.13fF, C₀=2.5pF.

Figure 3.11: Equivalent circuit simulation of SAWR around its resonant frequency (433.92MHz)
• Increasing the number of finger pairs in the IDT increased the separation between the series and parallel resonance modes. The series mode is required in this application to minimise the impedance at the resonant frequency, and the two modes should be separated to avoid distortion.

• Increasing the reflectivity of the gratings has a marked effect on performance, sharply decreasing the impedance at resonance while providing a steeper phase response. Both of these effects are beneficial for the sensors.

• Changing the aperture only produced small changes to the frequency response. This is to be expected, as the width of the wavefront primarily affects the SAW amplitude rather than the frequency of the resonant response.

The devices on the larger die were mainly created from combinations of the devices on the standard die. These larger die were reserved for more experimental configurations, most requiring two resonators. The devices were not intended for use as sensors but rather to test different SAWR parameter values. Of the 18 larger die, 16 were designed as pairs of identical sensors, while the last two die were individual designs. The following divisions were used:

• Die 1 to 10 each have two SAWR connected electrically in series as illustrated in [69]. This is designed to create two different resonances, each of which can be identified. The frequency response of a SAWR is dependent not only on its configuration and physical effects but also on the radio channel and communications equipment (antennas, cabling etc.) used. The two resonators on Die 1 to 10 each have different designs (and hence different frequency responses), but are subject to the same strain state. However, as both are interrogated by the same RF signal, a differential measurement of frequency shift could be used to effectively remove the effects of the RF channel [122]. In this project, however, the aim was merely to investigate the properties of the static response. The various pairs of die have different combinations of standard die connected together (see Appendix B), which is designed to give a wide variety of frequency responses.

• Die 11 to 16 also have two resonators per die, but these SAWR as not connected, with each having its own bond pads. These three pairs of die are
used to investigate extremes of IDT finger pairs, reflector lengths and apertures. As the SAWRs are separate, each element can be analysed individually if necessary or the responses can be combined.

- Die 17 and 18 were deliberately put at poor propagation angles (45° and 60° relative to the other devices) to investigate the degradation in performance, as mentioned earlier. These were produced by simply rotating a standard die about its centre, without any reference to the mask design grid.

The same bond pads were used in all of the die for simplicity, and were slightly displaced from the IDT in an effort to reduce parasitics from the large metal areas.
Each die was numbered for identification, and a border with standard orientation marks was provided for alignment as strain gauges. Figure 3.12 shows the completed mask layout with the die details added; Appendix B has a complete listing of the properties of each die as designed. Figure 3.13 shows a rendering of standard Die 02 on a quartz substrate. The thin strip in the centre of the die is the electrode area where the surface waves propagate, while the large square areas on either side are the bond pads. Figure 3.14 shows a closeup of the IDT structure from the same die. It should be noted that the reflectors are slightly wider than the SAW aperture: this is designed to reflect more of the SAW energy as it diffracts through the grating.
3.3.6 Photomask design and production

The mask design was created using AutoCAD 2000 software[^123] to the 8.33nm design grid. A dark-field binary design (a single chrome layer etched with the sensor layouts) was selected for simplicity. The design was then exported in DXF format to the photomask manufacturer. The data was converted to the GDSII format used by the mask writer, and then fractured into primitives for the actual writing. Fused quartz was chosen as the mask substrate due to its temperature stability, while the layout is formed from a thin chrome layer deposited on the substrate surface.

The control of dimensions on the mask is of paramount importance, as errors in the layout cannot be rectified by other fabrication steps. Given the huge number of individual features found on a modern photomask, it is impractical to measure each dimension after manufacture. Instead, the client specifies certain critical
dimensions (CDs) [115] which must be kept within a specified tolerance: all other dimensions are uncontrolled and are assumed to be within specification. In this project, the electrode linewidths are the most critical dimension, and the smallest linewidths were selected for measurement. Figure 3.15 shows the measured error in linewidth across an electrode section: the nominal linewidth is 1.80761 µm. The mean linewidth (and standard deviation) across this section is 1.821 ± 0.016 µm, which is within the specified ±0.05 µm tolerance. It should be noted, however, that this measurement is significantly larger than the design value (almost as large as the largest design linewidth), especially when the small differences in design linewidth are considered: the effect of this will be discussed in Section 3.5. In addition to the dimensional tolerances, the maximum size of defects and their density on the mask is specified. The price of photomasks is generally based on their writing and inspection times, and thus reasonable dimensional tolerances and defect sizes were selected to avoid excessive expense.

3.4 Microfabrication of sensors

Ideally the integrated system could be continued in order to model the fabrication process. This would allow the mask layout to be included in a ‘virtual clean-room’ simulator, allowing the effects of process variables on final devices to be evaluated. Such a simulator would be particularly useful in this project, given the extremely limited access to cleanroom facilities. Although huge advances in microfabrication simulation have taken place in recent years [116, 124], no system was found to be suitable for use in this project. The LAVA suite of programs from UC Berkeley [125] was evaluated, in particular the SAMPLE-2D and SAMPLE-3D components. While the 2D version was useful for basic lithography simulation, the full 3D program was unsuitable for this project (see Section 3.4.4). A commercial lithography simulator (PROLITH 8.1.2 [126]) was also tested. While both simulators give the same results for basic simulations [127], PROLITH has much better support for process components in common use. However, in common with SAMPLE, its 3D model is unsuitable. Therefore all of the fabrication relied on experimental techniques.

The most common process used to create SAW devices (or indeed any μm-
scale component) is photolithography. This involves using ultraviolet radiation to transfer a device design from a 2D pattern on a photomask to a polymer film called the resist. Selective parts of the film can then be removed, forming a 3D representation of the layout in the resist. The resist pattern can then be used to form devices on the underlying substrate. Pattern definition is a two-stage process involving the exposure of the device layout and subsequent development of the resist layer, and should be considered as a whole \cite{128}. Some simple exposure and development models are given in \cite{116}, but they are not essential for this work. An excellent introduction to the fabrication of SAW devices is provided in \cite{129}, which was used as a guide for the manufacturing.

Several different types of photolithography exist (proximity, projection etc.), but contact lithography was chosen for this project as it provides the highest resolution on the MJB3 mask aligner. Figure 3.16 shows the exposure scheme \cite{128}.

![Figure 3.15: Linewidth error across a grating section](image-url)
In contrast to other types of photolithography, contact lithography requires that the mask and resist layer be in contact. For thin resist films, the method offers the highest resolution of any lithographic process. The theoretical resolution of a regular grating (equal lines and spaces) using contact lithography is:

\[ b_{\text{min}} = \frac{3\sqrt{0.5\lambda_r z}}{2} \]  

where \( b_{\text{min}} \) is the minimum resolvable line or space width, \( \lambda_r \) is the wavelength of the light (typically 300-400nm) and \( z \) is the thickness of the resist film (typically about 1\( \mu \)m). In practice, however, process variations reduce this resolution considerably. The main problem with this technique is that the mask degrades over multiple uses due to the contact with wafers. Particles between mask and wafer or lack of flatness can lead to gaps which cause diffraction and thus reduce the resolution across areas of the wafer. While the wafer damage problem is a serious issue for volume manufacturers, it is less important for a small scale research project.

The fabrication process uses the resist pattern as a basis for creating the devices. Several processes exist for creating devices, with etching probably being the most common. For this project, however, a lift-off process was selected. As noted in [29], the lift-off process offers high resolution for small electrode widths, high yields and precise dimensional control. It requires tight lithographic
3.4. MICROFABRICATION OF SENSORS

Cleaning Resist coating Exposure

Development Metallisation Lift-off

Figure 3.17: Fabrication steps in lift-off process

constraints, however, with vertical sidewalls in the resist to produce successful devices. Figure 3.17 gives an overview of the process [130]: details of each step are provided in the following sections.

Fabrication was first attempted in the SFI Trinity Nanoscience Laboratory [131], where hands-on experimentation was performed. Later fabrication runs were performed by the Tyndall National Institute [132], with manufacturing steps provided by the author. Although these fabrications were performed separately, the respective steps are presented together.

3.4.1 Wafer cleaning

Wafer cleaning is the first step of the manufacturing process, and is essential to the success of the final SAW sensors. A clean, residue-free surface optimises the pattern quality, electrode adhesion and SAW propagation properties. Quartz generally has poorer adhesion properties than silicon, and this is a particular problem given that the electrode structure will be strained. In many cases cleaning is
performed using a local ‘recipe’ which is known to be good, but several procedures have been documented in the literature. A comprehensive process is given in [129], which is designed to remove both organic contamination and small particles: contamination sources are explained in [128]. The RCA and Piranha procedures, commonly used in IC manufacture, are outlined in [133]. In relation to quartz, a general guide to substrate cleaning is given in [134], while cleaning for BAW resonator substrates is explored in [135]. An interesting application of ultra-clean quartz surfaces is given in [89], which uses a combination of RCA and Piranha cleaning; a possible application of this is discussed in Section 3.2.3.

The quartz wafers were cleaned in the TCD lab using a modified Piranha clean \((\text{H}_2\text{SO}_4(97\%):\text{H}_2\text{O}_2(35\%), 3:1)\) followed by a DI water rinse and air drying. Tyndall used a standard Piranha clean and included a detergent step before the DI rinsing; a dehydration bake was used for drying.

### 3.4.2 Resist coating

The resist layer is a polymer film used to define the device layout on the wafer. It contains a photoactive compound which is sensitive to radiation at particular wavelengths: resist chemistry is discussed in many lithography references such as [116] and [133]. As mentioned above, adhesion to the quartz surface can be a problem, in this case causing large sections of the resist layer to slide off during development. The probable cause of most of the adhesion problems was retained moisture after cleaning, and so the wafers were vapour primed using HMDS at the TCD lab to form a hydrophobic surface. This approach was only partly successful, and so the Tyndall fabrication also used a 5nm Au adhesion layer over the entire wafer: this was applied using a Leybold LAB600 evaporator.

The need for vertical sidewalls in the resist film is a challenging requirement. The ‘Metallisation’ part of Figure 3.17 shows the ideal case, with vertical profiles and discontinuous metal coverage. In practice, however, single-layer resists often have sloping sidewalls, leading to continuous metal films. At the lift-off stage such films can completely detach from the wafer, stripping off both the electrode structure and the excess metal. An alternative approach is to use lift-off resists: some early work is documented in [136]. Microchem’s lift-off resist system [137]
3.4. MICROFABRICATION OF SENSORS

LOR applied Imaging resist applied Exposure

Development Metallisation Lift-off

Figure 3.18: Processing steps for bi-layer resists using LOR

was used (LOR1A in TCD, LOR3A in Tyndall): Figure 3.18 shows the processing steps. The lift-off resist is applied after cleaning, followed by the imaging resist which is used to define the device layouts. Following exposure of the wafer, both layers are developed together. The lift-off resist develops isotropically to create a undercut resist profile, which should ensure a discontinuous metal film: the rest of the fabrication steps are as normal. Spin coating was used to create 150nm (LOR1A) and 350nm (LOR3A) layers on the wafers, with a prebaking step to remove the solvent.

Shipley’s MicroPosit S1800 series was chosen as the imaging resist (diluted S1813 in TCD, S1805 in Tyndall). This is a positive resist, i.e., sections exposed to radiation become more soluble in developer than unexposed sections. In contrast to the lift-off layer, the imaging resist is designed to develop anisotropically in order to replicate the mask pattern. The S1800 series was chosen to match both the linewidths of the devices and the exposure equipment (see below). 500nm films were spin coated over the lift-off layers and prebaked as above.
3.4.3 Exposure

The Karl Süss MJB3 UV400 mask aligner [102] was the key piece of equipment to consider during fabrication, and it influenced much of the integrated design and manufacturing process (see Section 3.3). The mask aligner determines the following parameters:

- **Type of lithography**: as detailed above, contact lithography on the MJB3 should be used to optimise resolution.

- **Achievable feature size**: the minimum resolvable feature size is quoted as 600nm, but this is heavily dependent on the layout of the device (see below) and on the substrate type. A working resolution for individual features of 1µm was expected.

- **Mask and substrate dimensions**: a 4” square mask was required, and wafers of up to 3” diameter can be used.

- **Resist type**: the MJB3 primarily uses the G-line radiation (λr = 436nm) from its Hg lamp, and thus G-line resists like the S1800 series must be used.

The aim of the exposure step was to provide enough energy to the exposed sections so that they can be sufficiently developed. Ideally, only the resist areas directly below the mask patterns would be irradiated, but in practice diffraction causes degraded mask images: a discussion of optical effects may be found in [128]. In some cases there is an interaction between the resist-covered wafer and the exposure equipment, and between devices on a mask, leading to reflections and standing waves which change the effective exposure energy. Another complication is that the exposure density is affected by the lamp condition, as ageing lamps become progressively dimmer. The number of variables involved underlines the need for simulation techniques (see below), but in practice experimental testing is usually used to determine exposure parameters.

Several different exposure times were investigated in the TCD lab, ranging from 0.8 to 2.2s. Control of exposure energy proved to be a problem, with fluctuations in lamp power leading to different exposure densities. The Tyndall fabrication used a Süss MA1006 mask aligner with a regulated exposure density.
(10mW/cm$^2$) which produced better results. Optimum exposure time was 4.2s under 365/405nm UV radiation.

3.4.4 Development

As mentioned above, the exposure and development steps should be treated together as both are integral to pattern definition. Developing liquids dissolve exposed areas of positive resist at a much faster rate than unexposed areas, ideally revealing a projection of the mask patterns in the resist layer. However, the diffracted image described above may cause areas beside the mask patterns to also be developed, thus reducing the linewidth definition. As a rule of thumb, development times should be inversely proportional to exposure times, as strongly exposed areas will develop more quickly: experimental testing was again used to find the optimum development time. Shipley MF-319 developer was used to develop the TCD wafers, with development times between 20 and 60s. The same developer was used in Tyndall with a development time of 27s.

The quality of the resist pattern largely determines the quality of the finished devices, and so the developed wafers were examined to check the process parameters. Several fabrication runs were performed in the TCD lab up to this stage, initially with Si wafers before moving to quartz substrates. Microscope and SEM analysis was used to examine the resist layers after each run, with the results used to refine the subsequent fabrications. Two major problems became apparent:

- **Resolution of isolated electrodes**: the IDT may be divided into an area of dense electrodes (where the electrodes from the two sections overlap) and two smaller areas of isolated electrodes (near where the electrodes connect to the busbars). It became clear that these different areas were developing at different rates, even though they were exposed together for the same period. Figure 3.19 shows a portion of an IDT and reflector grating: purple areas are developed sections while green areas are resist-covered. The reflector sections and the overlapping IDT electrodes appear to well defined, while the isolated electrodes are barely noticeable. Increasing the exposure time caused the isolated sections to correctly form, but overexposed the dense electrodes, destroying the gratings. This behaviour was related to an effect
known as the iso-dense print bias \([139]\), where isolated lines are created wider than dense lines of the same design. This is because the diffracted images from each dense grating section interfere and increase the effective exposure density in exposed areas. Similar proximity effects in contact lithography are described in \([140]\), which notes that diffraction effects from multiple apertures (such as in a grating) can reverse the polarity of the image depending on the phases of the diffraction components: this will be explored below. Increasingly dense layouts in IC design mean that proximity effects now need to be examined at the design stage, and algorithms have been developed to automatically adjust designs \([141]\). However, in this case the mask was already created and could not be changed. It was also noted that a few relatively good resist patterns were being produced, which suggested that resolving the isolated sections wasn’t a fundamental design problem. Figure 3.20 shows another IDT and reflector section from a quartz fabrication, where isolated electrodes are more apparent.

- **Grating polarity:** close examination of Figure 3.19 shows that although the dense sections appear to be correctly defined, they are in fact in the wrong positions. Comparison with the mask design shows that the IDT busbar and isolated electrodes are correctly placed, but the dense sections have reversed polarity, i.e., areas which should be resist-covered are not and vice versa. The pattern in Figure 3.20 has the correct polarity throughout the structures. It was assumed that the same proximity effects detailed above were causing the image reversal, as the behaviour was local to the dense sections.

Analysis of the better-quality die revealed that almost all were located on the edge of the wafer, rather than near the centre as would be expected. It was hypothesised that a lack of contact between the mask and the centre of the wafer was causing both of the above problems. Three possible causes of contact failure were identified:

1. **Edge bead:** during spin coating a small amount of resist is placed near the centre of the wafer and is spread by centrifugal force. As the resist drys
near the edge of the wafer its viscosity increases, causing an build-up of polymer near the perimeter known as edge bead. If this bead is sufficiently large it would mean that patterns near the perimeter of the wafer would be in contact with the mask, while those nearer the centre would have a gap between mask and wafer.

2. *Lack of wafer and/or mask flatness*: it is possible (if unlikely) that the wafers and/or mask were bowed, leading to contact near the wafer perimeter with a gap in the centre. No bow measurements were available for either the wafer or mask.

3. *Insufficient contact pressure from the mask aligner*: the MJB3 has 3 contact modes – soft, hard and high precision. All of the TCD samples were made using the hard contact mode, where nitrogen is used to press the wafer
against the mask. High precision mode forms a vacuum between mask and substrate, ensuring the best possible contact; unfortunately this feature was not operational when the fabrications were taking place.

Any gap between mask and wafer would have the potential to cause the proximity and polarity effects shown above. Given the limited cleanroom time available, it was decided to investigate some lithography simulators to see if this behaviour could be replicated. As mentioned above, both SAMPLE-3D [125] and PROLITH 8.1.2 [126] were evaluated, but neither was found to be suitable for this project. SAMPLE-3D’s SPLAT imaging software uses far-field waves to model projection lithography, rather than the near-field analysis required for contact simulation. Similarly, PROLITH only models projection lithography and so could not be used. In light of these problems it was decided to halt the TCD work at this stage and begin fabrication at Tyndall, where more advanced production equip-
3.4. MICROFABRICATION OF SENSORS

ment might alleviate some of the problems. The resist patterns from the Tyn-
dall fabrication did prove to be successful and were used for the later lithography
stages.

3.4.5 Metallisation

The metallisation step involves depositing a metal layer over the entire wafer sur-
face, part of which will be used to form the electrode structures. Evaporation is
the preferred deposition method for lift-off as most of the metal arrives normal to
the wafer surface [129]; an analysis of the effect of deposition conditions on film
resistivity may be found in [142]. The wafers were hard baked at 90° for 30 mins
following development and then etched to remove the Au resist adhesion film in
the developed areas (15s in KI(8g):I2(2g):DI(160ml)). An Ar plasma process was
used to further clean the developed areas down to the wafer surface, which should
improve the adhesion of the electrode metallisation. The electrodes consist of a
bi-layer structure evaporated using the LAB600, with a 15nm Cr layer next to
the substrate and a 150nm Al layer above as the primary metallisation. The Cr
layer is used as an adhesive film between the quartz substrate and the Al metalli-
sation, as these generally demonstrate poor bonding properties. A total electrode
 thickness of 165nm (c. 2% of the SAW wavelength) was chosen as a compro-
mise between the weak reflective behaviour of thin electrodes and that of thicker
structures, which exhibit larger mass loading, non-linear effects etc.

3.4.6 Lift-off

Once the metal layers were deposited, the last lithographic task was to remove the
resist and excess metal from the wafer. In an ideal case the excess metal is only
attached to the resist, and thus can be easily removed to leave the finished wafer.
MicroPosit 1165 resist remover was used to remove the resist, with ultrasonic
agitation to remove stubborn sections. The Au resist adhesion layer was then
etched as above to complete the lithography.
3.4.7 Dicing

The final fabrication stage was the dicing of wafers into individual die. A resist layer was applied to the wafer before cutting in order to protect against chip damage; this was removed after dicing. The dicing was performed using a Disco wafer saw with a blade optimised for quartz cutting with minimal chipping, and a polymer film was used to hold the diced devices together for transport.

3.5 Finished devices

Five wafers of devices were produced in total, of which three were specified as using ST-X (0°) propagation (marked as Wafers 1-3) and two with ST-(X+35°) (35°) propagation (Wafers 4 and 5); the angles refer to $\psi$ in Section A.3 as before. It was discovered during testing, however, that the resonant frequencies of the Wafer 1 die were considerably higher than the nominal design values (see Section 5.1.5), which was surprising given that the measured linewidths were larger than the design values (see below), and thus the devices should resonate at lower frequencies. Careful inspection of Wafers 1-3 revealed that the wafer flat, which should be normal to the SAW propagation direction for 0° propagation (see Figure A.3), was actually parallel to the propagation direction, and thus the SAW propagation direction is approximately ST-(X+90°); errors in the wafer cut and in the photomask orientation relative to the wafer account for the uncertainty. Figure 3.21 illustrates the problem. Although wafer orientation markings were provided on the photomask (see Section 3.3.5), it appears that these were misinterpreted during fabrication. The implications of this misorientation will be discussed in Section 5.1.5 Wafers 4 and 5 appear to be correctly fabricated using ST-(X+35°) propagation.

Figure 3.22 shows a typical standard die: some damage to the right bond pad may be noted. Each of the wafers was examined under a microscope to check the pattern quality and to detect any obvious faults. SAW devices act as distributed structures, and apart from clear IDT shorts (which would stop any surface wave generation) and large-scale damage (which would stop SAW propagation), it is often difficult to determine whether a device will be successful purely from vi-
3.5. FINISHED DEVICES

Figure 3.21: Design orientation of Wafers 1-3 (left) for 0° (i.e., ST-X) SAW propagation and actual wafer orientation (right) with 90° (i.e., ST-(X+90°)) propagation; note the positions of the wafer flats. SAW propagation in both cases occurs in the north-south direction for the standard die (see Figure 3.12).

Visual inspection. Such visual examinations are useful to spot-check the fabrication quality, but ultimately the success of a particular die is determined by its frequency response. Figure 3.23 shows a typical IDT structure, with good electrode definition and some isolated damage which appears to be metal loss. By contrast, Figure 3.24 shows the same IDT on a different wafer, with more extensive damage to the IDT and reflectors of a different colour (probably due to widespread metal loss). A wide variety of minor faults were also observed (scratches, pinhole defects etc.), but most of these were not regarded as fatal.

A selection of the sensors were imaged using SEM in order to measure some of the fabricated dimensions (see Table 3.2). These devices all displayed resonant behaviour during electrical testing (see Section 5.1) and represent each of the design linewidths and the rotated designs. The majority of the selected die were positioned near the perimeter of the wafer, the most common location for poor-quality die [133], and thus should represent the ‘worst case’ measurements.
Figure 3.22: Photo of Die 30, Wafer 4

Figure 3.23: Photo of standard Die 10, Wafer 5 at approx. 200x magnification
3.5. FINISHED DEVICES

Figures 3.25 and 3.26 show the same standard die on Wafers 1 and 5, while Figures 3.27 and 3.28 depict the same large die from Wafers 1 and 3. Some general points may be made:

- Most of the electrodes appear to be well defined, with consistent linewidths across each section and no obvious shorts. However, there appears to be considerable variation from wafer to wafer. Although the same die design is shown in both Figures 3.25 and 3.26, the Wafer 5 example has 18% wider electrodes than those on Wafer 1 (see Table 3.2). Such changes in linewidth will mean that even nominally identical die from different wafers will have different frequency responses; the implications of this will be discussed in Section 5.1.

- As is typical of devices made by photolithography, sharp corners in the design are rounded in the final devices: note the ends of the isolated electrodes. More interesting is the wavy appearance of the electrode edges, especially in Figures 3.27 and 3.28: the cause of this is unknown, but it is possibly an artifact of the metal deposition process. Neither of these effects were
considered to be critical flaws.

- Minor damage is evident on most of the IDTs, but this is unlikely to have a major effect of device performance. Figure 3.27 shows more serious damage, with discoloured electrode sections and poorly-defined structures. It should be noted that a resonant response (albeit weak) was still demonstrated by this device.

An important task was the measurement of actual structure dimensions, in particular the linewidths. Table 3.2 shows the measured dimensions of the IDT and reflector features: the design linewidths and measured values of the IDT lines and spaces, reflector lines and spaces, periods lengths $p$ and metallisation ratios $\eta$ (see Section 2.4.1) are tabulated. Mean values and standard deviations are presented for multiple measurements across the features. The accuracy of individual measurements is estimated as $\pm 5\%$ [143]; this error is not included in Table 3.2.
should be noted that the measurements were taken over a small number of electrodes (typically 5 to 10) in each structure as it was difficult to accurately locate the electrode edges in larger areas. Measurements of average periods lengths over complete structures would be more representative of the complete devices, and should be used in future work [88]. The dimensions tabulated in Table 3.2 are usually the most critical in determining the frequency response. All of the devices are designed to have dense lines and spaces of equal widths (i.e., \( \eta = 0.5 \)), with the isolated lines having the same widths as the dense ones. The measurements, however, show large variations both from die to die and from wafer to wafer. A number of features may be noted:

- All of the line features (with the exception of the reflector lines on Die L17, Wafer 3) are wider than their design values: this effect is most obvious on the Wafer 5 die. Width increases range from 3\% for the best of the Wafer
Table 3.2: Dimensions of periodic IDT and reflector features (mean and standard deviation) in µm. *L* denotes large die. Individual IDT Space and Line Widths are quoted. These values are accurate to ±0.5%.

<table>
<thead>
<tr>
<th>Die Width (µm)</th>
<th>IDT Length (µm)</th>
<th>Reflect Line Space (µm)</th>
<th>Reflect Line Width (µm)</th>
<th>IDT Space (µm)</th>
<th>IDT Line Width (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.072</td>
<td>1.22 ± 0.14</td>
<td>1.11 ± 0.10</td>
<td>2.79 ± 0.01</td>
<td>45</td>
<td>32</td>
</tr>
<tr>
<td>0.094</td>
<td>1.44 ± 0.07</td>
<td>1.39 ± 0.03</td>
<td>4.47 ± 0.01</td>
<td>18</td>
<td>5.06</td>
</tr>
<tr>
<td>0.12</td>
<td>2.72 ± 0.10</td>
<td>2.25 ± 0.11</td>
<td>2.52 ± 0.04</td>
<td>32</td>
<td>18.59</td>
</tr>
<tr>
<td>0.14</td>
<td>3.96 ± 0.17</td>
<td>3.94 ± 0.15</td>
<td>2.85 ± 0.09</td>
<td>25</td>
<td>18.59</td>
</tr>
<tr>
<td>0.16</td>
<td>5.19 ± 0.24</td>
<td>5.12 ± 0.19</td>
<td>3.19 ± 0.11</td>
<td>18</td>
<td>5.06</td>
</tr>
<tr>
<td>0.18</td>
<td>6.42 ± 0.31</td>
<td>6.40 ± 0.26</td>
<td>3.52 ± 0.14</td>
<td>25</td>
<td>18.59</td>
</tr>
<tr>
<td>0.20</td>
<td>7.65 ± 0.37</td>
<td>7.64 ± 0.31</td>
<td>3.86 ± 0.16</td>
<td>18</td>
<td>5.06</td>
</tr>
<tr>
<td>0.22</td>
<td>8.98 ± 0.44</td>
<td>8.97 ± 0.40</td>
<td>4.20 ± 0.19</td>
<td>25</td>
<td>18.59</td>
</tr>
<tr>
<td>0.24</td>
<td>10.21 ± 0.51</td>
<td>10.20 ± 0.46</td>
<td>4.54 ± 0.23</td>
<td>18</td>
<td>5.06</td>
</tr>
<tr>
<td>0.26</td>
<td>11.44 ± 0.57</td>
<td>11.43 ± 0.53</td>
<td>4.88 ± 0.27</td>
<td>25</td>
<td>18.59</td>
</tr>
<tr>
<td>0.28</td>
<td>12.67 ± 0.63</td>
<td>12.66 ± 0.60</td>
<td>5.22 ± 0.31</td>
<td>18</td>
<td>5.06</td>
</tr>
<tr>
<td>0.30</td>
<td>13.90 ± 0.69</td>
<td>13.89 ± 0.65</td>
<td>5.56 ± 0.35</td>
<td>25</td>
<td>18.59</td>
</tr>
<tr>
<td>0.32</td>
<td>15.13 ± 0.75</td>
<td>15.12 ± 0.71</td>
<td>5.90 ± 0.39</td>
<td>18</td>
<td>5.06</td>
</tr>
<tr>
<td>0.34</td>
<td>16.36 ± 0.81</td>
<td>16.35 ± 0.77</td>
<td>6.24 ± 0.43</td>
<td>25</td>
<td>18.59</td>
</tr>
<tr>
<td>0.36</td>
<td>17.59 ± 0.87</td>
<td>17.58 ± 0.83</td>
<td>6.58 ± 0.47</td>
<td>18</td>
<td>5.06</td>
</tr>
<tr>
<td>0.38</td>
<td>18.82 ± 0.93</td>
<td>18.81 ± 0.89</td>
<td>6.92 ± 0.51</td>
<td>25</td>
<td>18.59</td>
</tr>
</tbody>
</table>

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*Note:* The values are given in µm with standard deviation ±0.5%.
3.5. FINISHED DEVICES

3 die to 55% for the worst example from Wafer 5. Given that the mask linewidths are presumed to be within specification (i.e., within ±0.05µm of the design values, see Section 3.3.6), most of the dimensional variation can be attributed to the manufacturing process. As a general rule dimensional tolerances should be controlled to between ±10% and ±20% of the minimum (or critical) feature size in an IC production process [128], but greater variation is to be expected during prototyping. Linewidth control is mainly dependent on the exposure and development processes, and given the relatively good results from the Wafer 3 die it should be possible to improve the tolerances through optimisation. It would be expected that the widening of the dense line features would lead to a corresponding narrowing of the dense spaces, but in most cases this has not happened. Instead it appears that all of the features have been scaled up, i.e., the electrode periodicity
$p$ has increased. The line features may additionally have been subject to diffraction, which would account for the higher $\eta$ values, but this cannot be confirmed.

- Although the mean linewidths are significantly different from the design values, the small standard deviations indicate that they are relatively consistent within each structure. The IDT and reflector dimensions are similar for each individual die, demonstrating that the variation in linewidths is a general grating effect rather than one local to the IDT.

- The lines on the Wafer 1 die are consistently narrower than the corresponding ones on Wafer 5, while the dense spaces are wider. Although different orientations were used for each wafer, this should have no effect on linewidth control: variations in the fabrication process are a more likely
Table 3.3: Dimensions of other device features (mean and standard deviation) in µm. ‘L’ denotes large die. Individual measurements are accurate to ±5%.

- The basic IDT analysis presented in Section 2.4.1 presumes that $\eta = 0.5$, which produces a frequency response proportional to equation (2.42). There is, however, considerable variation in the measured $\eta$ values, which will have an effect on device performance. The modelling of such devices is discussed in the next chapter.

Some of the other device dimensions were also measured. These are not subject to grating effects, and show whether the dimensional variation is local to the electrode fingers or is a more general effect. Table 3.3 shows the design and measured values of the isolated IDT lines (see Section 3.4.4) and the IDT-reflector separation, along with the IDT busbar width. While there are some differences between the widths of isolated and dense lines, there doesn’t appear to be a definite pattern like that shown in Section 3.4.4 again, the lines on the Wafer 1 die are narrower than the corresponding ones on the Wafer 5 die. All of the sensors were designed with the same busbar width (12.495µm), but again there were significant differences between the measured dimensions. As with the linewdths above, all
of the die have wide busbars, with the Wafer 3 devices being closest to specification. The IDT-reflector separation (the distance between the ends of the IDT and reflector busbars) is a function of the electrode linewidth (see Section 3.3.5). All of the large die have greater separations, while those of the standard die are generally smaller than the design values.

When the measurements are considered as a whole, it is clear that the exposed mask features are larger than the design dimensions. The large busbar widths and narrow IDT-reflector separations are a good indication of this, given that they are less likely to be affected by proximity effects. The significance of this scaling will be examined in Chapter 5 where the electrical testing of these devices will be described.

### 3.6 Conclusion

In this chapter, the design and manufacture of SAW strain sensors was examined. An innovative integrated design and manufacture process was introduced, managing the development of SAW sensors from basic specifications to finished devices while increasing process visibility and lowering costs relative to traditional processes. The resulting devices have thus been custom designed for a demanding multi-sensor environment. Fabrication steps for such devices were detailed, along with some comments on the finished sensors.

In the next chapter, the modelling and simulation of such sensors will be introduced.
Chapter 4

Modelling and Simulation of SAW Sensors

The modelling and simulation of SAW strain sensors is the second major part of this project (see Section 1.4), complementing the design and manufacturing work discussed in Chapter 3. Accurate prediction and description of sensor response is key to the success of any measurement project. This allows the estimation of device performance, evaluation of sensor design decisions and can guide future design improvements.

In this chapter the scope of the model parameters are first defined, and current deficiencies in the modelling of SAW strain sensors are discussed. This is followed by an introduction to common SAW device modelling techniques. A new custom simulation scheme is then proposed, leading to a discussion on coupling-of-modes (COM) analysis. Modifications to the basic COM model are then presented which allow the sensor response to be evaluated.

4.1 Model parameters

An important first step is to select the parameters which will be included in the model. This involves the identification of the dominant influences on device performance. Three main contributors were identified for the SAW sensors:

1. The design parameters of each device (e.g., number of reflectors, finger
2. The properties of the interrogation signal (e.g., frequency, amplitude etc.)

3. The applied biases on the sensor (e.g., stress, strain, temperature etc.)

While the first two factors are important for all SAW sensor types, the significance of the various applied biases are heavily dependent on the application in question (see Section 4.5). For example, the applied stress and strain should be the dominant biases (through design) for SAW strain sensors. Temperature effects may also be important, even for substrates with low temperature sensitivities (see Section 3.3.2), but these are outside the scope of this work. Many other factors may influence the response of the devices, but only the above items will be considered in this study. This restriction on the number of model variables should ensure a better understanding of fundamental sensor operation.

The issue of which performance parameter(s) of the sensors to model must also be addressed. In theory, any measure of device performance may be used provided it varies appropriately with the applied bias. However, it is useful to pick generic (i.e., non SAW-specific) parameters which can be easily used across different applications: this will be discussed in Section 4.3. Such an approach is particularly important in the overall RTWIM project, as the sensors represent only part of the measurement system (see Section 1.3). The SAW sensors have been designed as 1-port resonators, for which frequency response methods are usually employed. It was decided to model the impedance (or admittance as convenient) of the devices as a function of frequency, which should give good insight into device behaviour. The experimental testing of impedance for such RF devices will be introduced in Section 5.1.1.

In this project the key relationship to be modelled is that between the frequency response of the sensor and the applied strain. Typical SAW strain sensor papers (e.g., [69]) present a basic outline of SAW theory, followed by a presentation of experimental results. Some excellent work (e.g., [144]) has been presented on the frequency sensitivity of SAW devices to strain, but to date this has not been linked to a general model of SAW sensor behaviour. The aim of this work is to develop a model that predicts the frequency response of a SAW sensor and the effect of an external bias on this: Section 4.3 outlines such a model.
4.2 COMMON MODELLING TECHNIQUES

As noted in Section 3.3, SAW modelling schemes require accurate experimental values to predict device response, which were not available in this project until after fabrication. However, the modelling should allow subsequent sensor designs to be characterised before production.

4.2 Common modelling techniques

Many different modelling approaches are used for SAW devices: a general review is given in [145]. All of the methods concentrate on IDT modelling, as these structures determine much of the frequency response. Three main models were used for early SAW devices [40]:

1. **Delta-function model**: this method (introduced in Section 2.4.1) models the IDT as a set of discrete delta-function sources, and can be used to get an approximate frequency response [62]. Its basic design means that no information is given on impedances, insertion loss, acoustic reflections from fingers etc.

2. **Crossed-field model**: based on earlier simulation work on BAW devices [29], the crossed-field model treats the IDT as a three-port electrical network, with the two acoustic ports represented by their equivalent electrical parameters. While impedances can be calculated, the basic model assumes that the electrodes are reflectionless.

3. **Impulse-response model**: often used to extend the delta-function approach, this model can be used to model broadband or chirped devices [146]. Fourier transform relations can be used to determine the impulse response (and hence IDT layout) from the desired frequency response (see Section 2.4.1).

As SAW device frequencies grew towards 1GHz, 2nd order effects (e.g., electrode reflections) became much more important, and thus new modelling schemes were required. Four different models are now used for the bulk of SAW devices:

1. **Equivalent circuit model**: this extension to the crossed-field model uses cascaded transmission lines to represent the propagating surface wave [147].
Differences in the characteristic impedance and transmission properties of each line segment are used to represent reflections, piezoelectric effects etc., while lumped elements may be introduced to model energy storage effects. This model is distinct from the equivalent circuit used in Section 3.3.5, which is merely a simple representation of a device’s frequency response.

2. **S-matrix model**: scattering matrices are widely used in microwave circuit design [148], and are utilised here to model the incident and reflected voltages at each IDT port. As with the crossed-field model, the IDT is treated as a three-port electrical network, with each S-matrix element representing a ratio between incident and reflected voltages. These can be used to find transmission and reflection coefficients of IDTs for acoustic analysis. The use of S-parameter measurements will be detailed in Section 5.1.1.

3. **P-matrix model**: this is a widely-used variant of the S-matrix model, which uses mixed units in the matrix instead of dimensionless figures [149]. It allows physical parameters to be included in the model (rather than inferred electrical quantities), thus creating a more natural description of the IDT.

4. **Coupling-of-modes (COM) model**: this approach models the forward and backward propagation of waves through a distributed structure, incorporating their coupling interactions (see Section 4.4). It can be combined with the S- or P-matrix techniques to describe device elements analytically; numerical modelling may be used for more complex devices.

The choice of model to use largely depends on the type of device. For example, a delta-function model may be acceptable where the device is a simple two IDT delay line; however, if the electrodes are thick, the significant reflections created will not be included. It has been shown that, for Rayleigh SAW on quartz, all of the modern models above give excellent results [145].

All of the above techniques were designed to model SAW devices as communications components (e.g., filters or resonators). Thus externally-applied substrate strain (or any other applied bias) is not included in the models, and at best is treated as a small error source external to the model. With this in mind, it was
decided to investigate a custom simulation scheme for the SAW sensors, which will be detailed in the next section.

### 4.3 Custom simulation

Given the limitations of the above models, it was decided to explore alternative approaches. For this project, two different simulation approaches seem appropriate: device level and system level. In device level modelling, the sensor is treated as a complete electro-mechanical body, i.e., a composite structure consisting of a piezoelectric substrate with deposited metallic electrodes and reflectors, subjected to mechanical and electrical loads. The sensor is modelled and analysed as a whole, with the SAW propagation and external loads treated together. Analytic solution methods for such a model were investigated, but given the complexity of the wave propagation, the electrode layout and the substrate properties, these solutions would almost certainly be unworkable. A common alternative is to use Finite or Boundary Element methods. Such techniques are increasingly used in SAW devices to investigate general periodic structures, electrode/substrate interfacial stresses and acceleration sensitivity, among other effects. Advanced FE packages (e.g., ANSYS MultiPhysics) commonly support piezoelectric materials and the combined electrical/mechanical inputs required for SAW sensor modelling. The FE device level approach has the following advantages:

1. **Excellent insight into device behaviour**: the model could be investigated at any point to analyse stress components, electrical fields etc.

2. **Clearly defined simulation steps**: although the simulation itself would be quite complex, there is a clearly defined path to a solution. Most FE packages have comprehensive support and validation examples, so a simple model could be progressively refined over time.

3. **Easy dynamic analysis**: the model inputs could vary both with time and frequency, allowing dynamic effects to be analysed.
Chapter 4. Modelling and Simulation of SAW Sensors

The main disadvantage of the approach is that the processing time of such complex simulations could be excessive. Many Finite Element analyses of SAW devices use the periodic nature of the electrodes to reduce the simulation domain, typically to $\lambda/2$ in length. This allows a relatively dense mesh to be used, which is required to capture the surface wave behaviour. SAW sensors, by contrast, may experience position-dependent loads (e.g., from a point contact [154]) and thus modelling of larger domains is often preferable. The combination of dense meshes and relatively large simulation domains leads to a large number of nodes, and thus very large computational resources would probably be required.

In system level modelling, the SAW device is treated as a part of a larger system, effectively a ‘black box’ which receives inputs from one part of the system, processes them and then outputs the results back to the system. A basic version is shown in Figure 4.1. The interrogating signal is produced by an interrogator model and applied to the sensor block. Independent biases (e.g., applied strain, temperature etc.) are also applied, and the response signal is evaluated.

A system level approach has the following advantages:

1. **General application**: the model can be configured in many different ways to integrate with the rest of the measurement system. This allows easy integration with models for interrogation systems, wireless channels, antennas etc.

2. **Wide variety of modelling packages**: the sensor block is basically a transfer function, which makes it compatible with virtually every modelling package. For example, the block could be prototyped in MATLAB, before being
ported to an electronic design package for circuit analysis.

3. Previous work: all of the existing modelling schemes detailed in Section 4.2 use a system level approach, which has proven successful for existing SAW devices.

4. Existing data: parameters for equivalent circuits are widely available (see Section 3.3.5) and could be used as a basis for sensor models.

There are, however, some disadvantages to the system modelling approach:

1. No direct information on the strain state of the device: as the model is abstracted from mainly electrical parameters, strain values are inferred rather than directly calculated.

2. Existing work only covers unstrained devices: as previously mentioned, existing analysis approaches are designed for filters, and assume that the substrate is unstrained. Most of the published work on SAW sensors is experimental in nature, and so the models would need to be expanded.

Given that neither the device level nor the system level approach is ideal for the project, it was decided to incorporate both in a new custom simulation [155]. A coupling-of-modes model (see Section 4.4) was chosen as the core simulation tool, augmented where appropriate with device level modelling (see Section 4.5).

COM has the following advantages for this project [156]:

- **Transparent, modular structure:** of all the system level models, COM offers arguably the most natural approach, being based on wave physics rather than circuit theory. This is especially true for SAW resonators, where the interactions between incident and reflected SAW are crucial to device operation. Additional physical effects such as strain can be added to the model as required, and the modular structure allows different device configurations to be easily tested.

- **Accurate simulation of narrowband devices:** the SAWR strain sensors may be classed as narrowband Rayleigh wave devices with weak coupling, and the COM approach is very accurate for these components.
• Small computational requirements: in many cases analytical solutions can be obtained for device parameters, thus enabling fast processing of simulations.

Naturally, some disadvantages must also be contended with:

• Accurate COM parameters required: as with other phenomenological methods, the accuracy of the model is dependent both on the quality of the assumptions made (e.g., the surface wave type) and on the precision of the independent parameters. Care was taken at the design stage to have the devices operating in well-defined modes (see Section 3.3), which strengthens the assumptions, but the independent parameters must still be determined.

• Only surface waves simulated: the coupled waves are represented by a single quantity (usually the normalised power), and thus additional disturbances such as bulk waves are not normally simulated. The formulation could be extended to cover different wave types within a single model, though for SAW devices the surface wave behaviour is dominant by design.

• One-dimensional analysis: the basic COM approach is one-dimensional, and thus effects such as diffraction are not modelled. An additional COM model could be used to model transverse waves in the SAW structures, but this is generally not required.

• No modelling of parasitics: COM modelling deals exclusively with wave propagation, so electrical parasitic effects (e.g., from bond wires, packaging etc.) must subsequently be added with equivalent circuits.

The device level approach is mainly used in the determination of the independent COM parameters (see Section 4.5). FE or conventional elastic analysis can be used to examine the complex biasing fields near the substrate surface which occur when the sensor is loaded. This analysis can be static or low frequency in nature, given that the measurand varies far more slowly than the SAW field, and allows arbitrary biasing conditions to be applied. The results are then used to calculate the COM parameters and biased device geometry. Therefore only these components,
rather than the basic model itself, need to be sensitive to external loads. This technique combines the advantages of both the device and system level approaches while minimising the main disadvantages. It should be noted that a similar technique has recently been independently developed for liquid sensors \[157,158\].

A pressure sensor designed using the COM model has also been reported \[159\], though here the applied biases are not integrated into the COM parameters, nor are they used to predict device performance. Both of these applications emphasise the flexibility of the approach.

### 4.4 COM analysis

The coupling-of-modes approach was introduced by Pierce in 1954 \[160\] to model the interaction between wave modes in arbitrary media. The analysis was general in nature and lent itself in particular to the study of wave propagation in periodic media, where coupling is an important consideration. This field of wave propagation covers a huge number of phenomena: a comprehensive review may be found in \[161\], while a modern review of coupled-mode approaches to the theory may be found in \[162\]. The COM approach can be used to analyse modes coupled in time or, as is the case for SAW devices, in space. The spatial description actually describes coupled waves rather than modes: each mode of a waveguide consists of a forward and a backward wave \[163\]. COM was first used to analyse surface wave devices in 1976 \[164\], and has developed into a popular modelling tool; some useful introductions to the technique for SAW work may be found in \[40\] and \[93\]. The nomenclature and approach used in this section follows the excellent paper by Plessky and Koskela \[156\], with references to other works where appropriate.

#### 4.4.1 COM fundamentals

When a wave is incident on a periodically perturbed region (such as a grating), strong reflections occur if the period of the grating \( p \) is equal or close to half of the wavelength, i.e., \( \lambda \approx 2p \). This is known as the Bragg condition and is fundamental to all types of waves; SAW nomenclature has been used here for convenience. A
weak perturbation is presumed, and the wavenumber $\beta$ is defined as:

$$\beta = n\frac{\pi}{p} + q$$  \hspace{1cm} (4.1)

where $n$ is an odd integer harmonic number and $q \ll \pi/p$: $q$ is used to represent small deviations from the structure wavenumber $\pi/p$. The reflected waves from the periodically perturbed region are in phase and constructively interfere. This means that even if the reflection coefficient of each perturbation is small, almost total reflection of the incident wave can be achieved with a sufficient number of reflectors. Wave propagation in a perturbed medium may be described by the loaded wave equation \[161\], the solutions to which may be decomposed as an infinite set of discrete Floquet harmonics. It can be shown that these harmonics are not independent but are in fact coupled to each other, implying that an infinite system of linear equations must be solved in order to obtain a full solution. Algebraic methods can be used to truncate high-order harmonics, thus allowing numerical solution of a simpler system: full details may be found in \[156\]. A more popular approach (detailed below) uses differentiation to linearise the truncated equations: this allows local wave changes to be modelled, and is more useful for practical SAW device work.

The coupled-mode analysis only considers wave behaviour in a narrow frequency range around the centre frequency $f_0 = v/2p$ (see Section 2.4.1). Although the Floquet harmonics are usually only weakly coupled, this choice of frequency range means that two harmonics (the incident wave component and its Bragg reflection, i.e., $n = 1$ and $n = -1$ in equation (4.1)) interact very strongly and dominate the wave field. Thus only these harmonics need to be modelled, and the wave field as a function of position $x$ may then be represented as:

$$\psi(x) = \psi_+(x) + \psi_-(x) = \psi_+ e^{-iqx}e^{-i\pi x/p} + \psi_- e^{-iqx}e^{i\pi x/p}$$  \hspace{1cm} (4.2)

An $e^{i\omega t}$ time dependence is assumed throughout this analysis. Figure 4.2 depicts an IDT with the counter-propagating waves $\psi_+$ and $\psi_-$, applied voltage $V$ and busbar current $I(x)$. Note that the period $p$ is defined as the distance between the centreline of each electrode. The field $\psi(x)$ may be used to represent any wave amplitude quantity (e.g., displacement, stress, potential etc.), but is usually
4.4. COM ANALYSIS

normalised to the wave power, i.e.:

\[ P(x) = \frac{|\psi_+(x)|^2 - |\psi_-(x)|^2}{2} \]  

(4.3)

The \( e^{\pm i\pi x/p} \) components of equation (4.2) vary much more quickly than the \( e^{-iqx} \) components as \( q \ll \pi/p \), and these represent the normal phase behaviour of the wave. By contrast, the \( e^{-iqx} \) components effectively show the frequency response as the wavenumber is varied. It is thus useful to express the counter-propagating waves as follows:

\[ \psi_+(x) = R(x)e^{-i\pi x/p} \]
\[ \psi_-(x) = S(x)e^{i\pi x/p} \]  

(4.4)

where \( R(x) \) and \( S(x) \) represent the slowly-varying wave fields. Following differentiation and back substitution into the loaded wave equation, it may be shown that the COM equations for a general SAW device structure are given by [156]:

Figure 4.2: IDT with COM wave parameters
These equations represent the core of the COM model. To model the behaviour of a particular structure, five parameters must be independently determined:

- The effective SAW velocity \( v \)
- The SAW attenuation \( \gamma \)
- The electrode reflectivity \( \kappa \)
- The transduction coefficient \( \alpha_s \)
- The capacitance \( C \)

The detuning parameter \( \delta \) provides basic frequency response information and is defined as:

\[
\delta = \frac{2\pi(f - f_0)}{v} - i\gamma
\]  

Asterisks in equations (4.5) denote complex conjugation. The electrode resistance could also be added to the model as an extra parameter, but it was decided to treat this separately (see Section 5.1.7). It should be noted that only dummy COM parameters will be used in the following sections for illustrative purposes (unless stated otherwise): estimation of the actual parameter values will be discussed in Section 4.5.

In the most general case, the COM parameters are functions of position, but for the uniform structures used in this project they may be treated as constants. Therefore equations (4.5) become an inhomogeneous system of linear first-order differential equations. The general solution to this system consists of linear combinations of the homogeneous solution and a particular solution [19]. The homogeneous solution corresponds to the case where waves are incident on a shorted
structure (i.e., \( V = 0 \)), while the particular solution describes the behaviour when no waves are incident and the structure is driven by \( V \). In this treatment the structure is assumed to be lossless as power losses are generally small. For the homogeneous solution, all of the excitation and transduction terms are removed to simulate a shorted grating, producing a pair of coupled homogeneous first-order differential equations:

\[
\frac{dR(x)}{dx} = -i\delta R(x) + i\kappa S(x) \tag{4.7}
\]

\[
\frac{dS(x)}{dx} = -i\kappa^* R(x) + i\delta S(x)
\]

The solutions are assumed to be of the form:

\[
\begin{bmatrix}
R(x) \\
S(x)
\end{bmatrix} = \begin{bmatrix} R_0 \\ S_0 \end{bmatrix} e^{iqx} \tag{4.8}
\]

Equation (4.8) is substituted into (4.7), and by equating the determinant of the coefficient matrix to zero the homogeneous solution is given by:

\[
\begin{bmatrix}
R(x) \\
S(x)
\end{bmatrix} = c_1 \begin{bmatrix} 1 \\ \kappa^* \end{bmatrix} e^{-iqx} + c_2 \begin{bmatrix} \kappa \\ q+\delta \end{bmatrix} e^{iqx} \tag{4.9}
\]

with arbitrary coefficients \( c_1 \) and \( c_2 \) determined by the boundary conditions. The eigenvalues of the above system may be used to evaluate the behaviour of \( q \) around \( f_0 \):

\[ q = \pm \sqrt{\delta^2 - |\kappa|^2}, \quad \Im(q) \leq 0 \tag{4.10} \]

This is known as the dispersion equation, which shows how \( q \) varies around the structure wavenumber \( \pi/p \). Figure 4.3 plots this important equation for a frequency range around \( f_0 \). At large values of \( \delta \) (i.e., for frequencies away from \( f_0 \)), the wavenumber approaches that of the uniformly-loaded case, where no periodic perturbations are present. Close to \( f_0 \), however, the real part of \( q \) goes to zero while a strong imaginary component appears. Physically this imaginary part corresponds to the appearance of Bragg reflections, with the largest response at \( f_0 \). The choice of sign in equation (4.10) ensures that the incident wave does not
grow in the direction of propagation and that the reflected waves have an opposite phase velocity. Both the width of the stopband and magnitude of reflected waves are determined by $\kappa$, with larger reflection coefficients producing stronger dispersive effects.

The particular solution for the excited field is found by solving the first two equations of (4.5) to obtain:

$$
\begin{bmatrix}
R_E(x) \\
S_E(x)
\end{bmatrix}
= \frac{1}{q^2} \begin{bmatrix}
\delta \alpha_s + \kappa \alpha_s^* \\
\delta \alpha_s^* + \kappa^* \alpha_s
\end{bmatrix} V \quad (4.11)
$$

Combining equation (4.9) and (4.11) produces the general solution:
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4.4.2 P-matrix representation

While equations (4.5) completely describe the wave behaviour in a SAW structure, their differential nature makes them awkward to use for practical work. However, as the differential equations are linear they can be re-cast as linear equations with defined boundary conditions. Figure 4.4 shows an IDT as a three-port network, with acoustic ports at \( x_1 \) and \( x_2 \) (ports 1 and 2) and a single electrical port (port 3). Although the choice is largely arbitrary, usually the incident waves \( \psi_+ (x_1) \) and \( \psi_- (x_2) \) and the applied voltage \( V \) are taken as stimuli, with \( \psi_- (x_1), \psi_+ (x_2) \) and \( I \) treated as the structure’s response. It should be noted that due to the definition of \( p \) (see Figure 4.2), the locations of \( x_1 \) and \( x_2 \) (known as the reference planes) are displaced from the physical ends of the structure: this is used to determine the reference phases of the waves. The length of the structure is given by \( L = Np \), where \( N \) is the number of fingers, \( x_1 = 0 \) and \( x_2 = L \). The relationship between incident and response waves may be described using a P-matrix [149]:

\[
\begin{bmatrix}
R(x) \\
S(x)
\end{bmatrix} = c_1 \begin{bmatrix}
1 \\
\frac{\kappa}{q + \delta}
\end{bmatrix} e^{-iqx} + c_2 \begin{bmatrix}
\kappa \\
1
\end{bmatrix} e^{iqx} + \frac{1}{q^2} \begin{bmatrix}
\delta \alpha_s + \kappa \alpha_s^* \\
\delta \alpha_s^* + \kappa \alpha_s
\end{bmatrix} V
\]  
(4.12)

with \( c_1 \) and \( c_2 \) again determined by the boundary conditions. This solution will be used in the next section to determine the frequency response of the structure.
As mentioned in Section 4.2, P-matrices use mixed units to describe the structure’s response; each matrix element is also frequency-dependent. Although P-matrix modelling is a technique in its own right (e.g., see [145]), it is very useful for implementing the COM approach in practical devices. It should be noted that some differences in notation exist between authors depending on whether peak (as used here) or RMS values are used: some reference results are given in [93]. The $2 \times 2$ submatrix in the upper left of the P-matrix describes how incident waves are scattered by the structure, while the other terms describe the transduction and admittance behaviour. Each P-matrix element may be calculated from the general solution of equation (4.12) with appropriate boundary conditions [165]. The boundary conditions for the scattering terms are that $V = 0$ and that incident waves on the structure are described by equation (4.4):

$$R(0) = \psi_+(0)$$
$$S(L) = (-1)^N \psi_-(L)$$

Similarly, the transduction terms presume that the structure is driven by $V$ and that no incident waves are present. For example, $P_{11}$ (the reflection coefficient at port 1) is the ratio of the reflected waves (propagating right-to-left) to the incident waves (propagating left-to-right) at port 1, with no incident wave at port 2:

$$P_{11} = \frac{\psi_-(x_1)}{\psi_+(x_1)}, \quad \psi_-(x_2) = 0$$

As no transduction is taking place (waves are simply reflected), the general solution of equation (4.12) reduces to that of (4.9). Applying the boundary condition allows $c_1$ and $c_2$ to be calculated, and after extensive simplification it may be shown that:

$$P_{11} = \frac{i \kappa^* \sin(qL)}{q \cos(qL) + i \delta \sin(qL)}$$
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Figure 4.5: Magnitude of reflection coefficient $|P_{11}|$ for different normalised reflectivities $\kappa L$

Figure 4.5 shows the behaviour of $|P_{11}|$ (which is dimensionless) around the centre frequency for different values of reflectivity $|\kappa L|$; it should be noted that in general all P-matrix elements are complex. The normalised reflectivity $\kappa L$ is used here as $P_{11}$ depends on both $\kappa$ (see Section 4.5.4) and the length of the particular structure; negative $\kappa$ values will be used in this section for illustrative purposes. It is clear that as $|\kappa L|$ is increased a distinct stopband appears around $f_0$ with a fractional bandwidth of $\Delta f/f_0 = \pm \kappa p/\pi$, within which $|P_{11}| \to 1$ as $|\kappa L| \to \infty$; the phase is linear through $f_0$. The reflection coefficient at port 2 may be found in a similar manner:

$$P_{22} = \frac{i\kappa \sin(qL)}{q \cos(qL) + i\delta \sin(qL)}$$  \hspace{1cm} (4.17)
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The $P_{12}$ and $P_{21}$ elements are the dimensionless transmission coefficients, which give the ratio of the transmitted waves at one port relative to the incident wave at the other port:

$$P_{12} = \frac{\psi_-(x_1)}{\psi_-(x_2)}, \quad \psi_-(x_1) = 0$$

$$P_{21} = \frac{\psi_+(x_2)}{\psi_+(x_1)}, \quad \psi_-(x_2) = 0$$ (4.18)

SAW devices exhibit reciprocity (i.e., device characteristics are unchanged if input and output ports are exchanged [93]), and thus it may be shown that $P_{12} = P_{21}$. Following a similar procedure to that used for $P_{11}$, the transmission coefficients may be defined as:

$$P_{12} = P_{21} = \frac{(-1)^N q}{q \cos(qL) + i \delta \sin(qL)}$$ (4.19)

The sign term in the numerator denotes whether the fields are equal at both ends of the structure (for an even number of electrodes) or opposite (for odd $N$) [156]. Figure 4.6 shows the transmission behaviour near $f_0$ with the same parameters as used in Figure 4.5. When operated away from the centre frequency, almost total transmission is achieved (i.e., $|P_{12}| \approx 1$), but the reflective behaviour near $f_0$ means that only a small fraction of the incident wave power is transmitted.

The transduction terms are slightly more complicated in that the particular solution of equation (4.11) must be used, but the solution procedure is broadly the same. $P_{13}$ and $P_{23}$ denote the conversion efficiency (voltage-to-SAW) of the structure (in units of $\sqrt{\text{A/V}}$), while $P_{31}$ and $P_{32}$ denote the SAW-to-current conversion efficiency (in the same units). $P_{13}$ and $P_{23}$ may be defined as:

$$P_{13} = -L \frac{\sin(qL/2)}{qL/2} \frac{(\delta \alpha_s^* + \kappa \alpha_s) \sin(qL/2) - i \alpha_s q \cos(qL/2)}{q \cos(qL) + i \delta \sin(qL)}$$ (4.20)

$$P_{23} = -(-1)^N L \frac{\sin(qL/2)}{qL/2} \frac{(\delta \alpha_s + \kappa^* \alpha_s) \sin(qL/2) - i \alpha_s q \cos(qL/2)}{q \cos(qL) + i \delta \sin(qL)}$$ (4.21)
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Transmission coefficient behaviour around $f_0$

Figure 4.6: Magnitude of transmission coefficient $|P_{12}|$ for different normalised reflectivities $\kappa L$. 

$|P_{12}|$

$\frac{f-f_0}{f_0}$

- $\kappa L = -0.5$
- $\kappa L = -1.0$
- $\kappa L = -5.0$
Reciprocity can again be used to reduce the number of independent elements, thus producing $P_{31} = -2P_{13}$ and $P_{32} = -2P_{23}$. When the structure is non-reflective (i.e., $\kappa = 0$), the $|P_{13}|$ behaviour is similar to that shown in Figure 2.9 with a symmetric, sinc-like response about $f_0$ and a peak magnitude proportional to $L$. Figure 4.7 shows the effect of reflectivity on the $|P_{13}|$ response. The reflectivity not only increases the voltage-to-SAW transduction efficiency but shifts the maximum response to a slightly lower frequency (as $\kappa < 0$). As noted in [166], internal reflections in a transducer shift the maximum response towards the low-frequency edge of the stopband (for $\kappa < 0$): this property will become significant when whole SAW resonators are considered in the next section.

The $P_{33}$ element is perhaps the most important for analysis as it gives the admittance $Y = G + iB$ of the structure in the absence of incident waves. This
is inverse of the impedance, and is measured in $\Omega^{-1}$. In the same way that the resistance of a strain gauge changes in response to loads, the frequency response of the impedance (or admittance) may be used for SAW sensor measurements. $P_{33}$ may be defined as \[156\]:

$$P_{33} = P_{33}^{sc} + P_{33}^E$$

where:

$$P_{33}^{sc} = -\frac{4}{q^3} \left( \frac{\left(\delta^2 + |\kappa|^2\right)|\alpha_s|^2 + 2\delta \Re(\kappa^\ast \alpha_s^2)}{q \cos(qL) + i\delta \sin(qL)} \right)$$

$$+ \frac{4i}{q^3} \left( \frac{\delta |\alpha_s|^2 + \Re(\kappa^\ast \alpha_s^2)}{q \cos(qL) + i\delta \sin(qL)} \right)$$

$$P_{33}^E = -L4i \frac{\delta |\alpha_s|^2 + \Re(\kappa^\ast \alpha_s^2)}{\delta^2 - |\kappa|^2} + i\omega CL$$

The first term of equation (4.22) describes the electrical response due to non-uniform SAW distribution along the structure, in particular that caused by end effects: these are generally small for long structures. The second term, which models the excited field response, is dominant for most practical structures where $|\Im(q)L| \gg 0$ \[166\]. Figure 4.8 plots the $P_{33}^E$ behaviour of an IDT near the centre frequency. In common with $P_{13}$, the response is downshifted from the nominal centre frequency of the structure due to reflectivity effects. The resonance occurs at the low-frequency edge of the structure’s stopband due to constructive interference of the counter-propagating waves; no distinct response is observed at the high-frequency edge due to destructive interference.

It should be noted that considerable simplification in the transduction and admittance P-matrix terms is possible if a bidirectional, uniform structure is considered: details are given in \[156\]. This, however, requires that both the IDT and the propagating waves act bidirectionally. In general the COM parameters are complex and vary considerably with propagation direction (see Section 4.5), thus some asymmetry will typically be found. In particular cases this can be used to advantage in unidirectional devices with conventional IDTs \[167],[168\]: an intro-
4.4.3 SAW device response

One of the most useful properties of the P-matrix approach is that individual structures can be cascaded. All practical SAW devices consist of at least two SAW structures (IDTs, reflectors etc.) which interact to give the total device response. The 1-port SAW resonators used in this project, for example, consist of a single IDT and two reflector gratings which are designed to resonate at a particular frequency. Cascading is performed by electrically connecting the structures in parallel, while at least one of the acoustic ports is common to both structures (e.g., port 2 of the IDT is equivalent to port 1 of the reflector grating). Formulae for cascading arbitrary structures are presented in [169], while combining large
numbers of identical P-matrices is considered in [170]. These techniques allow complicated structures to be described by their simpler constitutive parts. For example, each electrode in an apodised IDT (see Figure 2.10) could be described by an individual P-matrix, which may then be cascaded to form the total transducer response. The total admittance $Y$ of a 1-port resonator using P-matrix cascading is given by:

$$
\begin{bmatrix}
0 \\
0 \\
Y
\end{bmatrix} =
\begin{bmatrix}
(P_{11}^r P_{22}^r - 1) & P_{12}^r P_{11}^r & P_{13}^r \\
(P_{22}^r P_{11}^r - 1) & P_{23}^r \\
-2P_{13}^r P_{22}^r & -2P_{23}^r P_{11}^r & P_{33}^r
\end{bmatrix}
\begin{bmatrix}
\psi(x_1) \\
\psi(x_2) \\
1
\end{bmatrix}
$$

(4.25)

where the IDT extends from $x_1$ to $x_2$ and the $r$ superscript refers to reflector P-matrix elements; all of the others belong to the IDT. In most cases the reflectors are physically displaced from the IDT reference planes, thus introducing a $e^{-i2\omega x/v}$ phase term to the reflector P-matrix elements [156]: $v$ in this case is taken as the SAW velocity between the IDT and reflector structures. Figure 4.9 shows how the IDT-reflector gap distance $g$ is defined, with the reference planes of the structures offset from the physical structure as before. Equation (4.25) can be evaluated analytically for bidirectional structures, enabling very fast calculation of a device’s frequency response. In general, however, numerical methods must be used for more complicated devices, especially those with more than one transducer.

As introduced in Section 3.3.5 two different types of SAW resonator are used in this project: optimal and synchronous. Each of these resonator types is imple-
mented in the device designs by varying $g$. Optimal designs position the reflectors such that the resonant response is maximised through in-phase reflection of the incident waves. This requires that the total phase shift of the SAW within the resonant cavity is a multiple of $\pi$ \cite{40}. If $\kappa$ is assumed to be real and IDT reflections are ignored (as was the case here), optimal sensors may be implemented by having $g = 3.5a$, where $a$ is the electrode linewidth. It should be noted, however, that $\kappa$ is complex for most propagation directions (see Section 4.5.4) and reflections may be significant in some IDTs, both of which would affect the optimal $g$. While having the optimal resonant performance is obviously desirable, there are some practical problems with the design. The resonant frequency is dependent on the reflectivity of the electrodes \cite{72}, which varies due to fabrication tolerances (see Section 4.5.4), and thus exact frequency responses can be difficult to predict. A second issue is that $g$ must be tightly controlled, which can be challenging when high-frequency devices (with narrow linewidths) are to be fabricated. Figure 4.10 plots the admittance response of an optimal device. Device dimensions and COM parameters in this case were taken from \cite{171}, which fitted theoretical parameters to experimental measurements of synchronous SAW resonators with excellent results. The one-port synchronous SAWR in this study used the ST-X quartz propagation direction with $p = 3.932\mu m$, $W = 200p$, 50 IDT pairs, 300 reflectors per grating, Al electrodes with $h = 160nm$ and $\eta = 0.5$. An optimal response was simulated in Figure 4.10 by setting $g = 3.5a = 1.75p$. The behaviour is similar to that of the IDT shown in Figure 4.8. Some ripples may be observed, caused by the finite lengths of the structures, and both the conductance and susceptance curves are DC shifted by the device’s resistance and capacitance, respectively.

Synchronous designs use reflector sections which directly follow the periodicity to the IDT, i.e., $g = 2a$. These devices are easier to manufacture than optimal designs as the resonator is effectively one long grating. Another advantage is that the periodicity of the reflectors is the same as that of the IDT; optimal designs often have different period lengths in each structure, though this feature was not used for the optimal sensors in this project. The constant periodicity means that the resonant frequency is almost independent of the reflectivity, and thus tight frequency tolerances can be achieved. A major disadvantage of these devices is that the resonant behaviour is degraded due to the imperfect placement of the reflec-
Admittance behaviour of an optimal SAWR near $f_0$. COM parameters taken from [171]: $\nu = 3146.3621$ (m/s), $\kappa_p = -0.014973$, $\alpha_p = 2.705 \times 10^{-4}$ ($1/\sqrt{\lambda \Omega}$), $C = 1.9474$ (pF), $\gamma_p = 3.823 \times 10^{-4}$ (Neper/$\lambda$), $R = 21.6397$ ($\Omega$). The $p$ subscript is explained in Section 4.5.4.
Figure 4.11: Simulated admittance behaviour of a synchronous SAWR near $f_0$. COM parameters are the same as those in Figure 4.10.

tors. Figure 4.11 shows the admittance response of a synchronous device with the same parameters as that shown in Figure 4.10, only $g$ was changed. Strong ripples can now be seen on the low-frequency side of the stopband: these are due to the resonance occurring near the edge of the band. The conductance peak is much smaller than that of the optimal device, and some small ripples may be seen on the high-frequency stopband edge. The results plotted in Figure 4.11 show excellent correlation with those presented in [171] for the same COM parameters, thus verifying the model used here.

Figures 4.10 and 4.11 demonstrate the power and flexibility of the COM approach for modelling SAW devices. In comparison to other techniques such as equivalent circuits, COM provides detailed frequency response information from a relatively simple model: compare, for example, the response given in Figure
3.11 to those produced by COM. While simpler models may be sufficient in some applications, SAW sensor networks with multiple devices require the most accurate response information, particularly where the sensors have small frequency separations. In this case, ripples in the frequency response of one device can degrade the responses of others, even if the primary resonant responses are distinct.

In the next section, modifications to the COM model to account for biasing effects will be discussed.

4.5 COM modelling of SAW strain sensors

The basic COM analysis presented in Section 4.4 addresses two of the modelling factors mentioned in Section 4.1, i.e., the design parameters of the sensors and the interrogation signal properties. The effect of the applied biases must be dealt with through modifications of the model. To the author’s knowledge, the coupling-of-modes approach has not been used to model the response of SAW strain sensors to measurands, though liquid sensor applications have been reported (see Section 4.3). Some excellent work on the strain sensitivity of SAW devices as a function of temperature is presented in [15]. Although this paper does not provide a model of strain and temperature effects, its treatment of the loaded piezoelectric equations inspired much of the work below.

As mentioned in Section 4.3, the effects of applied biases on the SAW sensors will be implemented by modifying the independent parameters in the COM model (see equation (4.5)) and the device geometry. The approach detailed in Section 4.4 is general in nature, and thus only minor additional assumptions are required to model biasing effects:

- **Small loading effects:** the COM approach is based on small perturbation theory, and thus the loading effects should be small. For example, large strain fields causing gross distortion of the substrate may introduce waveguiding effects which would not be modelled. This is not an issue for the SAW sensors as they are substrate-limited to strains of $< 0.002$ (see Section 3.3.2). Other biasing effects (e.g., extreme temperatures or strong electrical fields)
may be included through the higher-order coefficients of the substrate material if required.

- **Homogeneous biasing fields within each COM structure**: as mentioned in Section 4.4.1 the COM parameters are constants for uniform, unbiased structures. To retain this relationship, it is useful to assume that the biasing fields within each structure are also uniform. Even if the applied biases on the substrate are homogeneous, some stress concentrations may occur at the electrode-substrate interfaces (see Section 4.5.1), but these are assumed to be local and not to affect the performance of the structure as a whole. Similar effects are expected at the substrate-component interface, but these are distant from the active SAW region. It would be possible to split the P-matrices of the structures into regions where individual loading effects are present and then use cascading [158], but this was considered unnecessary here as small biasing field gradients are assumed. The basic COM model already allows each structure to have different properties, and thus the biasing fields in each reflector grating, for example, may be different from those in the IDT.

The determination of the independent parameters is a very important aspect of any COM model, and several different approaches have been developed:

- **Classical methods**: these use perturbational and variational theory to model devices with thin electrodes: some of these approaches are detailed in the following sections, and extensive references are given in [156]. The main advantage of these classical approaches, especially for sensor applications, is that the COM parameters are often expressed in terms of the device dimensions (e.g., the relative electrode height) or the properties of the propagating waves. Thus, if the responses of these dimensions and wave properties to applied biases are known, the COM parameters can (in theory) be made sensitive to the biases. The assumption of thin electrodes with small perturbations limits these methods to certain classes of SAW device, and naturally can only account for a limited number of factors affecting the COM parameters. Nevertheless, they provide valuable information on the behaviour of these variables.
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- **Experimental fitting**: this can be used to fit the COM model to measured electrical responses, thereby revealing the COM parameters [172], and is usually the most accurate method. However, the results are generally only valid for the particular fabrication system (at best), and often only for the device under test. An interesting implementation of this approach is given in [171], where nonlinear numerical optimisation is used with good results. It should be noted that some of the fitted parameters in this study differed by almost 30% from those predicted by classical methods. No information is given on the bias sensitivity of the COM parameters, and optimisation routines must be carefully constrained to give valid results.

- **Numerical methods**: most modern techniques for COM parameter extraction use numerical methods, especially where thick electrodes are employed. Finite and Boundary Element approaches are the most popular, and estimation of just the COM parameters is much faster than the complete numerical simulations mentioned in Section 4.3. However, the accuracy of the results is often insufficient for design work, generally because the exact parameters of a real device are not known [156], a disadvantage shared with the classical methods.

The following sections detail the application under consideration and how the COM parameters are sensitive to this. While the frequency response of the impedance (the measurand) is sensitive to all of the parameters, the magnitudes of these sensitivities vary considerably, and their relative importance depends on what aspect of the frequency response is being analysed. For 1-port SAW resonators, the key feature is usually the peak in the admittance response (see Figures 4.10 and 4.11), though the results developed in the following sections are applicable to any aspect of the response.

### 4.5.1 Modelled application

Given the range of potential applied biases (e.g., mechanical, electrical, thermal etc.), it is important to consider a particular application for analysis. It should be
noted that any applied bias could be considered provided that it affects the COM parameters in some fashion.

Figure 4.12 shows the application under consideration. The SAW sensor is bonded to a beam which is under flexure from applied forces $F$. This is the loading case used in the main international standards for strain gauge calibration ([173] and [174]), which will be discussed in Section 5.2.1. A biased state is induced in both components by a combination of applied loads on the beam and temperature effects. It is important to note that the desired measurand is the strain on the beam surface caused only by the applied loads, not the total strain or that caused by temperature. Many modern foil resistive strain gauges are specified as being ‘self-temperature-compensated’. These devices use foil materials with approximately the same coefficient of thermal expansion as the component’s material [4]. This means that the thermal output of the gauge (the strain caused by thermal expansion) is minimised and can be compensated for.

For this particular application, some assumptions have been made to simplify
the analysis:

- **Absence of temperature effects**: as mentioned in Section 4.1, the modelling of temperature effects is outside the scope of this work. The experimental testing was performed at room temperature (see Section 5.2.1). This is significant as the material constants of the sensor materials are most commonly determined (and therefore most accurate) at this temperature, while the temperature derivatives of these are more difficult to quantify: a discussion is given in Section A.2. Although temperature effects could be included in the model in a straightforward manner, the clarity of the model is improved by omitting them in this discussion.

- **Mechanical-only biases**: it is presumed that only mechanical biasing fields are present during testing, and that biasing terms from other sources (e.g., electrical, magnetic etc.) are ignored. Again, this closely matches the experimental setup. Quartz has weak coupling to these other sources in any case, and so their effects would be small.

- **Perfect interfacial bonds**: the electrode-substrate and substrate-beam bonds are assumed to be perfect in order to simplify the bias modelling.

In preparation for its use in the COM parameters, the mechanical biasing state for this application was investigated. Analytical treatments of such states in anisotropic materials are challenging, even for simple beam bending scenarios; analysis of equivalent isotropic scenarios are, by contrast, elementary. Formative work on the deformation of anisotropic crystals was performed by Mindlin [175], [176], which treated the vibrations of anisotropic plates in various modes; further details may be found in [34]. While these analytical techniques are useful for simple geometries and loading cases, they are cumbersome to use for SAW sensor installations such as that shown in Figure 4.12. In this case the sensor is indirectly loaded through its bonding to the beam, and thus defining the stress state is more difficult. Force equilibrium along the sensor/beam cross-section could be used to find both the stress and strain states, but again this is complex for anisotropic materials with arbitrary symmetry. Many analyses of strain gauge
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applications simply consider that the effect of the sensor on the strain state is negligible (as ideally it should be), and that the strain on the gauge is identical to that on the strained component’s surface. Given that the SAW sensors have thick, stiff substrates (relative to conventional strain gauges), it was decided to analyse the sensor and beam as a composite body.

The device level modelling introduced in Section 4.3 can be used to analyse such a composite body. The sensor/beam composite has large differences in scale, e.g., ratio of electrode thickness to substrate thickness to beam thickness is about 1:3000:70000. Therefore, the modelling was performed in two stages:

- The substrate/beam composite was modelled first in order to find the general stress/strain behaviour in the SAW propagation region.
- The substrate/electrode composite was then modelled to determine the local influence of the structures. Applied loads on the substrate were determined from the substrate/beam model.

For a simply-supported beam of an isotropic material in pure bending, the normal stress along $x_1$ is given by [1]:

$$T_{11} = -\frac{M_3 x_2}{I_3} \quad (4.26)$$

where $M_3$ is the bending moment about the $x_3$ axis caused by the applied forces (see Figure 4.12), $x_2 = 0$ is at the midpoint of the beam thickness and $I_3$ is the 2nd moment of area about the $x_3$ axis. This simple result was used to validate an ANSYS v8.1 [153] model of the bending beam. The effect of mounting holes along the beam’s neutral axis (see Section 5.2.1) on the stress/strain behaviour at the beam surface was found to be negligible, and thus these were excluded from the model. A substrate/beam model was then created using an attached quartz volume with appropriate stiffnesses. For simplicity, only linear elastic, rather than piezoelectric, behaviour was modelled. The model size was reduced to the region in the centre of the beam where the SAWR is attached. It should be noted that although symmetry about the $x_1 = 0$ and $x_3 = 0$ planes could be employed in some cases, this was not used here as arbitrary substrate orientations were to be modelled. Bending stresses were calculated from equation (4.26) and the beam geometry;
Figure 4.13: Contour plot of $T_{11}$ for substrate/beam composite under bending stress; applied stresses are normal to the YZ plane of the beam.

these were then applied to the positive and negative $x_1$-faces of the beam. Figure 4.13 shows a plot of $T_{11}$ through substrate/beam composite; numerical results will be discussed in Section 5.3. As expected, the attached substrate only had a local effect on the stress/strain behaviour of the beam, given that its stiffnesses are much lower than those of the beam material (typically steel). The variable stress through the beam thickness can clearly be seen, as can the stress discontinuities at the substrate/beam interface. No large $T_{11}$ gradients were evident in the SAW propagation region, though the stress does change rapidly near the substrate edges. The applied $T_{11}$ on the beam induces an essentially biaxial stress state at the centre of the substrate surface: $T_{11}$ is dominant, while $T_{33}$ is only significant for some orientations, and the shear stresses are generally small.

The substrate/electrode model was created in the same fashion to analyse the effect of the electrodes on this stress state. A substrate volume $\lambda$ long, $\lambda/2$
Substrate with Attached Electrodes

Figure 4.14: Contour plot of $T_{11}$ for substrate/electrode composite under uniaxial stress; applied stresses are normal to the YZ plane of the substrate

wide and $\lambda/2$ thick was used, with appropriately-scaled Al electrodes; symmetric boundary conditions were used at the $x_3$ faces. The uniaxial stress from the substrate/beam model at $x_1 = 0$ was applied to the substrate ends. Figure 4.14 shows a contour plot of $T_{11}$ at the electrode/substrate interface. The metallised sections of the substrate surface demonstrate significantly lower stresses than the free surface, as would be expected: the effects of electrode loading will be discussed in Section 4.5.3. By contrast, the thin electrodes have a negligible effect on the overall stress state in the substrate. Therefore it was decided to treat the bias state in the SAW sensor as being equal to that of its substrate, with loading effects of the electrodes contained in the biased SAW velocity.
4.5.2 Geometric effects

The COM model requires only a few dimensional parameters: the width $a$ and height $h$ of each electrode, the SAW wavelength $\lambda$, the aperture $W$ and structure length $L$. For the IDTs designs used in this project $\lambda = 4a$, $W = 45\lambda$ and $L = Np = 2Na$. Each electrode may be treated as a long, thin strip: the ratio of $a$ to $h$ for the electrodes used in this project is about 11:1, while the ratio of $h$ to $\lambda$ is about 0.02:1. This latter ratio is important as perturbation methods for determining COM parameters presume that the electrodes are thin ($h/\lambda \approx 0.01$), which is a fair assumption here. It may also be assumed that the electrodes are homogeneous Al as the Cr adhesion layer is very thin (see Section 3.4.5), and that the material properties are isotropic given that the Al was deposited using evaporation.

The strain due to the applied mechanical bias is given by the generalised Hooke’s law of equation (2.13):

$$S_{ij} = s_{ijkl}T_{kl}$$

(4.27)

where $S_{ij}$ is the strain due to applied loads, and the compliance (i.e., the inverse stiffness \[^{[18]}\]) $s_{ijkl}$ of the material is used here to invert the original formula. The only unknown here is the substrate stress $T_{kl}$, which depends on the loading conditions of the substrate (see Section 4.5.1). $S_{ij}$ is used to find the strained values of $a$ and $h$, which are related to the other dimensions as above. Increased values of $a$ reduce the resonant frequency of a SAW resonator in the COM model, as would be expected, and also lead to small increases in the peak conductance magnitude, with small decreases in the frequency separation of ripples at the stopband edges. Similarly, increased values of $h$ also decrease the resonant frequency.

4.5.3 Strained SAW velocity

In order to calculate the effective SAW velocity $v$ used in the COM model, and to make it sensitive to strain, the free-surface SAW velocity procedures outlined in Section 2.3 must be revisited. These assume that the substrate is unbiased, and thus that the velocity $v$ depends only on the substrate’s material properties and
boundary conditions. However, the velocity of acoustic waves in elastic media can display stress dependence, a coupling known as acoustoelasticity \[177\]. The first reference to the change in SAW velocity with strain was made in 1973 where it was used to change filter behaviour \[178\]: sensor applications were introduced in \[78\]. Measurements of strained SAW velocity for different quartz cuts were presented in \[179\], which demonstrated that the strain sensitivity changed significantly with substrate orientation. Much of the early modelling work was performed by Nalamwar and Epstein, who proposed that the change in velocity was the resultant of changes in elastic constants, density and the equations of motion \[180\]. It was shown that although these changes almost cancel out for some crystal orientations, the net effect can be significant, particularly for layered substrates \[181\].

The approach used in this project is based on that originally presented in \[182\]. Rather than empirically adding the effects of strain to the velocity as was done previously, this work includes the strain effects in the fundamental piezoelectric equations (see Section 2.2). It is a particular case of the seminal work presented by Baumhauer and Tiersten \[183\], which deals with small fields superposed on a bias in electroelastic (i.e., nonlinear piezoelectric) media. In the absence of biasing fields, the piezoelectric equations presented in Section 2.2 are the correct linear limit of the properly invariant equations of nonlinear electroelasticity (the most general description of piezoelectricity) for infinitesimal deviations from an ideal reference state. However, if such biasing fields exist, the constitutive equations are not those of linear piezoelectricity, and higher-order terms must be considered even though the total fields (bias plus small deviation) may be within the linear range of the material \[184\]. Baumhauer and Tiersten’s approach includes higher-order biasing fields in the nonlinear constitutive equations, which are then linearised around the biasing state to form tractable expressions. Thus ‘effective’ material constants are formed which can be used in equations (2.18) and (2.19). This approach has given excellent predictions of device behaviour in previous works, with close correlation between experimental and theoretical results over a range of biasing states (e.g., \[182\], \[185\] and \[144\] etc.). These studies assumed that the biased state of the SAW device is equal to that of the substrate, as was detailed in Section 4.5.1 For the SAW strain sensors, three substrate states may
be defined:

1. The initial state, where no external loads are applied and no SAW propagation exists.

2. The intermediate state, where applied loads on the substrate cause static biasing fields (i.e., the biased state).

3. The final state, where both the external bias and SAW propagation exist.

It should be noted that the analysis of biased electroelastic bodies is extremely general in nature: an excellent modern review of the field is given in \[186\]. For an arbitrary bias, all three sets of material constants (i.e., $c_{ijkl}$, $e_{kij}$ and $\varepsilon_{ij}$, see Section 2.2) in the piezoelectric equations will have higher-power biasing terms. However, as was done in Section 4.5.1, the complexity of these terms can be reduced by consideration of the target application. The analysis below only includes the linear effect of the mechanical biasing field on the surface waves as the applied strains are assumed small. Similarly, products of the biasing field and the piezoelectric constant are neglected due to the low piezoelectric coupling of quartz. With these simplifications in mind, only the second-order elastic stiffnesses $c_{ijkl}$ of the strained substrate need to be modified, and these may be redefined as \[182\]:

$$c_{ijkl}^* = c_{ijkl} + T_{il} \delta_{jk} + c_{ijklmn} S_{mn} + c_{ijpl} w_{k,p} + c_{ipkl} w_{j,p}$$

(4.28)

where $T_{il}$ is the static biasing stress, $\delta_{jk}$ is the Kronecker delta, $c_{ijklmn}$ are the third-order elastic stiffnesses, $S_{mn}$ is the static biasing strain and $w_i$ is the substrate displacement due to the static bias. It should be noted that the $c_{ijkl}^*$ are now dependent on arbitrary biasing fields rather than just the substrate orientation as before, and thus will generally display less symmetry than $c_{ijkl}$.

The nature of the applied bias has a significant bearing on how the SAW velocity should be calculated. For homogeneous biases, such as those caused by extensional stresses, the $c_{ijkl}^*$ components are also homogeneous. This means that the procedure given in Section 2.3 can be applied as normal; it is assumed that $T_{il}$ and $S_{mn}$ have been calculated previously. It has been shown that a homogeneous infinitesimal three-dimensional rotation does not produce any change in SAW velocity for homogeneous biases \[187\] and therefore can be omitted, thus $w_{j,i} = S_{ij}$.  


However, if the biases are inhomogeneous (e.g., from flexural stresses), the substrate stiffness may vary with position in both the $x_1$ and $x_2$ directions (see Figure 4.12). This is a problem for the determination of $v$ as such variation was not considered in Section 2.3 when $v$ was originally calculated. Although the SAW fields are tightly bound to the substrate surface, these do occupy a finite volume and thus the effect of the changing stiffnesses should be examined. Figure 4.15 shows a substrate with a propagating SAW and applied forces $F$ as an example: this is similar to Figure 4.12 although here the SAW substrate is directly loaded. The forces induce $T_{11}$ which, from equation (4.26), is invariant in the $x_1$ direction but varies linearly in the $x_2$ direction, with a maximum compressive value on the top surface and a maximum tensile value on the bottom surface. If the ratio of substrate thickness to SAW wavelength (and thus to SAW penetration depth, see Section 2.3) is small, $c_{ijkl}^*$ can vary considerably through the surface wave depth, and thus the SAW velocity calculations must be modified. Perturbation procedures, which can treat spatially-varying biasing fields provided the velocity change is small, are outlined in [188] and [189]. However, it is shown in [185] that, for the ratio of substrate thickness to SAW wavelength used in this project’s sensors ($\approx 70$), the perturbation procedure and the ordinary SAW velocity calculation produce almost the same results even if the substrate is directly flexed. In this application, the substrate is only attached to a much thicker beam under flexure, rather than under direct flexure itself, and thus the biases can be considered homogeneous: Figure 4.15 gives an example of this.

The use of $c_{ijkl}^*$ means that the biasing terms are naturally included in the SAW velocity calculation. Therefore the boundary conditions (see Section 2.3.2) are still applicable, and thus the procedure in Section 2.3 can be reused to find the biased $v$. It should be noted, however, that the full $c_{ijkl}^*$ tensor terms rather than the contracted $c_{ij}$ notation should be used in the determination of the biased $v$ due to the reduced material symmetry. The $c_{ijklmn}$ terms must be rotated to the propagation direction (see Section A.3), while the substrate density $\rho$ is only required in its initial, unstrained form.

The frequency of the biased wave on the free substrate surface will be affected by changes in both the SAW velocity and the wavelength. From equation (2.40), the change in frequency for an $x_1$-propagating wave is given by:
\[ \Delta f = f - f_0 = \left( \frac{v + \Delta v}{\lambda + \Delta \lambda} \right) - \frac{v}{\lambda} \] (4.29)

Simplification produces:

\[ \frac{\Delta f}{f_0} = \left( \frac{\Delta v/v - S_{11}}{1 + S_{11}} \right) \approx \frac{\Delta v}{v} - S_{11} \] (4.30)

for \( S_{11} \ll 1 \); \( S_{11} \) should be retained in the numerator as it is usually of the same order as \( \Delta v/v \). The numerator term in equation (4.30) is the fractional change in the ‘natural’ velocity \([190]\), and it is this velocity which is calculated in the biased SAW velocity procedure. It takes into account both the change in actual wave velocity and the deformed wave path. The actual fractional change in velocity for \( x_1 \) propagation is given by \([191]\):

\[ \frac{\Delta v}{v} = \frac{\Delta v_{\text{natural}}}{v} + S_{11} \] (4.31)

Although biased velocity results are usually given as natural velocities (and thus \( \Delta v_{\text{natural}}/v = \Delta f/f \)), here actual velocities will be presented. This is done in order to separate the effects of geometry change (see Section 4.5.2) from those due to changes in propagation properties, as required by the COM model used here.
An analysis of the stress results from the FE modelling (see Sections 4.5.1 and 5.3) revealed that only \( T_{11} \) (and to a lesser extent \( T_{33} \)) are significant at the substrate surface: this biaxial stress state is consistent with previous work \([192]\). Thus only the sensitivity of the velocity to these two stresses is required. Figure 4.16 shows these sensitivities as a function of propagation angle for ST-cut quartz.

The stresses are applied along the local \( x_1 \) and \( x_3 \) SAW axes which rotate in the ST plane. It is clear that the overall sensitivity varies considerably depending on the propagation angle and the magnitudes of \( T_{11} \) and \( T_{33} \). For example, a tensile \( T_{11} \) applied to a SAW propagating at 0° will cause a drop in wave velocity, while a tensile \( T_{33} \) applied at the same angle will cause an increase in velocity; the sensitivity to both stresses is about the same at 90°. Superposition can be used to find the total fractional change in velocity, i.e.:

![Graph showing actual velocity sensitivity to \( T_{11} \) and \( T_{33} \) for ST-cut quartz](image)
It should be noted that for ST-X propagation (i.e., at 0° and 180°), the results plotted in Figure 4.16 agree with those presented in [192], but for other angles they do not. The cause of this behaviour is unknown; model testing using results presented in [182], [185] and [144], which utilise a variety of loading cases but with the same modelling approach, produced excellent results.

The velocity results above refer only to the free-surface SAW velocity (see Section 2.3.3), rather than that found in each COM structure. The presence of electrodes introduces a loading on the surface which in turn induces a velocity shift. This velocity change due to a periodic array of thin electrodes may be described as a power series expansion on the relative electrode thickness [156]:

\[
\frac{\Delta v}{v} \approx \left( \frac{\Delta v}{v} \right)_e \left( \frac{K^2}{2} \right) + \left( \frac{\Delta v}{v} \right)_{m1} \left( \frac{h}{\lambda} \right) + \left( \frac{\Delta v}{v} \right)_{m2} \left( \frac{h}{\lambda} \right)^2 + \cdots \tag{4.33}
\]

The first term represents the change in velocity due to the shorting of the electrical fields by the electrodes (see Figure 2.6). \((\Delta v/v)_e\) is always negative, and as the term is proportional to \(K^2\) it is usually small for weakly-coupled substrates such as quartz. The coefficient may be related to the metallisation ratio \(\eta\) [193], [194]:

\[
\left( \frac{\Delta v}{v} \right)_e = -\frac{1}{2} \left( 1 + \frac{L_{0.5}(-\cos(\pi \eta))}{L_{-0.5}(-\cos(\pi \eta))} \right) \tag{4.34}
\]

where \(L_n(x)\) is the Legendre function of order \(n\) [42]. \((\Delta v/v)_e\) is a function of \(\eta\) only and thus is independent of the propagation direction and of homogeneous biases. The second term in equation (4.33) denotes the velocity shift due to the mass loading induced by the electrodes, and is proportional to \((h/\lambda)\). Variational or perturbational techniques may be used to derive \((\Delta v/v)_{m1}\): an analysis of these methods is given in [195]. In this project the perturbational approach presented in [194] is used, where \((\Delta v/v)_{m1}\) is given by:
\[
\left( \frac{\Delta v}{v} \right)_{m1} = \frac{\eta \pi K^2}{C_n} \left( \left| \frac{u_1}{\varphi} \right|^2 (c_1 - \rho' v^2) - \left| \frac{u_2}{\varphi} \right|^2 \rho' v^2 + \left| \frac{u_3}{\varphi} \right|^2 (c_2 - \rho' v^2) \right) \quad (4.35)
\]

where \( C_n \) is the normalised capacitance (see Section 4.5.6) and \( \rho' \) is the density of the electrode material. The coefficients \( c_1 \) and \( c_2 \) are related to the Lamé constants of the electrode material; stiffness values for Al may be found in \([45]\). An advantage of this particular form is that the biasing effects are naturally included in \( u_i \) and \( \varphi \) through the calculation of the biased \( v \) (see Section 2.3.2). The anisotropy of the substrate is also included, which has been shown to be important in the determination of \( (\Delta v/v)_{m1} \) for quartz \([195]\). Figure 4.17 shows the \( (\Delta v/v)_{m1} \) behaviour for ST-cut quartz, indicating that although considerable variation is apparent for different propagation directions, the magnitudes of the coefficients are small. Similarly, the sensitivity of \( (\Delta v/v)_{m1} \) to applied stresses was found to be negligible and can be neglected.

The third term in equation (4.33) denotes the energy storage effects due to discontinuities on the SAW propagation surface \([196]\). A perturbational procedure for metallic electrodes was presented in \([197]\) (subsequently modified in \([198]\)) which allows \( (\Delta v/v)_{m2} \) to be calculated. There are, however, significant differences between the calculated \( (\Delta v/v)_{m2} \) values presented in \([198]\) and the limited experimental measurements available (e.g., in \([40]\)), thus it is preferable to calculate \( (\Delta v/v)_{m2} \) experimentally.

The relative importance of the different \( (\Delta v/v) \) coefficients depends on the particular substrate/electrode combination \([156]\). The velocity shift for strongly piezoelectric substrates with thin electrodes is usually dominated by \( (\Delta v/v)_{e} \), for example, while for quartz the mechanical terms have a greater influence. Calculated values of \( (\Delta v/v) \) using all three of the above terms accurately predicts the ST-X behaviour measured in \([171]\) (c. -0.37%), while omitting the \( (\Delta v/v)_{m2} \) term reduces the predicted value by about half; it is clear that the velocity shift is small in either case. To the author’s knowledge, no \( (\Delta v/v)_{m2} \) results have been published for quartz orientations other than ST-X.

The biased values of \( h \) and \( \lambda \) (see Section 4.5.2) can thus be used to calculate
the electrode loading effects. Therefore, in order to calculate the correct SAW velocity for the COM model, the effect of the applied bias on the free-surface velocity must first be considered, followed by the effect of the electrode structures. It is assumed that, as the electrodes are thin, interactions between these two effects are small and thus they can be treated separately. As would be expected, increasing \( v \) in the COM model leads to an increase in the resonant frequency; the magnitude of the response is essentially unchanged.

### 4.5.4 Electrode reflectivity

The reflectivity of the COM structures has a major influence on the frequency response of the complete device. Of the reflection mechanisms outlined in Section 2.4.2 geometric discontinuity along the wave path has the greatest effect for ST
quartz substrates with thin aluminium electrodes [40], followed by the effect of piezoelectric shorting. In a similar manner to that used for the effects of electrodes on the COM velocity, the reflectivity of a periodic array may be described by a power series expansion on the relative electrode height [193],[168],[156]:

\[ \kappa \approx \frac{1}{p} \left( (\kappa)_e \left( \frac{K^2}{2} \right) + (\kappa)_{m1} \left( \frac{h}{\lambda} \right) \sin(\pi \eta) + \cdots \right) \]  

(4.36)

where:

\[ (\kappa)_e = -\frac{\pi}{2} \left( \cos(\pi \eta) + \frac{L_{0.5}(\cos(\pi \eta))}{L_{-0.5}(\cos(\pi \eta))} \right) \]  

(4.37)

\[ (\kappa)_{m1} = -\frac{\pi K^2}{C_n} \left( \left( \frac{u_1}{\varphi} \right)^2 (c_1 + \rho' v^2) + \left( \frac{u_2}{\varphi} \right)^2 \rho' v^2 + \left( \frac{u_3}{\varphi} \right)^2 (c_2 + \rho' v^2) \right) \]  

(4.38)

Here the first term accounts for piezoelectric shorting, while the second term includes mass loading and the effect of geometry changes. Expansions of \( \kappa \) to first order are usually sufficiently accurate. It should be noted that, unlike \( \Delta v/v \), \( (\kappa)_{m1} \) (and thus \( \kappa \)) may be complex, implying that incident waves may be phase shifted as well as reflected by a COM structure. Figure 4.18 shows the real and imaginary components of \( (\kappa)_{m1} \) for ST-cut quartz with Al electrodes and \( \eta = 0.5 \), demonstrating the considerable variation in reflective behaviour with propagation angle. The calculated value for ST-X propagation \( (\kappa)_{m1} = -0.50 \) is the same as that reported in [193]. For the parameters given in [171], the calculated value of \( \kappa_p \) is about -2.1%, which is larger than the fitted experimental value of -1.5%. The \( p \) subscript is used to denote COM parameters which are normalised to a unit period \( \lambda \) [156], e.g., \( \lambda = 2p \) for a conventional IDT.

The effect of biasing mechanical fields can be implemented in a similar manner to those in \( \Delta v/v \), and thus \( \kappa \) can be made sensitive to biases. \( (\kappa)_e \) is independent of propagation direction and applied biases, and like \( \Delta v/v \), it is a function of \( \eta \) only. Figure 4.19 plots the complex sensitivity of \( (\kappa)_{m1} \) to applied \( T_{11} \) and \( T_{33} \), which is analogous to the velocity sensitivity presented in Figure 4.16. The increased magnitudes at c. 35° and 145° are caused by the low unbiased \( (\kappa)_{m1} \)
of these orientations rather than increased inherent sensitivity. In general, the real and imaginary components of the sensitivity have different values, implying that applied stresses change both the magnitude and phase behaviour of $(\kappa)_m$. Some discontinuous behaviour may be noted between $80^\circ$ and $100^\circ$ which may be traced to computational issues rather than actual wave behaviour.

As demonstrated in Section 4.4.3, the distances between the COM structures, and specifically the distances between the reference planes of the IDT and reflectors, can have a major effect on device performance. This is because the phase of the reflected waves is determined both by the distances between the structures (i.e., from normal wave propagation) and by $\kappa$.

In terms of the COM model, increasing the value of $|\kappa|$ increases the peak resonant magnitude and shifts the resonant frequency, with the sign of the shift...
Figure 4.19: \((\kappa)_{m1}\) sensitivity to \(T_{11}\) and \(T_{33}\) for ST-cut quartz. The legend refers to the real and imaginary parts of the sensitivity, e.g., \(\text{Real}(T_{11})=\text{Real}(d(\kappa)_{m1}/((\kappa)_{m1}T_{11}))\).

determined by \(\kappa\). It increases the stopband width (see Section 4.4.1), while also changing the ripple behaviour. The complex nature of \(\kappa\) means that significant differences in reflective behaviour may be observed for difference propagation angles. Changing the reference plane separation also affects both the magnitude and frequency of the resonant response.

### 4.5.5 Transduction coefficient

The transduction coefficient \(\alpha_s\) determines the coupling between the excited SAW and the applied voltage. This may be decomposed into components related to the substrate properties, the SAW aperture and the electrode layout [199]. For the IDTs used in this project, the magnitude of \(\alpha_s\) as a function of the wavenumber \(\beta = \omega/v\) is given by:
\[ |\alpha_s(\beta)| = \left| \frac{Q_F(\beta)}{\lambda} \right| \sqrt{\left( \frac{W}{\lambda} \right) \left( \frac{\pi \Delta v}{\varepsilon_s(\infty)} \right)} \]  \hspace{1cm} (4.39)

where \( \Delta v \) is the difference between the free and metallised SAW velocities (see Section 2.3.3), and \( \varepsilon_s(\infty) \) is the effective permittivity of the substrate at infinite slowness [42], [53] (see Section 2.3.2). The IDT element factor \( Q_F(\beta) \) details the electrostatic charge contribution of a single IDT ‘cell’ [199], and for the IDTs used here is given by [200]:

\[ Q_F(\beta) = 2\varepsilon_s(\infty) \frac{L_m(\cos(\pi \eta))}{L_{-s}(-\cos(\pi \eta))} \sin(\pi s) \]  \hspace{1cm} (4.40)

where \( m \) is an integer and \( 0 \leq s \leq 1 \). For a particular wavenumber \( \beta \), the values of \( m \) and \( s \) may be determined from \( m + s = \beta p/(2\pi) \). The phase of \( \alpha_s \) is determined by that of \( Q_F(\beta) \). Figure 4.20 plots \( \sqrt{\Delta v \varepsilon_s(\infty)} \), which represents the substrate-dependent factor of \( |\alpha_s(\beta)| \): its general form resembles that of the electromechanical coupling coefficient \( K^2 \) (see Figure 2.7), though the drop in transduction is more pronounced near 90°. The calculated value of \( \alpha_p = |\alpha_s(\beta_0)|\lambda \) (i.e., the transduction magnitude normalised to \( \lambda \) for \( \beta = \beta_0 = \pi/p \)) using the parameters given in [171] is \( 2.83 \times 10^{-4} \sqrt{1/\Omega} \) for ST-X quartz, which is in good agreement with the experimental value of \( 2.705 \times 10^{-4} \sqrt{1/\Omega} \).

The inclusion of \( \varepsilon_s(\infty), \Delta v \) and the device geometry means that bias sensitivity of \( \alpha_s \) can be evaluated. This was found to be small relative to the orientational sensitivity shown in Figure 4.20 and can be neglected as was done with \( (\Delta v/v)_{m1} \). In common with the attenuation \( \gamma \) (see Section 4.5.7), \( \alpha_s \) affects the magnitude of the peak admittance response rather than its frequency, and is often measured experimentally for particular IDT forms.

### 4.5.6 Capacitance

The IDT electrodes in a SAW device act as distributed capacitors, and thus capacitive effects must be considered in the COM model. For weakly piezoelectric materials such as quartz, the normalised capacitance of the IDT may be approximated by its static capacitance:
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\[ \sqrt{\Delta \varepsilon_s(\infty)} \text{ for ST-cut quartz} \]

Figure 4.20: \( \sqrt{\Delta \varepsilon_s(\infty)} \) for ST-cut quartz

\[ C = \frac{C_n W}{\lambda} \]  
(4.41)

where \( C_n \) is the capacitance per electrode pair per unit aperture length [40]. For the IDTs used in this project, \( C_n \) may be determined from [42]:

\[ C_n = \varepsilon_s(\infty) \frac{L_{-0.5}(\cos(\pi \eta))}{L_{-0.5}(-\cos(\pi \eta))} \]  
(4.42)

For ST-X quartz with \( \eta = 0.5 \), \( C_n \approx 50 \text{pF/m} \). Unlike some of the other COM parameters, \( C_n \) is only weakly dependent on the propagation direction, though it does increase almost linearly with \( \eta \) around \( \eta = 0.5 \). As with most of the other COM parameters, the dependence of \( C \) on the device geometry (and on \( \varepsilon_s(\infty) \)) renders it sensitive to applied biases. It was found, however, that \( C_n \) was insen-
sitive to applied $T_{11}$ and $T_{33}$. This may be because $\varepsilon_s(\infty)$ effectively only characterises the material’s static behaviour (as it is evaluated for $v \approx 0$), neglecting wave-based capacitance effects; capacitive effects for strongly piezoelectric materials are discussed in [156]. In terms of device performance, the static capacitance is manifested as a DC shift in the susceptance response. It is also affected by parasitic effects (from busbars, bond wires, packaging etc.), and thus experimental measurements are often required.

### 4.5.7 Attenuation

Although a single-crystal substrate was chosen to minimise SAW propagation losses (see Section 3.3.2), some wave attenuation is inevitable. For a free surface, this attenuation is due to two main factors [42]:

- **Air loading of the substrate**: air loading (or loading from another gaseous medium) causes attenuation which is proportional to the frequency of the wave. The loss mechanism in this case is the excitation of acoustic waves in the gas medium [201, 202]. Most modern SAW devices are sealed in hermetic packages (see Section 3.2.3), which both protects the devices and allows them to operate in a vacuum.

- **Thermal phonon interactions**: these are the unavoidable interactions of the wave with the crystalline structure of the substrate, and produces attenuation proportional to the square of the wave frequency.

For ST-X quartz, the COM free-surface attenuation from these two sources is given by [42]:

$$\gamma \approx \frac{0.47 + 2.62 \times 10^{-9} f}{8685.9 \lambda} \quad (4.43)$$

where $\gamma$ is measured in Nepers (1 Neper $\approx 8.6859$ dB): the equation is sensitive to biases through $\lambda$ as above. However, in the COM technique this parameter must account for all acoustic loss mechanisms in a structure, including surface defects, attenuation in metal films, bulk wave parasitic modes etc. [156], which are difficult to model near the frequency ranges of interest. Losses from beam
steering and diffraction should also be considered (see Section 3.3.5). Recent work [203] has proposed more complete attenuation modelling, but in practice this parameter is usually measured experimentally. Increasing attenuation degrades an IDT’s peak admittance response (see [204] for details) and reduces the ripple magnitudes, but has little effect on the frequency of the resonant response.

4.6 Conclusion

In this chapter the modelling and simulation of SAW devices was examined, with particular reference to SAW strain sensors. Following an evaluation of existing modelling techniques, a custom simulation method was proposed. This combines existing modelling schemes to predict the biased frequency response of SAW sensors. Its modular nature means that the bias-sensitive parameters may be calculated through a variety of theoretical or experimental methods, thus increasing its flexibility.

In the next chapter, experimental results from the devices detailed in Chapter 3 and simulated results based on this chapter’s work are compared.
Chapter 5

Experimental and Simulation Results

The experimental testing of the prototype SAW sensors is the last major project objective (see Section 1.4). Such testing is key to any new sensor project: here it is used to evaluate both the design and manufacturing work of Chapter 3 and the modelling schemes of Chapter 4. The comparison between the experimental and theoretical results is used to assess the validity of the modelling.

In this chapter the unstrained experimental testing is first described, including a description of the testing methods, protocols and results. The unstrained COM parameters are then extracted from these measurements. This is followed by the strained testing results, including an analysis of common sensor parameters. Comparisons between the predictions of sensor response from the COM model and the experimental results are then provided.

5.1 Unstrained experimental testing

It is essential to evaluate the performance of the devices as ordinary, unstrained, 1-port SAW resonators before their implementation as sensors. Given the small biases applied to the sensors, their gross frequency response is almost entirely due to their unstrained behaviour, and thus only those devices with acceptable performance may be useful as sensors. It was decided to test all of the die as basic
1-port SAWR, and then select some of the devices for strain testing; this process is detailed below.

5.1.1 S-parameter testing

As mentioned in Section 4.1, device impedance (or admittance) is the main output of the sensor model, and thus it is natural to use the same quantity for the experimental testing. DC or low frequency impedance measurements of devices are relatively straightforward as the electrical wavelength is much longer than the device size, and thus the phase of the incident signal is essentially constant. By contrast, at RF frequencies the device’s electrical length can be comparable to the signal wavelength, and the wave nature of the signal must be considered. For the sensor frequencies used in this project (c. 433MHz), microwave analysis techniques are commonly used to analyse device behaviour; an excellent introduction to such methods may be found in [148]. These methods employ transmission line theory to model the electrical fields in a device, and can account for the high frequency boundary conditions commonly encountered.

Most microwave devices (filters, waveguides, resonators etc.) are treated as N-port electrical networks for measurement. Such networks may consist of a single component or a complete microwave circuit, while transmission line ports are used rather than those defined in Section 4.4.2. The measurements refer only to the electrical response at the ports: the network itself may have arbitrary linear behaviour internally. Although several network analysis techniques exist [205], the most common is the scattering matrix (or S-matrix) approach [148], mentioned in Section 4.2 for the analysis of SAW devices. The S-matrix elements (S-parameters) characterise the reflection and transmission properties of a device at a given frequency. S-parameter analysis has the following advantages in this project:

- **Good linkage with P-matrix techniques:** in addition to being consistent with transmission line theory, the S-parameter approach naturally integrates with the P-matrix modelling detailed in Section 4.4.2. The P-matrix technique is actually derived from the S-matrix method (see Section 4.2), and thus it is usually simple to link the two together.


- **Relatively simple measurements**: network analysis instruments commonly measure S-parameters directly (see below), reducing the complexity of measurements.

- **Good error correction**: instruments which employ S-parameter test sets offer better error correction features than those using simpler transmission / reflection hardware [206], thus improving the quality of the measurements.

For a 2-port electrical network with port locations $x_1$ and $x_2$, the S-matrix is given by:

$$
\begin{bmatrix}
V_-(x_1) \\
V_+(x_2)
\end{bmatrix} = 
\begin{bmatrix}
S_{11}(f) & S_{12}(f) \\
S_{21}(f) & S_{22}(f)
\end{bmatrix}
\begin{bmatrix}
V_+(x_1) \\
V_-(x_2)
\end{bmatrix}

(5.1)
$$

where $V_+(x_1)$ and $V_-(x_2)$ are the incident voltages at the ports. Note that conceptually this is almost identical to the P-matrix definition of equation (4.13), except that in this case the port quantities are voltages and the S-parameters are dimensionless. Therefore, the methods used to analyse the P-matrix elements can also be used for the S-parameters. For example, $S_{11}$ (the voltage reflection coefficient at port 1) is the ratio of the reflected voltage to the incident voltage at port 1, with no incident voltage at port 2:

$$
S_{11} = \frac{V_-(x_1)}{V_+(x_1)}, \quad V_+(x_2) = 0

(5.2)
$$

Similarly, $S_{12}$ (the voltage transmission coefficient at port 1) is the ratio of the transmitted voltage at port 1 to the incident voltage at port 2, with no incident voltage at port 1:

$$
S_{12} = \frac{V_-(x_1)}{V_-(x_2)}, \quad V_+(x_1) = 0

(5.3)
$$

The voltage boundary conditions are implemented by terminating the appropriate port with a characteristic impedance $Z_0$ [148], which is generally the same as the input or output impedance of the network (often 50Ω). In common with P-matrix elements, S-parameters are usually complex.

The 1-port SAW resonators used in this project may be considered either as 1-port or 2-port electrical networks, depending on the desired measurand(s). In a
2-port analysis, each bond pad (see Figure 5.13) is considered as a separate port, with off-die grounding. This allows the transmission properties of the device to be examined, as the effect of voltage excitations at one port can be analysed at the opposite port. While this is the most flexible analysis method, the impedance measurements can be performed more simply using 1-port testing. In this case, one bond pad is excited while the other is grounded, and thus only the reflection properties can be examined. The relationship between the load impedance \( Z \) on a transmission line and \( S_{11} \) is given by [205]:

\[
Z = Z_0 \frac{1+S_{11}}{(1-S_{11})} \tag{5.4}
\]

It should be noted that for passive devices (such as SAW sensors) \( 0 \leq |S_{11}| \leq 1 \).

Three basic loads may be considered:

- **Matched load**: for a perfectly-matched load, \( Z = Z_0 \) and thus \( S_{11} = 0 \), i.e., no waves are reflected back to the source. All of the incident power is seen by the load.

- **Open circuit**: \( Z = \infty \) in this case, thus \( S_{11} = 1 \). All of the incident waves are reflected back to the source, and no power is used by the load.

- **Short circuit**: \( Z = 0 \) for a shorted termination, thus \( S_{11} = -1 \). All of the incident waves are reflected back to the source, phase shifted by \( \pi \), and again no power is used by the load.

1-port SAWR operate between these extremes, depending on the excitation frequency. At off-resonance frequencies, the device approximates an open circuit, and thus its impedance is high. 1-port SAW resonators display two resonant features, with a minimum impedance at the series resonant frequency and maximum impedance the parallel resonant frequency: these can be seen in Figure 3.11. The series resonance was analysed for the prototype SAW sensors, where the impedance drops to a finite value dependent on the device parameters, and the behaviour approaches that of a matched load.
5.1.2 Test equipment and protocol

Electrical testing of prototype die is best performed using a network analyser with a probe station; facilities for this were kindly provided by the UCD Microwave Laboratory. Figure 5.1 shows the equipment used for the static testing, while Figure 5.2 shows the probe/die interface. An Agilent E8361A PNA vector network analyser was used to measure $S_{11}$ of the die. Such instruments can measure both the magnitude and phase of the $S$-parameters, allowing complex impedance behaviour to be investigated. Electrical probing of the die was performed using GGB ECP18-GS/SG-2500-EDP Picoprobes, which were calibrated using a CS-17 calibration substrate. Accurate calibration is essential for any network analyser measurement [206], as systematic errors can easily be induced by temperature changes, cable adaptors etc. 1-port SOL (Short-Open-Load) calibration was used for all of the experimental measurements as it provides excellent error correction (e.g., ±10ppm frequency accuracy) for 1-port testing: a good introduction to die testing issues is given in [207]. The probes and die were held in a Cascade Microtech Summit 9000 probe station.

It was decided to first use a 150MHz (350-500MHz) $S_{11}$ sweep of all of the devices to look for any resonant responses. The wide frequency range also allows the resonant response to be compared to the general broadband behaviour, while any spurious responses could be noted. Viable die were then tested with a 15MHz sweep to get more accurate frequency responses.

5.1.3 Measurement of commercial SAW devices

In order to evaluate both the testing system and the prototype devices, it was decided to test a comparable commercial SAW device. The Epcos R820 1-port SAWR [68] was selected as it is comparable to the sensors in resonant frequency (433.92MHz) and should demonstrate similar 1-port resonance characteristics. An added advantage is that its QCC4A package can be directly probed with the same equipment used for the sensors (see Section 5.1.2). Figure 5.3 shows the impedance behaviour of the two R820 devices measured and the predicted response from the device’s equivalent circuit. The experimental results show the excellent frequency tolerances of the devices: the deviations from the design
CHAPTER 5. EXPERIMENTAL AND SIMULATION RESULTS

Figure 5.1: Static testing equipment showing vector network analyser (left) and probe station (right)

Figure 5.2: Overhead view of probe and a section of wafer
resonant frequency are less than 40kHz in both cases. In general the resonant
behaviour is smooth, though three additional responses may be seen. The two
smallest responses probably correspond to the stopband edges, while the largest
response may be caused by a transverse mode [88] (see Section 3.3.5): as noted
in Section 5.1.2 the designs of commercial SAW devices are usually proprietary.
Apart from the production-standard fabrication quality, the devices’ excellent per-
performance can be attributed to their 50Ω impedance matching at resonance and
their hermetically-sealed packages. As mentioned in Section 3.3.5 impedance
matching was not used for the sensors as a variety of die designs were to be inves-
tigated, but such matching ensures optimum power transmission in RF devices
[205]. The sealed package reduces the effects of air loading on the propagat-
ion surface (see Section 4.5.7), thus improving the magnitude of the resonant
response. The frequency response predicted by the equivalent circuit model is in
excellent agreement with the experimental results, confirming the accuracy of the
testing system. As the model assumes a smooth RLC-type resonance, the three
small responses are not predicted.

5.1.4 Device yield

The preliminary broadband testing revealed wide variations in performance be-
tween the prototype devices, even between nominally identical die. While this
is obviously undesirable, it is inevitable given the differences in device dimen-
sions detailed in Section 3.5. The variations revealed the need to define what an
‘acceptable’ die is, both as a SAW device and as a sensor. Commercial 1-port
SAWR are typically characterised by the resonant frequency (and its tolerance),
the quality factor $Q$, the input/output impedance and the insertion loss (see Section
3.3.1); additional parameters may be specified for custom devices. For example,
an Epcos R820 1-port SAWR (see Section 5.1.3) has a resonant frequency of
433.92MHz±75kHz, $Q \approx 11500$, $Z = 50\Omega$ and minimum insertion loss of 1.2dB
[68]. Insertion losses are not applicable for the sensors in this project as trans-
mission measurements were not performed. Similarly, impedance matching was
not considered for the sensors (see Section 3.3.5), though in general this is an im-
portant consideration for wireless devices where matching to antennas and other
equipment is required. Thus the resonant frequency and $Q$ are the more important device parameters. It quickly became clear that few (if any) of the die would meet the frequency requirements outlined in Section 3.3 (no $Q$ requirements were presented), yet the devices are still useful as prototype sensors. It was therefore decided to evaluate the devices qualitatively by comparison with other devices on the same wafer. As noted in Section 5.1.1, 1-port SAWR should demonstrate $|S_{11}| \approx 0\text{dB}$ at off-resonance frequencies, with the minimum $|S_{11}|$ occurring at the resonant frequency. Therefore devices with no (or very small) resonant responses (typically disguised by the broadband response) or those with very low broadband $|S_{11}|$ values were omitted after the broadband testing. It should be noted that most of the desired characteristics given in Section 3.2.2 can still be met by the prototype devices, even though the resonant frequencies differ from the design values.
The device yield is defined as the percentage of working die on a wafer or series of wafers, and gives an indication of fabrication quality. Yields of prototype devices tend to be low by production standards as the manufacturing processes are often immature \[133\]. though the integrated design and manufacture process of Section 3.3 was designed to minimise problems where possible. Table 5.1 gives the number of acceptable die on each wafer. Note that some of the large die have 2 SAWR each, and that the number of acceptable die includes those with at least one good device. The standard die from Wafers 2, 3 and 4 displayed no resonant behaviour whatsoever: no die were retained after the broadband sweep. Similarly, with the exception of Wafers 4 and 5, very few acceptable large die were found. It is suspected that the primary cause of these low yields was a failure of the metallisation process and/or the lift-off process during the fabrication of these wafers (see Sections 3.4.5 and 3.4.6). As mentioned in Section 3.5, optical inspection of the finished devices revealed a large variety of defects, though few of these were considered critical to the resonant behaviour. This suggests that the fabrication of the die up to the development stage was largely successful - the presence of acceptable standard die on Wafers 1 and 5 supports this. However, the standard devices from Wafers 2, 3 and 4 have ‘dull’ sections where the metallisation should be, rather than the ‘bright’ layouts of Wafers 1 and 5, indicating a problem with the metallisation: compare the reflector sections in Figures 3.23 and 3.24. Although some acceptable large die were found on Wafers 3 and 4, the lack of any resonant behaviour from the standard die indicates that metallisation failure may have occurred over large areas of the wafers. The lower yields (in general) of the large die can be explained by their increased size and complexity relative to the standard die (see Section 3.3.5), thus rendering them more vulnerable to defects. For example, large Die 1-10 use two SAWR in series, and thus a serious defect in the connection between the resonators may cause failure of the whole die. Some of the large die also use extremes in device geometry and propagation direction, which may degrade the resonant response even if the fabrication is of sufficient quality.

Table 5.2 lists the die which were retained after the broadband testing, while Figure 5.4 shows the number of acceptable SAWR at each die location across all of the wafers. As is common in IC manufacture, the majority of the defective die
CHAPTER 5. EXPERIMENTAL AND SIMULATION RESULTS

<table>
<thead>
<tr>
<th>Wafer</th>
<th>No. of Acceptable Standard Die</th>
<th>No. of Acceptable Large Die</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>35 (73%)</td>
<td>2 (8%)</td>
</tr>
<tr>
<td>2</td>
<td>0 (0%)</td>
<td>0 (0%)</td>
</tr>
<tr>
<td>3</td>
<td>0 (0%)</td>
<td>2 (8%)</td>
</tr>
<tr>
<td>4</td>
<td>0 (0%)</td>
<td>12 (50%)</td>
</tr>
<tr>
<td>5</td>
<td>36 (75%)</td>
<td>10 (42%)</td>
</tr>
</tbody>
</table>

Table 5.1: Acceptable die from the fabricated wafers with percentage yields

<table>
<thead>
<tr>
<th>Wafer</th>
<th>Retained Standard Die</th>
<th>Retained Large Die</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1,3-5,7-10,12-20,22-23,25-28,30-34,37-38,41-43,45-46</td>
<td>17,18</td>
</tr>
<tr>
<td>2</td>
<td>None</td>
<td>None</td>
</tr>
<tr>
<td>3</td>
<td>None</td>
<td>17,18</td>
</tr>
<tr>
<td>4</td>
<td>None</td>
<td>1-9,11u,14u,15b</td>
</tr>
<tr>
<td>5</td>
<td>1-3,5,7-11,13-15,17-22,25-26,28,30-42,44-45</td>
<td>1-6,8,9,12b,15l</td>
</tr>
</tbody>
</table>

Table 5.2: Details of retained die from the fabricated wafers. The letters denote whether the (u)pper, (l)ower or (b)oth resonators on the large die were retained.

are near the perimeter of the wafer. It is useful to note that of the 34 unique SAWR designs on the photomask (24 standard die and 10 large die, see Section 3.3.5), only 2 failed to produce a resonant response on any wafer. The perimeter locations of these designs, used for standard Die 47 and 48 and the lower SAWR of large Die 13 and 14 (see Figure 3.12), means that their poor performance may be due to their locations on the wafers rather than inherent problems with the designs.

The success of the die designs validates the integrated design process detailed in Section 3.3. It is clear from Table 5.1 and Figure 5.4 that although serious yield problems were experienced with these five wafers, the manufacturing process outlined in Section 3.4 is capable of producing acceptable devices. Future improvements to the integrated design and manufacture process will be discussed in Section 6.1.
5.1.5 Standard die results

As mentioned in Section 5.1.2, all of the acceptable standard die were tested using a 15MHz sweep. Several objectives were defined for this testing:

- **Determination of device frequency response**: while the broadband testing was sufficient to detect the presence of resonant behaviour and its general form, the 15MHz sweep with a larger number of test points was designed to give detailed frequency response information.

- **Evaluation of device reproducibility**: although some die were omitted after the broadband testing, many nominally identical devices remain which can be compared. Consecutive odd and even standard die should be identical (e.g., Die 1 and Die 2).

- **Evaluation of die design decisions**: the experimental responses should reveal the effects of the die design decisions. With reference to Section 3.3.5.
and Appendix B, the standard die designs are subdivided by the linewidth, then by the number of IDT finger pairs, then by the reflector lengths and finally by resonator type.

### 5.1.5.1 Resonant frequencies

Figure 5.5 plots the resonant frequencies of the standard die on Wafer 1 grouped by the design linewidth \( a \); mean frequencies of each group and their confidence intervals are also given. It should be noted that the resonant frequencies of devices with the same linewidth may not be identical as this is also affected by the IDT and reflector size, type of resonance etc. - the mean frequencies merely give an indication of scatter. Some initial points may be made:
• The resonant frequencies can be grouped quite neatly by a. Note that the mean resonant frequencies are separated by 2.08 and 2.13MHz, which are close to the design separations of 1.98MHz and 2.00MHz, respectively. This indicates that although the design linewidths vary by only 8.33nm, the effect of this change can clearly be seen in device performance, even though the mask linewidth tolerance is ±0.05µm and considerable variation in the fabricated dimensions was observed (see Table 3.2). Thus the photomask linewidth decisions made in Section 3.3.3 have been vindicated. As mentioned in Section 3.5, these SAW devices act as distributed narrowband structures, and thus it is possible that variations in individual linewidths are averaged out in the frequency response.

• Considerable scatter is evident within each of the linewidth groups, and it is difficult to discern definite patterns of behaviour corresponding to particular designs. Some nominally identical die display closely-matched resonant frequencies (e.g., Die 41 and 42), while some do not (e.g., Die 19 and 20). No differences were observed between the optimal and synchronous die in this respect. This scattering of resonant frequencies for identical designs is primarily due to manufacturing variations. In general, die with indistinct resonant responses (e.g., Die 19 and 23) demonstrated greater deviations from the mean frequencies. The first eight die within each group have fewer IDT finger pairs than the second eight, but no discernable effect on the resonant frequency was observed; this may be because the IDT length mainly affects the magnitude of the resonant response rather than its frequency. Similarly, the effects of reflector length are not evident. In this case, the SAW decay (due to reflection and attenuation) within the reflector structures may be rapid, and thus no waves propagate in the outer sections, rendering long structures unnecessary. The synchronous devices do appear to have a lower resonant frequency than the corresponding optimal ones, especially for the largest linewidth. This behaviour matches that predicted by the COM model (see Figures 4.10 and 4.11).

It was noted during the testing that the resonant frequencies of the Wafer 1 die (c. 445.08, 447.16 and 449.29MHz) were about 3% higher than the nominal
design values (432.78, 434.76 and 436.76MHz). This was surprising given that
the measured period lengths (albeit over small numbers of electrodes) were larger
than the design values (see Section 3.5), and thus the devices should resonate at
lower frequencies; reflectivity effects should also reduce the resonant frequencies
below their nominal values. It was subsequently discovered that the actual prop-
agation direction of the Wafer 1 standard die is approximately ST-(X+90°) (see
Section 3.5). This orientation change has profound implications for the perfor-
mance of the devices. With reference to Section 2.3.1 Rayleigh SAW do not
demonstrate piezoelectric coupling for ST-(X+90°) propagation: this can also be
seen in Figure 2.7. Thus Rayleigh SAW cannot be generated or transduced by an
IDT, though they can propagate if excited by some other means. Clear resonant
behaviour was demonstrated by the Wafer 1 die, however, and thus a piezoelectric
wave (of some form) is propagating. For the exact ST-(X+90°) orientation, only
SH waves display piezoelectric coupling (see Section 2.3.1). These waves have a
free surface velocity of approximately 5100m/s (depending on the energy trapping
mechanism), so for a sample wavelength of 8µm (see Table 3.2) the resonant fre-
cquency of such a device should be about 638MHz (see equation (2.40)); reflective
effects only have a small influence on the gross resonant frequency and can be
ignored here. Retesting of some Wafer 1 standard die from 200MHz to 1.5GHz,
however, revealed no distinct resonant responses at the expected SH frequencies,
nor at any frequencies other than those originally measured. The possibility that
the responses were caused by other types of ‘pseudo’ SAW was considered, but
the orientation does not commonly support such modes; the frequencies would
also be higher in these cases than those measured [47]. Thus it can be assumed
that the original measurements represent the ‘true’ die results rather than a spuri-
ous response related to another wave mode.

Table 5.3 shows the SAW velocity \( v \) calculated from the measured resonant
frequency and wavelength for some Wafer 1 die using equation (2.40). The esti-
mated ±10ppm error in the frequency results is negligible compared to the ±5%
accuracy of the SEM measurements and can be ignored. It should be noted again,
however, that the measured electrode dimensions only refer to small areas of the
electrode structures, and may not characterise the structures as a whole (see Sec-
tion 3.5). Although there is considerable variation in the die dimensions and fre-
5.1. UNSTRAIN EXPERIMENTAL TESTING

Table 5.3: Calculated $v$ from measured parameters for Wafer 1 die. The IDT wavelength is $2p_{IDT}$ from Table 5.2.

<table>
<thead>
<tr>
<th>Die</th>
<th>Meas. Res. Freq. (MHz)</th>
<th>Meas. IDT $\lambda$ ($\mu$m)</th>
<th>Calculated $v$ (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>445.35</td>
<td>8.12±0.41</td>
<td>3616±181</td>
</tr>
<tr>
<td>18</td>
<td>447.50</td>
<td>7.88±0.39</td>
<td>3526±176</td>
</tr>
<tr>
<td>46</td>
<td>449.38</td>
<td>7.52±0.38</td>
<td>3379±169</td>
</tr>
<tr>
<td>L17</td>
<td>447.11</td>
<td>7.98±0.40</td>
<td>3568±178</td>
</tr>
<tr>
<td>L18</td>
<td>444.02</td>
<td>8.18±0.41</td>
<td>3632±182</td>
</tr>
</tbody>
</table>

The frequency results, the unbiased $v$ should be constant for a particular propagation direction, and thus the calculated velocities for Die 1, 18 and 46 should be equal. It is clear that although some variation is present, the calculated velocities are relatively consistent with those for Rayleigh SAW around the ST-(X+90°) propagation direction (c. 3525m/s, see Figure 2.6). The piezoelectric coupling around this orientation for Rayleigh SAW is virtually zero, however: this will be discussed in Section 5.1.5.2. The only other comparable wave type for this orientation is the slow shear bulk wave, which has a velocity of approximately 3780m/s [47]. This wave, however, does not satisfy the free surface boundary conditions [208], and would also result in higher frequency responses than those measured.

Results for large Die 17 and 18 are also presented in Table 5.3. Although these were originally designed to investigate suboptimal SAW propagation directions (ST-(X+45°) and ST-(X+60°) respectively, see Section 3.3.5), due to the wafer misorientation they now propagate along the ST-(X+135°) and ST-(X+150°) directions. Thus they provide useful measurement information as their orientation is known precisely relative to the standard devices; their design is also similar to that of Die 18. The theoretical $v$ values for these orientations are approximately 3282m/s and 3270m/s, respectively, however it is clear that the calculated values are considerably higher than these; they are also higher than the corresponding slow shear wave speeds. The velocities are similar to those displayed by the ST-(X+90°) die, which suggests that the behaviour is almost isotropic when in fact it should be anisotropic (as shown in Figure 2.6). This apparent behaviour may also be caused by problems with the measured dimensions. These die use propagation angles which are rotated from the symmetry axes, and thus the possibility
Table 5.4: Calculated \( v \) from measured parameters for Wafer 3 die. The IDT wavelength is \( 2p_{IDT} \) from Table 3.2.

The equivalent resonant frequency results for the Wafer 5 standard die are plotted in Figure 5.6; this wafer appears to be fabricated using the correct ST-(X+35°) orientation (see Section 3.5). The same basic features observed in the Wafer 1 die can also be seen here, with distinct frequency groups corresponding to the three design linewidths. Some increased scatter is apparent for devices with the smallest linewidth, though the results for the other two linewidths are comparable to those on the first wafer. In general the synchronous devices with the two larger linewidths display higher resonant frequencies than the corresponding optimal die, the opposite of the Wafer 1 behaviour, though the larger scatter makes this difficult to confirm. The increased scatter is at least partially due to the significantly weaker resonant responses compared to those of the Wafer 1 die (see Section 3.1.5.2). This means that the resonant response is often of the same order as the ripples either side of the stopband, thus making it difficult to determine the precise resonant frequency. The design resonant frequencies of the standard die on this wafer were 448.81, 450.87 and 452.95MHz (see Section 3.3.5), and in this case the experimental results are about 1% lower than these (c. 445.34, 447.77 and
5.1. UNSTRAINED EXPERIMENTAL TESTING

Figure 5.6: Resonant frequencies of standard die from Wafer 5 grouped by design linewidth. The solid lines represent the mean frequency of each group, while the dashed lines show the 99% confidence interval of the mean.

449.55MHz). Table 5.5 gives the calculated \( v \) from different die measurements; neither rotated die produced a resonant response on this wafer. The theoretical propagation velocity for the ST-(X+35°) orientation is c. 3276m/s, and again it is clear that the calculated velocities are considerably higher than this. It is interesting that the calculated \( v \) are similar to those of the rotated large die from Wafers 1 and 3, which have approximately the same theoretical velocity, though the large scatter makes it difficult to draw definite conclusions.

5.1.5.2 Magnitude of resonant responses

In addition to the resonant frequency, the magnitudes of the resonant responses are also important. Figure 5.7 plots the behaviour of the standard die from Wafers 1
<table>
<thead>
<tr>
<th>Die</th>
<th>Meas. Res. Freq. (MHz)</th>
<th>Meas. IDT ( \lambda ) (( \mu )m)</th>
<th>Calculated ( v ) (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>445.26</td>
<td>8.06±0.40</td>
<td>3589±179</td>
</tr>
<tr>
<td>18</td>
<td>447.90</td>
<td>7.72±0.39</td>
<td>3458±173</td>
</tr>
<tr>
<td>25</td>
<td>448.03</td>
<td>7.28±0.36</td>
<td>3262±163</td>
</tr>
<tr>
<td>31</td>
<td>447.37</td>
<td>7.38±0.37</td>
<td>3302±165</td>
</tr>
<tr>
<td>32</td>
<td>448.49</td>
<td>7.92±0.40</td>
<td>3552±178</td>
</tr>
<tr>
<td>45</td>
<td>449.23</td>
<td>7.80±0.39</td>
<td>3504±175</td>
</tr>
</tbody>
</table>

Table 5.5: Calculated \( v \) from measured parameters for Wafer 5 die. The IDT wavelength is \( 2p_{IDT} \) from Table 3.2.

| Wafer | Die | Wideband \( |S_{11}| \) (dB) |
|-------|-----|----------------|
| 1     | L17 | -0.04          |
| 1     | L18 | -0.08          |
| 3     | L17 | -0.09          |
| 3     | L18 | -0.11          |

Table 5.6: \( |S_{11}| \) behaviour of rotated large die from Wafers 1 and 3 at off-resonance frequencies

and 5 at off-resonance frequencies, interpreted in this case as the maximum value of \( |S_{11}| \) (expressed in dB) across the 15MHz sweep. This gives an indication of the broadband behaviour, and is mainly dependent on the resistance and static capacitance of the devices rather than their resonant properties; it also acts as a reference to calculate the magnitude of the resonant response. The majority of the Wafer 1 die display maximum \( |S_{11}| \) values of between -0.03 and -0.07dB, which is close to the open-circuit \( S_{11} = 1 \) (i.e., 0dB). Devices with more finder pairs (i.e., large IDTs) display smaller (i.e., more negative) values of \( |S_{11}| \) as the static capacitance is larger, though again considerable scatter is evident. Table 5.6 gives the wideband values for the rotated large die on Wafers 1 and 3, which are similar to those of the standard die. The broadband responses of the Wafer 5 standard die are also similar, though a number of devices (e.g., Die 25, 32 and 34) display significantly poorer behaviour.

The magnitudes of the resonant responses for the standard die on Wafers 1 and 5 are plotted in Figure 5.8. These are calculated by subtracting the maximum
value of $|S_{11}|$ (plotted in Figure 5.7) from the minimum $|S_{11}|$, which corresponds to the resonant response. Marked scatter is evident, with wide variations between nominally similar devices. In general the optimal devices produced stronger resonant responses, as would be expected (see Section 4.4.3): for example, all of the die with resonance magnitudes greater than 2.5dB on Wafer 1 are optimal. Similarly, devices with more finger pairs also demonstrated improved performance. Die numbers between 7 and 15 on both wafers display significantly better performance than other devices: the cause of this behaviour is unclear. Table 5.7 gives the response magnitudes for the rotated large die on Wafers 1 and 3. In common with the resonant frequency results, the corresponding rotated die on each wafer display similar magnitude behaviour, with the large Die 17 examples producing stronger responses. As before, there is significant variation between identical designs: the performance of large Die 17 on Wafer 1 considerably better than that
Table 5.7: Magnitude of $|S_{11}|$ resonant response of rotated large die from Wafers 1 and 3 on Wafer 3. Both examples of large Die 18 produced poor quality responses.

In general, the Wafer 1 die have larger resonances than those on Wafer 5. This is surprising given that the Rayleigh wave piezoelectric coupling coefficient for ST-cut quartz is maximised for $35^\circ$ propagation, while no coupling is predicted for $90^\circ$ propagation (see Figure 2.7 and Section 4.5.5). Thus not only should the Wafer 5 die display better results than the Wafer 1 die, but no coupling whatsoever should be seen from the Wafer 1 devices – clearly this is not the case. The results can be partially explained by recognising that the magnitude of the resonant response is determined by both the piezoelectric coupling and the reflectivity of the structures (amongst other factors). This means that resonant devices with strong coupling but weak reflectivity can display small response magnitudes, and vice versa: such behaviour has been demonstrated in NSPUDT devices [209]. The measured structures in Section 3.5 displayed relatively consistent periodicity (see Table 3.2), thus the reflectivity is dependent on $\kappa$ (see Section 4.5.4). Figure 4.18 shows that the reflectivity for $35^\circ$ propagation is low, which could lead to small response magnitudes (see Figure 4.7); by contrast, the reflectivity is maximised for $90^\circ$ propagation. Although this does not explain the existence of responses from the Wafer 1 die (which is discussed in Sections 5.1.5.4 and 5.1.7), it does demonstrate the complex nature of the response magnitude.

5.1.5.3 Quality factor and device impedance

The unloaded $Q$ results for Wafers 1 and 5 are plotted in Figure 5.9, while those of the rotated large die are given in Table 5.8. These were calculated from measurements of the conductance plot at the resonant frequency [209]. There is some correlation between the magnitudes of the resonant responses and the unloaded $Q$. 

<table>
<thead>
<tr>
<th>Wafer</th>
<th>Die</th>
<th>Resonance Mag. (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>L17</td>
<td>-3.50</td>
</tr>
<tr>
<td>1</td>
<td>L18</td>
<td>-0.48</td>
</tr>
<tr>
<td>3</td>
<td>L17</td>
<td>-1.23</td>
</tr>
<tr>
<td>3</td>
<td>L18</td>
<td>-0.46</td>
</tr>
</tbody>
</table>
which would be expected given that the broadband behaviour of the die across the wafers is relatively consistent. Although the \( Q \) performances are far lower than those of commercial SAW devices (see Section 5.1.4), they represent a reasonable result for the unmatched prototype sensors.

As a final comparison, the impedance frequency responses of some sample die were examined. Figures 5.10 and 5.11 show the frequency responses of some die
from Wafers 1 and 5, respectively, and the form of the responses can be considered as typical of devices from these wafers. All of the die in each plot have the same basic design (linewidth, IDT size etc.). However, the first two die in each plot use an optimal layout, while the second two use a synchronous one; each pair of die are nominally identical. In Figure 5.10 the resonant frequencies of Die 13 and 14 (i.e., the minimum of $|Z|$) are very close, but the magnitudes of the respective responses vary considerably. Similarly, the responses of Die 15 and 16 are quite different even though their designs are identical. The general form of the responses is similar to that demonstrated the commercial SAWR in Figure 5.3 though more ripples are evident in these devices. Due to the relatively short IDTs and the lack of 50Ω matching, the broadband values of $|Z|$ are larger than those shown in Figure 5.3. The Wafer 5 die display significantly poorer resonant behaviour, as was detailed above. It should be noted that the ripples in the responses
observed in both Figure 5.10 and 5.11 are of approximately the same magnitude, but the resonant responses of the Wafer 5 die are much smaller. Die 17 in Figure 5.11 shows the desired behaviour, while the identical Die 18 shows virtually no resonant behaviour; Die 19 and 20 are similar to Die 18.

5.1.5.4 Analysis of standard die results

Two main issues with the standard die results are apparent:

1. Performance variation between like devices: it is clear that there are large differences in performance between devices with identical (or very similar) designs. This could be predicted from the analysis of Section 5.5 which demonstrated the wide variety of fabricated dimensions. Given these variations, it is encouraging that the frequency separations between groups of
devices are correct, and that the effects of at least some of the design parameters can be seen in the results.

2. **Wave type uncertainty**: while performance variation is present in any SAW device production process, a more serious issue for this project is the uncertainty over the wave type. When both the frequency and magnitude results are considered together, it is not possible to prove the existence of Rayleigh SAW in the devices using the available results. This does no imply that another wave type is propagating, as Rayleigh SAW are almost certainly active, but rather that this behaviour cannot be demonstrated across the entire results set. For example, the calculated velocity results in Section 5.1.5.1 indicate that the wave velocities are almost isotropic and are generally higher than the theoretical Rayleigh SAW values for the measured orientations. As mentioned above, this calculated behaviour may be caused by the limited
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number of electrode dimension measurements, which may not be representative of the entire structure. The magnitude results are even more difficult to analyse as they are heavily dependent on distributed device dimensions and periodicity (see Section 5.1.2). The existence of responses for the precise ST-(X+90°) orientation is not consistent with Rayleigh SAW, but a possible explanation for the Wafer 1 die behaviour is given below. While the wave type uncertainty is not an issue for the experimental testing, it does represent a major problem for the COM device modelling; this will be discussed in Section 5.1.7.

Some possible causes of the unusual frequency and magnitude behaviour were investigated. Given that the experimental results differ from proven theoretical predictions, it was suspected that the wafer cut may have been incorrect. However, the actual cut of a sample wafer was checked and found to be within the manufacturer’s specification ($\phi = 0° \pm 15'$, $\theta = 42.75° \pm 30'$, see Section A.3): these tolerances are larger than those used for typical SAW device wafers [88]. The orientation of the devices relative to the wafer (i.e., the accuracy of $\psi$), caused by errors in the photomask alignment, was estimated as $\pm 5°$. Thus the Wafer 1 die may actually be using an arbitrary propagation direction around the ST-(X+90°) orientation, one which could support a Rayleigh SAW response. This theory is discussed in Section 5.1.7.

The possibility of a frequency bias in the measurements (i.e., that the measured resonant frequency was systematically different from the actual device frequency) was also considered. The excellent results from the commercial SAW devices (see Section 5.1.3) and the virtually identical results found for the die prior to strain testing using different measurement equipment (see Section 5.2.1) suggest however that gross measurement errors are unlikely.

Another factor which may affect the resonant responses is the residual bias state of the devices. The analysis above assumes that the devices are unbiased, i.e., that the residual stresses and strains in the wave propagation region are negligible. It has recently been shown, however, that ‘as supplied’ quartz wafers can demonstrate considerable residual strains (c. -10,000 $\mu$e at the lapped (reverse) surface) [210]. Section 4.5 demonstrates that such biases may affect the resonant properties of a given device, and thus even the ‘unstrained’ die may display biased
performance. The fabrication processes could also lead to residual biases. In particular, the metallisation process may lead to surface stresses; a good introduction to thin-film stresses in Al is given in [211]. Although both of these factors may be significant, the measurement of residual stresses is outside the scope of this project, and thus quantitative values were not considered.

5.1.6 Large die results

As introduced in Section 3.3.5, the large die designs are adapted from those of the standard die, and thus aspects of their performance should be the same. The yield of the large devices is poorer than that of the standard die (see Section 5.1.4), with only Wafers 4 and 5 producing a useful range of responses; the large Die from Wafers 1 and 3 were discussed in Section 5.1.5. The performance of the devices was analogous to the standard devices on Wafers 1 and 5, with the Wafer 4 die (using ST-(X+90°) propagation) producing better quality responses in general than those on Wafer 5 (using ST-(X+35°) propagation).

Large Die 1-10 use combinations of the standard die electrically connected in series (see Appendix B). Figure 5.12 shows the \(|Z|\) behaviour of large Die 1 and 2 from Wafer 4, each of which has two SAWR with a nominal frequency separation of 1.98MHz. Note that two distinct resonances are now present at approximately 445.6 and 447.6MHz, as opposed to the single resonances in Figures 5.10 and 5.11: this accurate frequency separation is similar to that shown by the standard die. The broadband impedances of the complete devices are also larger than those of a standard SAWR, and in this case the performances of the two die are consistent. Die 3 and 4 use optimal and synchronous SAWR with the same nominal frequency in order to get closely-spaced responses. Although distinct responses were seen on some die, in many cases it is difficult to distinguish between the stopband ripples of one device and the resonant response of another. Die 5-8 have devices separated both in frequency and in resonant magnitude, but again it is difficult to identify the stronger or weaker resonances in the experimental results. The large frequency separations used in Die 9 and 10 were accurately reproduced, with responses analogous to those shown in Figure 5.12.

Large Die 11-16 were designed to test extreme SAWR parameter values, but
unfortunately few devices provided useful responses. It is unclear whether this was caused by inherent design problems or by the manufacturing variations seen in the other devices: it is possible that both factors are involved. Die 11 and 12 use different IDT lengths, and on Die 12, Wafer 5 the longer IDTs reduced $|Z|$, which corresponds to the behaviour seen in the standard devices. The resonant responses of both devices on this die were too poor to check any effects on the resonant magnitudes. Die 13 and 14 were designed to analyse changes in reflector length, but no useable measurements were found on the fabricated devices. Die 15 and 16 test different aperture widths, and Die 15, Wafer 4 indicates that a wider aperture reduces $|Z|$ but also degrades the resonant response. While the reduction in impedance was expected, it is unclear whether the resonant magnitude was affected by the change in aspect ratio or by process variation.

In summary, the large die results show the potential of using multiple SAWR
or different parameter values to affect device performance, but also illustrate the fabrication and design difficulties. As the responses of the multiple SAWR die are linear superpositions of the standard die responses (in general), there is considerable flexibility for future designs. Although few changes in parameter values could be examined, the results of large Die 11-16 indicate that large variations in device design are possible.

### 5.1.7 COM parameter extraction

As discussed in Section 5.1.5.4, the existence of Rayleigh SAW in the prototype devices cannot be proven using the available results. This represents a major issue for the COM modelling as the independent parameters detailed in Section 4.5 assume that a Rayleigh SAW is propagating and can be analysed. COM analysis may be applied to general wave types (see Section 4.4), with the assumption that only one wave type is propagating (see Section 4.3); the relatively consistent device results suggest that this is the case for the prototype sensors. However, if the properties of the wave type or device structures are uncertain, the theoretical COM parameters (e.g., $v$) cannot be accurately evaluated, and thus device performance cannot be predicted. It should be noted that this behaviour is not particular to COM analysis: all phenomenological models require accurate wave descriptions and structure dimensions in order to predict device behaviour [156].

It was hypothesised in Section 5.1.5.4 that the existence of resonant responses from the Wafer 1 die may be due to the actual propagation direction differing from ST-(X+90°). As detailed in Section 5.1.5.2, the magnitude of the responses is determined by both the piezoelectric coupling and the reflectivity of the structures. Therefore small angular deviations from the ST-(X+90°) orientation could lead to a non-zero piezoelectric coupling, which when combined with the strong reflectivity of Rayleigh SAW near this orientation (see Figure 4.18) could create a resonant response. To test this theory, the theoretical COM parameters detailed in Section 4.5 were calculated over a range of possible propagation directions (i.e., $\phi = 0° \pm 1°$, $\theta = 42.75° \pm 1°$ and $\phi = 90° \pm 10°$); these are greater than the probable angular tolerances given in Section 5.1.5.4. Although differences in COM parameter behaviour were naturally observed for different values of $\phi$ and $\theta$ (e.g.,
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In magnitude, symmetry etc.), these were minor relative to those caused by $\psi$ and thus the ST-cut results presented in Section 4.5 are indicative of the general performance. Table 5.9 shows the calculated parameters near the ST-(X+90°) orientation. The $p$ subscript is explained in Section 4.5.4 while $\alpha_n = \alpha_p/\sqrt{W/\lambda}$ (see Section 4.5.5). The complex nature of $\kappa_p$ should be noted, as should the large variation in $\alpha_n$ with small changes in $\psi$.

The measured dimensions of Die 18, Wafer 1 (see Table 3.2) were used in the general COM model of equation (4.25) to simulate the admittance $Y = G + iB$ of the device over the range of possible propagation directions. This device demonstrated performance typical of those on Wafer 1. As noted in Section 3.5, the measured dimensions may be subject to error, but were used here to reduce the number of model variables. Although the theoretical COM parameters in Table 5.9 were used in the model, no significant resonant response was simulated for any of the possible orientations in the measured frequency range. There are a number of possible reasons for this behaviour. It is clear that $\alpha_n$ is extremely small: the maximum value within this range (i.e., for ST-(X+80°)) is only a quarter of the value for ST-X propagation. This weak transduction behaviour will naturally limit the magnitude of any resonant response. Another issue is the phase of $\kappa_p$. As noted in Section 4.4.3, optimal devices such as Die 18 were designed on the assumption that $\kappa$ is real and that IDT reflection effects may be ignored. It is clear though that the imaginary components of $\kappa_p$ for the possible orientations are as large as the real components, leading to a significant phase shift of the reflected waves. Thus the reflectors are not positioned optimally with respect to the IDT, leading to degraded responses. The IDT reflective behaviour may also be significant in these devices due to increased SAW decay within the reflective gratings. Such behaviour was noted in Section 5.1.5.1 where little change in the measured resonant frequency was observed for different reflector lengths. This suggests that the effective length of the reflective gratings is smaller than the actual length, due to a lack of wave propagation in the outer sections, and this may increase the importance of IDT reflective effects.

Although the theoretical COM parameters do not explain the Wafer 1 responses, it is possible to fit parameters (in a basic way) to the model developed in Section 4.4 from experimental results. Although these fitted parameters are less
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<table>
<thead>
<tr>
<th>Parameter</th>
<th>ST-(X+80°)</th>
<th>ST-(X+85°)</th>
<th>ST-(X+90°)</th>
<th>Fitted</th>
</tr>
</thead>
<tbody>
<tr>
<td>( v ) (m/s)</td>
<td>3503</td>
<td>3510</td>
<td>3513</td>
<td>3528</td>
</tr>
<tr>
<td>( \kappa_p )</td>
<td>0.0207+0.0256i</td>
<td>0.0226+0.0250i</td>
<td>0.0232+0.0248i</td>
<td>-0.011</td>
</tr>
<tr>
<td>( \alpha_n \left( \sqrt{1/\Omega} \right) )</td>
<td>6.92 \times 10^{-6}</td>
<td>3.51 \times 10^{-6}</td>
<td>1.06 \times 10^{-7}</td>
<td>2.4 \times 10^{-5}</td>
</tr>
<tr>
<td>( C_n ) (pF/m)</td>
<td>57.72</td>
<td>57.73</td>
<td>57.75</td>
<td>67</td>
</tr>
<tr>
<td>( R ) (Ω)</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>14</td>
</tr>
<tr>
<td>( \gamma_p ) (Neper/λ)</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>8 \times 10^{-4}</td>
</tr>
</tbody>
</table>

Table 5.9: Theoretical and fitted COM parameters for Die 18, Wafer 1 near the ST-(X+90°) orientation. An Al electrode thickness of \( h = 165 \text{nm} \) was used.

useful for sensor work than the theoretical predictions of the values (see Section 4.5), they can demonstrate the suitability of COM analysis for device modelling. Figure 5.13 shows the measured admittance of Die 18, Wafer 1 along with the fitted COM model; the parameters used are shown in Table 5.9. The experimental \( Y \) shows reasonable correlation with the theoretical optimal response (see Figure 4.10), though stronger ripples are present which may be indicative of additional dispersive behaviour. The COM model was manually fitted to the experimental response, with the measured electrode dimensions (see Table 3.2) again used to minimise the number of variables. It should be noted that, due to the jagged nature of the experimental response, key features such as the stopband edges cannot be accurately located, and thus the COM parameters are difficult to determine unambiguously. A bidirectional SAWR model was used to simplify fitting as many of the parameters were uncertain, though the more general COM model should be used if fewer parameters need to be determined. The following may be noted:

- The fitted velocity is in relatively good agreement with the Rayleigh SAW value for ST-(X+90°); \( v \) in this case includes the effect of the deposited electrodes as detailed in Section 4.5.3. It is also in excellent agreement with the calculated velocity in Table 5.3 as would be expected.
- The reflectivity and transduction coefficient results differ from the theoretical values, as would be expected from the above analysis. The positive, complex value of the theoretical \( \kappa_p \) indicates that the phase-shifted response should be moved towards the upper end of the COM stopband: this is not
supported by the experimental results. Similarly, while a significant transduction coefficient was indicated by the device, very little coupling is predicted in theory. It is interesting that the fitted values are in good agreement with those reported in [171] ($\kappa_p = -0.015$ and $\alpha_n = 2.7 \times 10^{-5} \sqrt{1/\Omega}$) for ST-X propagation with similar devices.

- $C_n$ and $R$ are used to fit the broadband responses to the experimental values. In common with the rest of the COM parameters, the fitted values describe the device as a whole (with busbars, bond pads, probe effects etc.) rather than just the active SAWR region, and thus some deviations from theoretical values are to be expected. With this in mind, the fitted $C_n$ is in relatively good agreement with theory. The resistance $R$ of the device was not included in the original COM model for simplicity (see Section 4.4.1), and
was implemented here as a simple resistor in series with the device.

- The normalised attenuation $\gamma_p$ is about four times larger than the theoretical free-surface value, which is unsurprising given that it includes all of the loss mechanisms (see Section 4.5.7). It is about twice the value reported in [171], which may be due to fabrication variations or surface imperfections.

The fitted results, while not as good as those reported in [171] and [212], are in reasonable agreement with the experimental results. As noted above, the failure of the COM model to completely describe the device response is due to uncertainties over the wave type and device dimensions rather than a fundamental model flaw. Figure 5.13 demonstrates the effectiveness of the COM approach for resonant SAW devices, producing detailed response information from relatively few parameters. With a better understanding of the active wave type and improved fabrication controls, it should be possible to improve model performance.

5.2 Strained experimental testing

Once the static behaviour of the devices was determined, a number were selected for strain testing. This was designed to give an insight into the general sensor behaviour; strain testing all of the acceptable devices was impractical due to time constraints. The following sections detail the testing process and results from some sample devices.

5.2.1 Test equipment and protocol

In the absence of any standards for SAW strain sensors, it was decided to adapt the two most common strain gauge standards ([173] and [214]) for use in this project. These standards are almost identical, and give procedures for the determination of strain gauge characteristics (gauge factor, transverse sensitivity, temperature sensitivity etc.). The most common loading case is shown in Figure 4.12 where the gauge is bonded to a beam under uniaxial stress: details of this are given in Section 4.5.1. This setup is used to find the gauge factor of the foil gauge, i.e., the fractional change in the resistance due to axial strain. It should be noted that the
uniaxial stress induces a biaxial strain state at the surface, and that in general the sensor will also be sensitive to transverse strains. This transverse sensitivity can be quantified using a uniaxial strain test rig.

In general, the characterisation of a particular type of sensor requires several identical devices, and due to the installation process these cannot be reused. However, the static testing of the SAW sensors revealed large performance variations between devices of the same design, and thus it was not possible to completely characterise the designs. As the gauge factor is of primary importance, all of the strain tests were performed with the uniaxial stress parallel to the SAW propagation direction: the transverse sensitivity was not measured. For strain gauges the transverse sensitivity is generally a small percentage of the gauge factor (c. 2%, see [4]), and thus only has a minor effect on the results. The modelling presented in Section 4.5 is defined in terms of stress rather than strain, thus biaxial strain effects are automatically included.

Figure 5.14 shows some of the equipment used for the strain testing. A simple test beam (120mm × 30mm × 12mm) was designed to mount the sensors, with an Instron servohydraulic testing machine used for loading as per Figure 4.12. This beam configuration provides a large surface area under homogeneous uniaxial stress, enabling the attachment of a SAW sensor and a conventional strain gauge in the same area. A disadvantage is that tensile and compressive tests cannot be performed in the same measurement cycle, due to the pinned mounting in the testing machine: the beam must be turned over. EN6A steel was selected for the beam due to its high yield strength, allowing testing over larger strain ranges compared to conventional mild steel. It was decided that the microwave probes used for the static testing were too fragile for use in a mechanical testing environment, therefore a coaxial receptacle was adapted for this purpose. The receptacle was attached to the beam’s neutral axis using nylon screws (see Figure 5.14), thus minimising its effects on the beam’s stress state and providing electrical isolation. Tinned copper wires were used as probes to connect the receptacle to the SAW sensor under test: these are similar to the BeCu tips of the microwave probes, and Cu-Al interfaces have been shown to provide good performance [213]. A disadvantage of such a probe is that no calibration standards are available for it, and thus the measurement system can only be reliably calibrated to the end of the network.
Figure 5.14: Photo of interrogation equipment used during strain testing, with an NI PXI-1011/PXI-8186 measurement platform (bottom module and monitor), Agilent E5061A vector network analyser (centre module) and test beam (in front of monitor).
analyser’s cable. Comparisons between frequency responses using the microwave probe and the receptacle, however, showed only minor variations in $|S_{11}|$ and no change in the resonant frequency of the SAW device. Conventional uniaxial foil resistive strain gauges in a quarter-bridge configuration were used as strain references: these were temperature compensated for steel specimens (see Section 4.5.1). Both sensors were bonded to the beam using standard cyanomethacrylate glue.

The standard test protocol was to statically load the beam in 1kN steps up to a total load of 10kN, with a similar unloading process. A reference measurement, with the unloaded beam placed on a flat surface, was performed before strain testing: this allows for strain nulling (see below) and establishes the unstrained resonant frequency $f_0$ for the installation (see Section 5.2.2). It should be noted that the strain gauge standards use fewer load steps (typically 3 or 5); extra data was collected for the SAW sensors as their likely performance was unknown. One measurement cycle comprised of compressive loading and unloading, with the sensors facing up (see Figure 4.12), followed by tensile loading and unloading with the beam turned over. Three measurement cycles were proposed for each sensor, though in some cases fewer cycles were used.

Measurement errors are inherent in any experimental testing, and can pose particular problems for new sensor types; an excellent discussion of strain gauge errors is given in [7]. In order to minimise systematic errors, the complete measurement system (see below) was calibrated before each test. The servohydraulic testing machine was load balanced to remove offset measurement values, and from the load cell specifications the static load accuracy was estimated as ±2% of the indicated load. In a similar manner, the strain gauge output was null balanced in software before loading to remove offset errors. As noted in Section 5.1.2 the calibrated frequency accuracy of the vector network analyser is estimated as ±10ppm. Other systematic errors within each test (sensor misalignment, bonding issues etc.) were minimised through the use of standardised installation procedures. In order to quantify the effect of random errors, 10 measurements were taken for each load point. Due to the small strain ranges involved, the strain accuracy of an individual measurement (with strain nulling) can be estimated as a constant ±16µε, though the overall accuracy is improved through the use of
multiple measurements. The mean values detailed and plotted in the following sections represent the best estimate of the true measurement values [214], while the error bounds are defined by the standard deviations. For clarity, the systematic errors are not tabulated, nor are error bars plotted: these can easily be calculated from the above.

An important task in the strain testing of the SAW sensors was their calibration against existing devices, in this case the conventional strain gauge. This was complicated by the fact that the different sensors require different interrogation methods and response measurements. In many cases, separate measurement systems are used for each device during the calibration of new sensor types. This can increase the cost and time required for calibration, and may also lead to more error sources. For this project an integrated measurement system was created using NI LabVIEW v7.1 [215]. This virtual instrument (VI) creates a central measurement point for both sensors, and was run on an NI PXI-1011/PXI-8186 measurement platform. Figure 5.14 shows some of the connectivity, with the strain gauge connected to the platform using SCXI-1520/SCXI-1314/PXI-6052E modules and an Agilent E5061A vector network analyser connected using the GPIB protocol. A block diagram of the VI is shown in Figure 5.15; this was adapted from an existing DAQmx VI used for strain gauging. The VI is designed to acquire a fixed number of measurement samples from each sensor on demand, and save these results to a text file. Continuous readings are taken from the sensors, but as the strain state is independently controlled, it is useful to save results only when required. The network analyser is controlled from the VI using NI-VISA v3.6 and a customised version its instrument driver. Specific measurement parameters, rather than complete traces, can be acquired: the resonant frequency and its magnitude were chosen for the strain testing. This means that a targeted data set can be created containing only the desired variables, which reduces the post processing of results and extends the functionality of the network analyser. GPIB instrument querying was used to synchronise the strain gauge and SAW sensor measurements, thus ensuring that they reference the same strain state and also optimising the sampling frequency.
Figure 5.15: Block diagram of integrated measurement VI
5.2.2 Sensor parameters

The SAW sensor and strain gauge results were analysed using a number of different parameters \[216,4\], which together give an indication of device performance. With the exception of the gauge factor, all of the following are defined as percentages of the full-scale range of the measurement:

1. **Gauge factor**: analogous to that defined for conventional strain gauges (i.e., \( \zeta = \Delta R/(RS_{11}) \)), the gauge factor \( \zeta \) for SAWR sensors with \( x_1 \) propagation was defined as the fractional change in resonant frequency with applied strain in the propagation direction:

   \[
   \zeta = \frac{f - f_0}{f_0 S_{11}} = \frac{\Delta f}{f_0 S_{11}}
   \]  

   where \( f \) is the measured resonant frequency, \( f_0 \) is the unstrained resonant frequency and \( S_{11} \) is the \( x_1 \) normal strain as before. Multiple load points were measured for each sensor, and both results sets were combined to calculate \( \zeta \). Least-squares fitting was used for both the \( S_{11} \) vs. load and \( \Delta f/f_0 \) vs. load results for each loading or unloading process (i.e., four per load cycle); the devices were assumed to act linearly. The nominal gauge factor for the strain gauges was 2 at room temperature.

2. **Nonlinearity**: the nonlinearity definition used here is the maximum deviation of the measured values from the least-squares lines defined above. Four values are defined for each load cycle.

3. **Hysteresis**: this is the maximum difference between the same measured point(s) in loading and unloading. The hysteresis is calculated over each half-cycle, i.e., two values per complete load cycle.

4. **Repeatability**: this is the maximum difference between the same measured point(s) over different load cycles, and is defined for each pair of loading or unloading processes.
5.2. STRAINED EXPERIMENTAL TESTING

<table>
<thead>
<tr>
<th>Die</th>
<th>Nonlinearity (%)</th>
<th>Hysteresis (%)</th>
<th>Repeatability (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.60±0.56</td>
<td>2.42±1.24</td>
<td>4.21±1.44</td>
</tr>
<tr>
<td>13</td>
<td>1.54±0.96</td>
<td>1.95±1.11</td>
<td>5.34±1.47</td>
</tr>
<tr>
<td>14</td>
<td>0.82±0.29</td>
<td>1.39±0.31</td>
<td>9.04±5.86</td>
</tr>
<tr>
<td>18</td>
<td>2.28±1.99</td>
<td>2.41±2.56</td>
<td>8.01±2.84</td>
</tr>
<tr>
<td>21</td>
<td>1.03±0.82</td>
<td>2.19±2.00</td>
<td>7.37±1.43</td>
</tr>
<tr>
<td>31</td>
<td>1.30±1.00</td>
<td>3.51±2.45</td>
<td>2.26±0.78</td>
</tr>
<tr>
<td>32</td>
<td>1.21±0.69</td>
<td>2.31±1.05</td>
<td>2.63±1.04</td>
</tr>
</tbody>
</table>

Table 5.10: Strain gauge $S_{11}$ parameters corresponding to the strained Wafer 5 die; mean values and standard deviations are shown.

5.2.3 Strained die results

A number of the Wafer 5 standard die (Die 10, 13, 14, 18, 21, 31 and 32) were strain tested. These devices were chosen at random from those detailed in Section 5.1.5 and have a variety of responses. In a similar manner to the SEM results presented in Section 3.5, the Wafer 5 die demonstrate poorer resonant performances than the corresponding Wafer 1 die, and thus they should represent the ‘worst case’ sensor performance measurements of the acceptable die. It should be noted that many devices which demonstrated good static performance were damaged during installation on the beam and thus could not be strain tested: this aspect will be discussed in Section 6.3.

An initial task was to analyse the strain gauge results, as these are used as the reference measurements for the SAW sensors. Table 5.10 shows the nonlinearity, hysteresis and repeatability results from the strain gauges corresponding to the different strained die. The following may be noted:

- All of the test results demonstrate relatively good linearity, confirming the fitting assumption made above. Each loading or unloading process can thus be modelled by the corresponding least-squares fitted line, which should be more indicative of the general behaviour than a given measured point. The fitted lines comprise of a strain sensitivity and a no-load offset value. Sensitivities for different loading processes are consistent across different load cycles for each die, though differences were observed in the compressive/tensile behaviour and between different die. For example, the strain
sensitivity for compressive loading of Die 10 ($4.06 \pm 0.04 \times 10^{-8}\text{N}^{-1}$) is about 14\% less than that for tensile loading ($4.62 \pm 0.03 \times 10^{-8}\text{N}^{-1}$). This is surprising given that the gauges and the test beams were expected to demonstrate the same sensitivity both in tension and compression, and indeed some of the gauges do. The small standard deviations across different measurement cycles indicate that the behaviour is systematic for this gauge rather than random; a possible cause is that the elastic properties of the particular test beam change slightly with different types of loading. Another possible error source is the accuracy of the applied load (see Section 5.2.1), which may be improved in the future through use of calibrated weights [88]. As both the strain gauge and SAW sensor use the same adhesive and installation technique for attachment to the test beam, and are subject to the same strain state, the results from both sensors may be compared while errors from attachment effects are minimised.

- The hysteresis values demonstrate that, in general, the performance is consistent both in loading and unloading for each half-cycle, though some variations are present. A compressive loading and unloading process changes the no-load strain value, i.e., the no-load strain is slightly different after the test compared to that before. Both positive and negative offsets appear to be equally likely, and the magnitudes are generally small. However, tensile loading and unloading increased the no-load strain in almost 70\% of the cases, indicating that some tensile residual strain may be present.

- Given the relatively good linearity and hysteresis results, the repeatability values are slightly poorer than expected, which indicates differences between results from different load cycles. Although the strain sensitivities for each die are consistent over different load cycles, the no-load offsets do vary. Together with the hysteresis effects, these degrade the repeatability. The main cause of these offsets was the reversal of the test beam to perform different tests: this produced similar behaviour to that shown in compressive loading and unloading, with small random changes in the no-load readings.

As an example, Figure 5.16 shows the measured $S_{11}$ corresponding to Die 10 as a function of load over three complete measurement cycles; this is indicative
of the general strain behaviour. Each plotted point in this and subsequent figures represents the mean of the 10 measurements taken for each load value (see Section 5.2.1).

The SAWR results detail both the frequency and magnitude of the resonant responses as functions of load. As may be expected from the static results of Section 5.1.5, the SAW sensors display greater variations in performance than the corresponding strain gauges, and the correlation between devices is lower. The tested die may be divided into those which display relatively consistent behaviour over different load cycles (Die 10, 14, 21, 31 and 32) and those which do not (Die 13 and 18). Table 5.11 gives the $\Delta f/f_0$ performance of the first group of die. The no-load values for Die 14 are significantly different from the die’s other test points, which could degrade both the linearity and the repeatability; such points were treated as outliers [214] and were removed. Some general points may be
made about the results:

- This group of die display reasonable linearity, though their performance is inferior to that of the strain gauges. It should be noted that the nonlinearity is caused by individual points (e.g., for Die 31) or by variations around the least-squares line (Die 32), rather than by a general nonlinear response.

- The hysteresis values are considerably poorer than those of the strain gauges, and need to be examined in more detail. As noted above, the strain gauges commonly demonstrate different sensitivities in tension and compression, but these are consistent for loading and unloading. By contrast, Die 10, 31 and 32 are more sensitive in a tensile unloading process than in a tensile loading process. For example, Die 10 demonstrates a $\Delta f/f_0$ sensitivity of $4.58 \pm 0.11 \times 10^{-8} \text{N}^{-1}$ for compressive loading and unloading, which is consistent across different measurement cycles. Similarly, the sensitivity to tensile loading is $4.56 \pm 0.20 \times 10^{-8} \text{N}^{-1}$. However, the sensitivity to tensile unloading is $5.16 \pm 0.11 \times 10^{-8} \text{N}^{-1}$, an increase of about 13%. Thus both the strain gauge and the SAW sensor (in this case) demonstrate roughly the same increase in sensitivity during tensile unloading, but only the strain gauge shows the same behaviour in loading. The increased tensile unloading sensitivity relative to that in loading means that the resonant frequency of the device after a tensile loading/unloading process is consistently lower than before the process; compressive loading and unloading does not affect the frequency in a consistent way. It should also be noted that subsequent tests are consistent with those performed before the tensile loading(s), ex-

<table>
<thead>
<tr>
<th>Die</th>
<th>Nonlinearity (%)</th>
<th>Hysteresis (%)</th>
<th>Repeatability (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.87±0.65</td>
<td>9.89±6.21</td>
<td>7.26±3.64</td>
</tr>
<tr>
<td>14</td>
<td>3.63±0.91</td>
<td>6.12±2.87</td>
<td>13.63±2.17</td>
</tr>
<tr>
<td>21</td>
<td>2.67±1.24</td>
<td>6.42±1.37</td>
<td>5.43±2.94</td>
</tr>
<tr>
<td>31</td>
<td>3.40±2.73</td>
<td>10.28±5.48</td>
<td>6.08±2.08</td>
</tr>
<tr>
<td>32</td>
<td>5.01±1.76</td>
<td>16.40±11.16</td>
<td>22.56±1.91</td>
</tr>
</tbody>
</table>

Table 5.11: SAW sensor $\Delta f/f_0$ parameters of some strained Wafer 5 die; mean values and standard deviations are shown.
cept for the no-load frequency shifts: if the SAW sensor was damaged during loading, it would be expected that these responses would be degraded. Figure 5.17 shows the $\Delta f/f_0$ behaviour of Die 10 over three complete measurement cycles, which may be compared to Figure 5.16; note the increased sensitivity in tensile unloading. Possible improvements in the test method to clarify these results are discussed in Section 6.3. The sensitivities of Die 14 and 21 are relatively consistent for loading and unloading, thus their hysteresis performance is determined more by individual measurement points than sensitivity variations. These die demonstrate lower hysteresis, as might be expected.

- Differences in the no-load offset values appear to be a greater issue for the SAW sensors than for the strain gauges. As well as the tensile effects noted
above, compressive loading and unloading raises the resonant frequency in about 68% of the tested cases, though the magnitudes of these shifts are smaller than those caused by tensile loads. This is in contrast to the strain gauge results, where compressive loading produced random strain shifts. Reversal of the test beam (either upside or upside down) increased the resonant frequency in the majority of cases, which is again different from the strain gauge behaviour. Thus there does not appear to be a correlation between the no-load results for a strain gauge and its corresponding SAW sensor, which suggests that the behaviour is not caused by the applied strain bias. Taken together, the hysteresis and offset effects markedly decrease the repeatability of the measurements relative to that of the strain gauges.

- The magnitudes of the resonant responses do not appear to change greatly with applied load. In general, tensile loads lead to a linear reduction in the resonant response, with the opposite behaviour for compressive loads. No marked changes in the magnitudes were noted over the different test cycles for most of the die, though the performance of Die 21 degraded over the third tensile load cycle. It was noted during the testing that flexure of the test cable shifted the entire frequency response, though the magnitude of the resonant response and its frequency remained constant. Changes in the test VI to improve the magnitude measurements will be discussed in Section 6.3.

The results from Die 13 and 18 are more difficult to analyse as the $\Delta f/f_0$ behaviour changes significantly over different cycles. Figure 5.18 shows the performance of Die 18 over three complete measurement cycles, which is similar to that of Die 13. A number of test points are missing due to testing errors, but the general behaviour is clear and may be summarised as follows:

1. 1st compressive cycle: this is analogous to that shown in Figure 5.17
2. 1st tensile cycle: displays only half the sensitivity of the above cycle; the unloading process shows the same behaviour noted in Die 10.
3. 2nd compressive cycle: similar to the first compressive cycle.
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Figure 5.18: $\Delta f/f_0$ vs. load plot for Die 18, Wafer 5

4. **2nd tensile cycle**: increased sensitivity relative to the first tensile cycle, roughly equal to that of the first two compressive cycles.

5. **3rd compressive cycle**: degraded sensitivity, equivalent to the first tensile cycle.

6. **3rd tensile cycle**: similar to the first tensile cycle.

The behaviour is interesting as the sensitivity varies over different load cycles, but in an inconsistent fashion. It should be noted that the corresponding strain gauge results are similar to those shown in Figure 5.16, so errors in the applied load are unlikely to be a factor. With such large changes in sensitivity, it was hypothesised that resonant response might vary considerably over different measurement cycles, but this does not appear to be the case. Each measured point in
Table 5.12: Gauge factors of some strained Wafer 5 die for different loading processes; mean values and standard deviations are shown.

<table>
<thead>
<tr>
<th>Die</th>
<th>Comp. Load</th>
<th>Comp. Unload</th>
<th>Tens. Load</th>
<th>Tens. Unload</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.21±0.08</td>
<td>1.16±0.06</td>
<td>0.96±0.05</td>
<td>0.84±0.10</td>
</tr>
<tr>
<td>14</td>
<td>0.40±0.15</td>
<td>0.34±0.20</td>
<td>1.72±0.24</td>
<td>1.76±0.30</td>
</tr>
<tr>
<td>21</td>
<td>0.98±0.04</td>
<td>0.93±0.07</td>
<td>1.23±0.10</td>
<td>1.17±0.11</td>
</tr>
<tr>
<td>31</td>
<td>0.83±0.03</td>
<td>0.80±0.03</td>
<td>0.85±0.04</td>
<td>0.78±0.06</td>
</tr>
<tr>
<td>32</td>
<td>0.77±0.08</td>
<td>0.73±0.06</td>
<td>0.64±0.01</td>
<td>0.48±0.14</td>
</tr>
</tbody>
</table>

Figure 5.18 displays about the same frequency stability, i.e., the standard deviation of each set of 10 measurements (see Section 5.2.1) is about 3kHz. The magnitude results are more difficult to interpret, but they show that the response is nonlinear, with decreased sensitivity at higher loads; they are consistent over the first two measurement cycles, however. It was discovered during testing than subjecting a die to large strains (c. 2000µε) not only seriously degraded the resonant response (indicating permanent device damage) but also reduced the load sensitivity \([217]\).

It is suspected that a less severe form of this behaviour may be occurring in Die 13 and 18, where the devices are progressively damaged over different load cycles: the reduced sensitivity in the third load cycles may be a resultant of the effects from the first two.

The gauge factor \(\zeta\) of the SAW sensors may be found by combining the results sets of the strain gauges and SAW sensors as detailed in Section 5.2.2. Mean measured values of \(\Delta f/f_0\) and \(S_{11}\), rather than the fitted lines, were used to assess \(\zeta\). As the no-load offsets of the frequency values are generally higher than the corresponding strain offsets, the gauge factors for small applied loads do not reflect the general behaviour, and it is more reliable to calculate \(\zeta\) based on larger loads: the upper half (5-10kN) of the loading was used. Table 5.12 shows \(\zeta\) for loading and unloading in compression and tension. A number of observations may be made:

- \(\zeta\) is positive, i.e., the resonant frequencies of the devices increase with tensile \(S_{11}\). This behaviour will be examined in the next section.
- There is lots of variation in the results, with no real sensitivity pattern. Die 10 and 32 are more sensitive in compression, while Die 14 and 21 show the
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opposite behaviour; Die 31 is equally sensitive to both load types. For some die (e.g., for Die 14), there are large differences between the compressive and tensile $\zeta$ values.

- In almost all cases, $\zeta$ is slightly lower in unloading than in loading. Although differences in loading and unloading were noticed in the $S_{11}$ vs. load and $\Delta f/f_0$ results, combining these results gives a better understanding of the SAW sensor behaviour.

- Although the SAW sensor’s gauge factor is only half that of the strain gauge, the potential resolution of the sensor is higher as small changes in frequency can be measured more easily than small changes in gauge resistance (or bridge output voltage). The exact resolution is dependent on the interrogation system used (see Section 3.3.1), which in turn depends on the measurement application.

As the $\Delta f/f_0$ behaviour of Die 13 and 18 varies significantly over different load cycles, no $\zeta$ results are presented for these devices. Figure 5.19 shows $\Delta f/f_0$ as a function of $S_{11}$ for Die 10, Wafer 5 as an example of a complete die performance.

5.3 Comparison of simulated and experimental results

In order to evaluate the performance of the strained COM model (see Section 4.5), the predicted sensor response was compared to the experimental measurements.

An initial task was to calculate the biased state of the test beam(s) (see Section 4.5.1). $S_{11}$ for the bending beam at the strain gauge location may be calculated from equation (4.26) with an assumed value of $E$. From the beam and loading geometry, the beam strain may be expressed as $S_{11} = \pm 8681P/E$, where $P = 2F$ is the total applied load on the beam (see Figure 4.12). Using the mean strain and load results indicates that the Young’s Modulus of the EN6A steel is approximately 200GPa, which is in good agreement with published values [218]: this
\[ \frac{\Delta f}{f_0} \] over different loading cycles

Figure 5.19: \( \frac{\Delta f}{f_0} \) vs. \( S_{11} \) plot for Die 10, Wafer 5

stiffness was subsequently used in the FE modelling. As was noted in Section 4.5.1, the behaviour of a simple finite element bending beam model was verified before the more complex substrate/beam model was constructed.

Once the beam properties had been accurately estimated, the biased state of the SAW substrate could be evaluated. Figures 5.20 and 5.21 plot the \( T_{11} \) and \( T_{33} \) behaviour (respectively) at the substrate surface along the SAW propagation direction, which was calculated by the substrate/beam model (see Figure 4.14): curves for different propagation directions are given. The stresses are proportional to the total applied load (\( P = -10 \)kN in this case), and results are given for the SAW propagation region of the substrate. All of the \( T_{11} \) curves show quadratic behaviour, with the maximum compressive stress near the centre of the substrate; it is slightly asymmetrical about the centre point. Considerable differences in
magnitude may be observed for different propagation directions: for example, the maximum $|T_{11}|$ for ST-(X+45°) propagation is almost 50% higher than that for ST-X propagation, given the same applied load. The $T_{33}$ results show different characteristics depending on the propagation direction, and the magnitudes are generally smaller than those of $T_{11}$. These results also demonstrate the symmetry of the material, e.g., the normal stress results for ST-(X+45°) and ST-(X+135°) propagation are equal. It was assumed in Section 4.5 that the COM structures were subject to homogeneous biasing fields, which is not the case for this particular application. A possible solution here is to average the stresses over the length of each COM structure. It was noted in Section 5.1.5.1 that the resonant frequencies did not vary with reflector length, indicating that little wave propagation was occurring in the outer sections. Thus although the stress gradients are highest in these sections, the lack of wave activity suggests that they will have little effect on the overall performance of these sensors. As was discussed in Section 4.5.1 the quartz substrates are considerably stiffer than those of conventional strain gauges, and this creates significant stress concentrations along the edges of the substrate/beam interface. Therefore it is important that the reference strain gauges be placed at least half a substrate width away from the SAW sensor, as they are designed to measure the unperturbed beam strain rather than that created by the stress concentration. All of the strain gauges used in the sensor testing were sufficiently displaced to measure the correct strain.

These calculated stresses may be applied to the biased COM model (see Section 4.5) in order to predict the strained performance of the sensors (see Section 4.3). The strained SAWR results discussed in Section 5.2.3 suggest that the device frequencies change in a relatively consistent manner with the applied bias, but the resonant magnitude results are more difficult to interpret. It was therefore decided to model only those COM parameters which contribute to resonant frequency shifts, neglecting those that only affect the magnitude of the response. Of the parameters outlined in Section 4.5 only the electrode geometry and SAW velocity need to be considered. The electrode reflectivity also influences the resonant frequency (see Section 4.5.4), but to a lesser degree. Given the poor correlation between the theoretical predictions and the fitted values of $\kappa$ exhibited in Section 5.1.7 it was decided to omit this parameter. When only the electrode geometry
and SAW velocity are considered, the COM model of the resonant frequency shift effectively reduces to that of equations (4.30) and (4.32):

\[
\Delta f = \frac{\Delta v}{v} - S_{11} = \frac{\Delta v}{v T_{11}} T_{11} + \frac{\Delta v}{v T_{33}} T_{33}
\] (5.6)

The change in velocity can be calculated from the procedure detailed in Section 4.5.3. The ‘natural’ velocity may be used here for convenience as the effects of changes in geometry and propagation properties need not be separated in this case. \(S_{11}\) may be found from the stress results and the material compliances (see Section 4.5.2). Table 5.13 gives the velocity sensitivities (see Figure 4.16) for ST-(X+35°) propagation, as well as the calculated stresses (from the centre of the substrate), derived strain, fractional frequency change and \(\zeta\). A number of points

Figure 5.20: \(T_{11}\) along the SAW propagation direction for different die orientations; \(P = -10\)kN in all cases.
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![Graph showing T_{33} along x_1 for different die orientations](image)

Figure 5.21: $T_{33}$ along the SAW propagation direction for different die orientations; $P = -10$ kN in all cases.

may be made:

- $\Delta v/(\nu T_{11})$ is positive for this orientation, and thus the compressive $T_{11}$ at the substrate surface will cause a decrease in SAW velocity. Similarly, $\Delta v/(\nu T_{33})$ is negative while $T_{33}$ is positive, therefore both stresses will cause a decrease in velocity.

- The SAWR $S_{11}$ is lower than that calculated at the beam surface ($S_{11} = -434 \mu \varepsilon$). This appears to be intuitively incorrect, as the SAWR propagation surface is displaced further from the beam’s neutral axis than the beam surface. However, it may be explained by the fact that the substrate is not in pure bending (due to its attachment), and thus it does not behave as a conventional composite beam.
Table 5.13: Theoretical frequency shift and gauge factor parameters for ST-(X+35°) propagation, with finite element stresses.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta v_{11}$ (m$^2$/N)</td>
<td>$1.094 \times 10^{-11}$</td>
</tr>
<tr>
<td>$T_{11}$ (MPa)</td>
<td>-46.90</td>
</tr>
<tr>
<td>$\Delta v_{33}$ (m$^2$/N)</td>
<td>$-1.042 \times 10^{-11}$</td>
</tr>
<tr>
<td>$T_{33}$ (MPa)</td>
<td>14.76</td>
</tr>
<tr>
<td>$S_{11}$ ($\mu$ε)</td>
<td>-394</td>
</tr>
<tr>
<td>$\Delta f/f_0$</td>
<td>$-6.67 \times 10^{-4}$</td>
</tr>
<tr>
<td>$\zeta$</td>
<td>1.54</td>
</tr>
</tbody>
</table>

- The theoretical $\Delta f/f_0$ is significantly larger than the measured values, which are typically around $-4 \times 10^{-4}$ for the same loading. As Figures 5.18 and 5.17 demonstrate, however, there are considerable variations in performance between die. Given these variations, it is difficult to determine whether the theoretical $\Delta f/f_0$ is an accurate sensitivity estimate for a ‘good’ die, though previous work has shown close correlations (see Section 4.5.3). Using the velocity sensitivities presented in [192] with the above stress results produces $\Delta f/f_0 = 3.96 \times 10^{-4}$, which demonstrates the discrepancy in results with this particular paper noted in Section 4.5.3.

- Due to the larger $\Delta f/f_0$, the theoretical gauge factor $\zeta$ is also larger than most of the measured values detailed in Table 5.12. In this case the beam $S_{11}$, rather than that on the surface of the substrate, is used for consistency with the experimental values. It is interesting to note that both the theoretical and experimental values of $\zeta$ are positive, i.e., tensile $S_{11}$ leads to an increase in the resonant frequency of the device. If the change in wave velocity is neglected in equation (5.6), the associated value of $\zeta$ is negative. This behaviour is intuitively correct: increasing the wavelength of a wave for a given velocity should reduce its frequency. The experimental and theoretical results above demonstrate, however, that the change in SAW propagation properties can be more significant than the wavelength change. These modelled results are a good demonstration of the biased velocity theory de-
5.3. **COMPARISON OF SIMULATED AND EXPERIMENTAL RESULTS**

Detailed in Section 4.5.3 illustrating the importance of modelling changes in propagation properties as well as geometry.

Given that the COM model does not recreate the static responses of the SAW devices with theoretical parameters (see Section 5.1.7), it is perhaps unrealistic to expect that the strained performance would be accurately predicted, as the biased parameters developed in Section 4.5 also require a well-defined wave type. While the strained geometry and bias state results appear to be accurate, the $\Delta v/(vT_{xx})$ results assume that a Rayleigh wave is propagating, which cannot be proven with the calculated ST-(X+35°) velocity results presented in Table 5.5. In the absence of a definite wave type, however, these represent the most likely sensitivities, and demonstrate how the COM model can be applied to SAW sensors. Another difficulty is that although the modelled results above are in qualitative agreement with the measurements, their quantitative value cannot be assessed as the experimental $\zeta$ results are inconsistent. The modular nature of the COM model means that the effect of each independent COM parameter on the frequency response can be isolated (see Section 4.5). Therefore, if only a particular aspect of the biased response (such as the change in resonant frequency) is required, only the relevant COM parameters need to be calculated. As such, the model can be scaled from the prediction of a single parameter to an entire frequency response, as required. This in contrast to device level methods (see Section 4.3), where the entire model must be evaluated, regardless of the desired output.

It is clear that, although the modelled behaviour cannot be verified by the experimental results, the biased COM model provides a flexible tool for SAW strain sensors. In common with the results presented in Section 5.1.7 the shortcomings in the modelled results do not appear to be caused by fundamental model issues but rather by the wave type uncertainty and the variations in the fabricated dimensions. It is expected that the biased performance of improved devices using a defined wave mode would be accurately simulated by the model.
5.4 Conclusion

In this chapter the experimental results of the prototype SAW sensors, both in unstrained and strained states, were examined. The test equipment and protocols associated with each test type were discussed, including a custom test platform for SAW strain sensor testing. Comparative simulation results from the COM model were also presented, illustrating some of the strengths and weaknesses of this modelling approach.

In the next chapter, the project as a whole will be discussed and evaluated.
Chapter 6

Discussion and Conclusion

An important aspect of any research project is the discussion and evaluation of the project as a whole, both from a technical and practical perspective. In this final chapter, the core research work detailed in Chapters 3, 4 and 5 is evaluated with respect to the project objectives outlined in Section 1.4. Possible improvements and future research themes are also discussed.

6.1 Analysis of the integrated design and manufacturing process

This process was designed as a framework for the design and manufacture of prototype SAW sensors, addressing the issues outlined in Section 3.3. In summary, the successes of the process are as follows:

- *Production of working resonant devices*: the most important success was the production of devices with clear resonant behaviour. Given the small linewidths, the design uncertainties and the fact that this was an initial production run, the working devices represent a significant success for the integrated process.

- *Clear indications of design parameter effects*: as well as demonstrating basic resonant behaviour, the results detailed in Section 5.1.5 show (to some extent) the effects of the design decisions made in Section 3.3. For example,
the separations between the resonant frequency groups (see Figures 5.5 and 5.6) closely correspond to the design values. Including such a wide range of design parameters would be prohibitively expensive for custom devices produced by a SAW manufacturer.

However, a number of significant problems were also encountered:

- **Large variations in device performance**: the fabricated dimensions detailed in Section 3.5 demonstrate large differences between different die, while the frequency results also show major variations. Although many design parameters were explored in the photomask layout, the failure of die with identical designs to produce similar results, and the differences in performance of die with the same basic designs proved to be a serious problem.

- **Uncertainty over the wave mode**: the Rayleigh wave mode was chosen in Section 3.3.2 as the preferred wave type, but the existence of this mode cannot be proven using the available results (see Section 5.1.5.4). This is primarily a problem for the device modelling work, which will be discussed in the next section.

- **Lack of derived design information**: an important aim of the process was to provide information for future design work. However, due to the issues mentioned above, the experimental results do not allow the die designs to be refined by any significant degree.

It is instructive to consider the design and manufacturing aspects of the process separately, even though they were implemented together. The design process worked relatively well overall, with good integration of the device designs with the target sensor application. As a full design tool was not available at the time, some of the design decisions made in Section 3.3.5 were necessarily based on rough estimates or on existing devices. While these were generally successful, the low reflectivity of electrodes for ST-(X+35°) propagation (see Sections 4.5.4 and 5.1.5.2) was not predicted, which contributed to the poorer resonant responses of the Wafer 5 die. As noted in Section 4.1, the COM model was not available until after device fabrication due to time constraints.
The manufacturing aspects of the integrated process proved to be the most challenging of the entire project, and most of the measured behaviour can be related to how the devices were made. Two core issues proved to be particularly difficult:

1. The exposure and development of resist patterns to sufficient accuracy.
2. The adhesion of metal layers to the substrate.

An assumption made during the design stages was that the MJB3 mask aligner could reliably expose features smaller than the design linewidths (see Section 3.3.1), and thus grating features could easily be produced. As demonstrated in Section 3.4.4, however, this proved not to be the case, with serious problems found in the resist patterns over a number of fabrication cycles. The mask was then used in a different fabrication process, for which it was not designed, in an attempt to make suitable devices. Thus the relatively poor fabrication quality evidenced in Section 5.5 is not a reflection on the mask design or on the fabrication quality control, but rather on the fact that neither the mask nor the fabrication equipment was used in its optimal state. The wafer misorientation was an unfortunate mistake, but one which is easily corrected. The issue of metal adhesion led to the loss of many die which may have been successful (see Section 5.1.4), and arguably affected the performance of the strained devices. The solution to both of these problems does not lie in the integrated process but rather in hands-on experimentation using tightly-controlled fabrication parameters; such work could not be performed in TCD due to the limited cleanroom access. Before any future design process, it must be proven that the fabrication equipment can produce complete SAW device features (rather than just isolated lines) to a specified resolution on a particular substrate. The discussion in Section 3.4.4 illustrates that the resolution for contact lithography is dependent on a number of parameters, all of which must be considered and optimised. It should be noted that any suitable lithography method may be used (see Section 3.4): the key consideration is whether the mask layout can be reproduced accurately in the resist layer. During the exposure and development experiments it was discovered that the quartz substrates demonstrated significantly different lithographic behaviour compared
CHAPTER 6. DISCUSSION AND CONCLUSION

to silicon wafers, and thus proven fabrication techniques may not be applicable to SAW sensor production. It is therefore recommended that the chosen substrate be used for fabrication testing as well as for the final devices.

Of the many possible improvements to the process, the single most important would be the integration of a preliminary device testing step immediately after fabrication. Given the variations in dimensions detailed in Section 5.5 and the frequency responses of Section 5.1.5, the most obvious course of action would have been to repeat the fabrication in order to create improved devices. However, as the devices were fabricated by an external body, each fabrication run is effectively a separate manufacturing project, and due to capacity constraints new devices could not be created within the required timeframe; it was thus decided to use the original devices in this project. Preliminary testing would remove the need to remanufacture by ensuring that only acceptable devices are released. This shifts the fabrication process from a project-based system, where the only requirement is that a set number of devices be created, to a performance-based one, where devices with defined characteristics are required. The key performance metric would be the frequency responses of the devices, with probe testing similar to that described in Section 5.1.2. This could take the form of a ‘pass/fail’ test, with criteria determined by the device modelling, in order to reduce the testing workload and improve repeatability. In addition, SEM imaging of the electrode layouts would assist in the modelling of the measured responses. Other possible improvements could include an increase in the number of examples of each design on the mask. Given the variations between like die observed from the first fabrication, it is unlikely that more examples of identical designs would have been useful in this project, but with improved fabrication control it should be possible to converge on a number of successful designs. These would be used in subsequent mask layouts with increased numbers of each design. Sensor packaging could also be investigated; this will be discussed in Section 6.3.

6.2 Evaluation of SAW sensor modelling

The aim of the modelling work was to produce a general SAW sensor model which could predict the device response to an applied bias (see Section 4.1). The
custom method outlined in Section 4.3 was designed as a balance between device level and system level modelling, integrating the bias simulation capabilities of the former with the flexible application of the latter. This work combines the COM model, which has been proven to give excellent results for static devices (see Section 4.4.3), with theoretical COM parameters designed to be bias-sensitive (see Section 4.5). Each element of the model has been verified in previous work, and the custom simulation aimed to combine these in a single modelling tool.

At its heart, COM modelling is a simulation technique for periodic structures, and thus its ability to model a SAW device’s response decreases with decreasing periodicity. Similarly, resonant SAW devices also require excellent structural uniformity to achieve maximum performance. Although the measured dimensions detailed in Table 3.2 show that the linewidths are relatively consistent within each COM structure, further refinements in dimensional control would therefore improve both the model validity and device performance. The fitted results detailed in Section 5.1.7 demonstrate that the basic COM model is capable of predicting device behaviour (in a general way), while the examples detailed in Section 4.4.3 show the accuracy of the method for high-quality devices.

Although the core COM model is suitable for the prototype sensors, the overall success of the modelling scheme is dependent on the accuracy of the COM parameters. As was mentioned in Section 4.5, the determination of these parameters is a challenging aspect of any COM model, and their complexity illustrates the importance of defining the application and the model appropriately, in order to remove minor or irrelevant biases. The modelled application defined in Section 4.5.1 and the assumptions made within it, appear to closely match the experimental setup. The validity of neglecting temperature effects is slightly degraded by the fact that arbitrary, rather than temperature-stable, SAW propagation directions were used, though this should not be a major issue as all of the testing work was performed at room temperature. Thus the COM parameters calculated for this particular application should be subject to the same biases as the actual devices. Some observations may be made:

- The bias results presented in Sections 4.5.1 and 5.3 accurately predict the beam behaviour, and thus should give a good indication of the sensor biases.
They also illustrate how the stress components can change significantly with propagation direction.

- The biased velocity method outlined in Section 4.5.3 appears to be appropriate for this work, and although the \( (\Delta v/v)_{m2} \) term is difficult to quantify, its effect on the SAW velocity is minor. Even though the general device behaviour makes it difficult to prove the existence of Rayleigh wave propagation (see below), the calculated static velocity shown in Section 5.1.7 and the velocity sensitivities demonstrated in Section 5.3 are in reasonable agreement with the experimental values.

- The reflectivity modelling detailed in Section 4.5.4 has been used successfully in other works, but in this project it does not predict the static device behaviour (see Table 5.9). A COM structure’s reflectivity is a function of the electrode periodicity, electrode height etc., all of which can vary locally, and as detailed in Section 5.1.7 the jagged nature of the experimental responses makes it difficult to identify specific response features.

- In a similar manner to the reflectivity, the transduction modelling does not match the experimental behaviour shown in Table 5.9. This again appears to be caused by the wave type uncertainty, rather than the calculation method, as Figure 2.7 demonstrates the same behaviour purely from the difference in free surface and metallised SAW velocities.

- The capacitance and attenuation results have been discussed in Section 5.1.7 but some additional comments may be made. Although the modelled capacitance values are relatively close to the fitted results, the agreement could be improved by reduction of parasitic capacitances, or by modelling these separately. In particular, integration of the IDT busbars and bond pads should be investigated as this may improve device performance. The wave attenuation could be reduced through improved fabrication and by using device packaging.

Although the classical methods outlined in Sections 4.5.3 to 4.5.7 represent some of the most accurate theoretical COM parameter techniques available, future work may compare the results of these to numerical methods, especially for
propagation directions with decreased symmetry. For complex bias states a consistent set of higher-order material constants is essential; these are discussed in Section A.2.

As has been previously mentioned, the failure of the COM model to simulate the responses of the devices is not due to a fundamental flaw but is mainly caused by the uncertainty over the propagating wave type; manufacturing variations also play a part, as described above. Despite the extensive research detailed in Section 5.1.5 the indications of Rayleigh SAW behaviour were not fully conclusive. Correlations with measured electrode dimensions, albeit over small areas, failed to provide a fully cohesive explanation of the wave behaviour, though some similarities between like devices were noted. A possible issue in this case is the use of point measurements to represent the dimensions of the entire IDT or reflector grating: the preliminary SEM imaging mentioned in the previous section would improve the quality of these. It is expected that, with better fabrication control and accurate wafer orientation, the active wave mode could be more easily identifiable. A consequence of the wave type uncertainty is that the COM model results detailed in Sections 5.1.7 and 5.3 are mixed, and for the current devices the accuracy of the model depends on the particular parameter of interest.

There appears to be good scope for future work on this topic. The COM model (at least for Rayleigh SAW devices) is mature, and thus once the appropriate wave type and COM parameters have been identified, it should be possible to use the model for sensor applications. At a device level, it could be used to investigate optimal device designs and propagation directions for strain sensitivity, temperature independence etc. Such searches for optimally-performing devices have been a hallmark of SAW research, though previously the work focussed on creating bias-insensitive devices for communications applications. Using the COM model for SAW sensors not only allows the bias sensitivity to be maximised (essentially the inverse of the previous work), but its modular nature means that the selectivity to particular biases (mechanical, electrical etc.) is improved over other models. At a system level, the modelled impedance/admittance response could be used as a component in simulations of multi-sensor systems, especially for wireless applications like RTWIM (see Section 1.3). As an example, the sensor model could be used to estimate the achievable strain resolution in a noisy RF channel, where
the interrogation signals may be degraded by environmental factors. Such applications illustrate the flexibility of the modelling tool, and it is possible that other useful implementations will emerge.

6.3 Evaluation of experimental testing and results

The experimental testing was used both to test the integrated design and manufacturing process and to assess the validity of the modelling. The S-parameter testing outlined in Section 5.1.1 proved to be a success, with enough flexibility to deal with different device designs and to integrate with the COM modelling. Although the static probe testing (see Section 5.1.2) provided excellent quality results, it leaves the die vulnerable to damage and requires specialist equipment. As mentioned in Section 6.1 sensor packaging should be investigated for future devices. Such packaging is successful for conventional SAW devices (as the results of Section 5.1.3 demonstrate), producing rugged components with good performance. Although strain sensor packaging is considerably more difficult than that for communications devices (see Section 3.2.3), it may be possible to implement the packaging as part of the design and manufacturing process after the preliminary testing. The packaging should protect the propagation surface of substrate and provide a rugged connection to coaxial receptacles, antennas etc. as required.

As detailed in Section 5.1.4 the overall yield from the five fabricated wafers is low, though working examples of almost every die design were created; possible improvement solutions have been discussed above. The preliminary testing outlined in Section 6.1 would allow more objective yield testing based on the devices’ design parameters rather than in comparison to other devices on the same wafer.

Although the static die results were extensively analysed in Sections 5.1.5 and 5.1.6 some brief comments may be made here. The resonant frequency results are generally more consistent than those related to the response magnitudes, and the wave type uncertainty has been discussed above. High $Q$ values are important for SAW devices deployed as wireless sensors (see Section 3.3.1), and while the results detailed in Section 5.1.5.3 represent a good starting point, future design work should be targeted to optimise this parameter. The impedance behaviour of
the devices demonstrates the variations in die performance, while the broadband performance could be improved by impedance matching during the design stage. Given the possibility of residual strains detailed in Section 5.1.5.4, examination of fabricated devices for inherent biases should be investigated in the future. The large die, which use combinations of resonators, appear to have good potential as sensors, but it is clear that their standard die components and interconnects need to be optimised first before this can be exploited.

The strained sensor testing detailed in Section 5.2 was designed as a natural extension of that used for conventional strain gauges. In general, the test protocol and approach outlined in Section 5.2.1 was effective, ensuring consistent, objective testing of the sensors. The SAW sensor installation proved to be relatively straightforward, in many cases easier than that of the strain gauges, but significant problems were found with receptacle attachment, leading to a large number of damaged devices. Using packaged sensors, as mentioned above, would significantly improve the durability of the devices. The sensor parameters outlined in Section 5.2.2 provide standardised measures of device performance, while comparing both the strain gauge and SAW sensor results against the applied load allows the characteristics of each device to be evaluated.

The results in Section 5.2.3 illustrate both the potential of SAW devices as strain sensors and the performance variations inherent in prototype devices. Using the sensor parameters allows the strain results to be analysed, and shows the value of examining the reference measurements in calibration work. These also give indications of how the test method can be improved, which will be discussed below. The SAW sensor results show more variation, as would be expected, but they also demonstrate clear strain sensor behaviour. Although the spread of the device results makes it difficult to analyse the die performances as a whole, or evaluate the strain modelling, they do indicate that high-quality SAW strain sensors are possible. With the improved fabrication and modelling detailed above, the full potential of these devices could be realised.

Future work would naturally include the strain testing of the remaining die, which could not be performed in this project due to time constraints. This testing could also benefit from improvements to the test rig. Changing the test beam loading from four-point bending (see Sections 4.5.1 and 5.2.1) to uniaxial loading
could aid the analysis of the tensile/compressive sensitivities and should remove the no-load offsets encountered during the beam reversal. Four-point bending has been preferred over uniaxial loading for strain gauge calibration due to the larger useable test area and the absence of torsional stresses, but with careful rig design both of these issues can be alleviated. A complete measurement cycle (or number of measurement cycles) could thus be performed without removing the beam from the testing machine, which would improve the overall quality of the results. Variations in the strain gauge results also indicate that an additional strain reference should be considered, such as an extensometer, which would verify the actual strain at the beam surface. Possible improvements in the test VI (see Figure 5.15) include better measurement of the resonant magnitude through analysis of the whole resonant peak (rather than just its maximum as is done currently) and better strain nulling of the strain gauge before each test. Logging of the applied load from the test machine should also be considered, particularly if dynamic or fatigue tests are to be performed. In light of the residual device strain mentioned in Section 5.1.5.4 the glued sensor attachment to the beam and its unknown bias state, the test beam should be cycled over a number of measurement cycles before calibration takes place; this is commonly performed with strain gauges.

6.4 Conclusion

For over 40 years, SAW devices have provided a rich research field, leading both to invaluable components used in everyday life and an improved understanding of the surface waves themselves. Their application as sensors is thus a natural evolution of their success as communications devices. The breadth of this project demonstrates their great potential for interdisciplinary research, incorporating ultrasonics, nonlinear electroelasticity, material science, manufacturing engineering and microwave testing amongst many other fields.

In summary, the project objectives outlined in Section 1.4 have largely been met, as discussed above. Although many problems were encountered during the course of the work, the research detailed in Chapters 3, 4 and 5 should lead to a better understanding of SAW strain sensors. It is hoped that this work will allow more SAW sensor applications to emerge.
Appendix A

Quartz properties and transformations

Quartz ($\alpha$-SiO$_2$) is one of the most common minerals found on earth, and is widely used as a substrate for SAW devices. Figure A.1 shows a single quartz crystal with the characteristic hexagonal cross-section and prismatic end. As mentioned in Section 3.3.2, quartz was among the first piezoelectric materials discovered by Pierre and Jacques Curie [25], and is still used in the bulk of piezoelectric devices. It occurs naturally in many different forms [219] and with varying levels of impurities, so most substrates for commercial devices are now artificially grown. These synthetic crystals can then be cut to suit each particular application.

In this chapter a brief introduction to crystallography is given to link crystal properties with the piezoelectric modelling of Chapter 2. Measured material values are then given, followed by a transformation procedure required in Chapters 2 and 4.

A.1 Quartz crystallography

Crystallography is a branch of science dealing with the formation and structure of crystals. It is frequently used to link the continuum mechanics description of piezoelectricity given in Chapter 2 with the physical properties of a given crystal [33]. Most crystals are classified into systems related to their natural symme-
APPENDIX A. QUARTZ PROPERTIES AND TRANSFORMATIONS

Figure A.1: Natural quartz crystal

Figure A.2: Axes of a right-handed quartz crystal [33]

try, which are then subdivided into smaller point groups; further details may be found in references such as [220]. Quartz is part of the trigonal system, with one three-fold axis and two two-fold axes. Figure A.2 shows the crystallographic axes for right-handed quartz (the standard form used in SAW substrates) and their associated Cartesian directions. The Cartesian $Z$ axis corresponds to the crystallographic three-fold axis, about which the crystal properties are invariant under rotations of $2\pi/3$. This give three possible $X$ axes, with each of these displaying two-fold behaviour (invariance under rotations of $\pi$). The $Y$ axis (the other two-fold axis) is then chosen to give a right-handed Cartesian coordinate system. The symmetry of the crystal considerably reduces the number of independent tensor components. For quartz, $14 \epsilon_{ijklmn}$, $6 \epsilon_{ijkl}$, $2 \epsilon_{kij}$ and $2 \epsilon_{ij}$ values are independent. The remaining values may be calculated from point diagrams of the symmetry conditions [33], or from other symmetry relations [221].
A.2 Constant sets and temperature dependencies

A key consideration in any SAW analysis is the selection of experimental material constants. Regardless of the analysis method in question, the accuracy of the results is dependent on the quality and consistency of these measurements. The properties of quartz have been extensively studied, and a recent work by Ballato gives an excellent overview of the field \[222\]. However, compendia of measurements such as \[221\] demonstrate not only the varieties of quartz which have been measured (natural, synthetic etc.) but also the differences between result sets for nominally similar materials. In general, these differences are attributable to small experimental errors, but in some cases different sign conventions are used: discussions on this are given in \[33\] and \[222\]. Serious errors may result if an incorrect axis system is used.

The linear constants (i.e., \(c_{ijkl}^{E}\), \(e_{ki j}\) and \(\varepsilon_{ij}^{S}\)) used in this work are those measured by Bechmann \[223\] for natural quartz specimens. This results set provides consistent values in a single study, and is the one most commonly used in SAW sensor research. The values shown below are given for left-handed quartz according to \[223\], in contracted notation, with \(c_{ijkl}^{E}\) in GPa, \(e_{ki j}\) in C/m\(^2\) and \(\varepsilon_{ij}^{S}\) in \((\text{F/m}) \times 10^{-11}\):

\[
c^{E} = \begin{bmatrix}
86.74 & 6.98 & 11.91 & -17.91 & 0 & 0 \\
6.98 & 86.74 & 11.91 & 17.91 & 0 & 0 \\
11.91 & 11.91 & 107.2 & 0 & 0 & 0 \\
-17.91 & 17.91 & 0 & 57.94 & 0 & 0 \\
0 & 0 & 0 & 0 & 57.94 & -17.91 \\
0 & 0 & 0 & 0 & -17.91 & 39.88
\end{bmatrix}
\]  \hspace{1cm} (A.1)

\[
e = \begin{bmatrix}
0.171 & -0.171 & 0 & -0.0406 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.0406 & -0.171 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]  \hspace{1cm} (A.2)
APPENDIX A. QUARTZ PROPERTIES AND TRANSFORMATIONS

\[ \varepsilon^S = \begin{bmatrix} 3.921 & 0 & 0 \\ 0 & 3.921 & 0 \\ 0 & 0 & 4.103 \end{bmatrix} \]  \hspace{1cm} (A.3)

The \( c_{12}^E \) entry above has been modified slightly to comply with the symmetry condition \( c_{12}^E = c_{11}^E - 2c_{66}^E \) [222]. The density of quartz is commonly given as \( \rho = 2649 \text{kg/m}^2 \).

Although the linear material constants have been extensively studied, there is a lack of published data on the higher-order parameters. Modelling approaches such as that used in Section 4.5.3 require higher-order terms to simulate the effects of biases, but complete data sets are rare. The third-order elastic stiffnesses for quartz were first measured in 1966 [225] and this set remains the standard; subsequent measurement sets have been conflicting and ‘true’ material values are difficult to determine [226]. The \( c_{ijklmn} \) values used in this project were taken from [225], but are not shown for brevity. Details of the symmetry conditions and thermodynamic basis for these constants may be found in [221] and [227].

Although temperature effects are not included in this project (see Section 4.5.1), the temperature derivatives of the material constants may be significant in some applications. Most material constants are measured at room temperature (c. 25°C), but their values can vary considerably with temperature. In common with their nominal values, derivatives of the linear constants demonstrate some variation between studies [228], especially for higher-order derivatives: a comparison of some results is given in [222]. It is noted in [15] that no temperature derivatives of \( c_{ijklmn} \) have been published, and thus experimental methods are still required to characterise the temperature behaviour of biased SAW devices. This represents a restriction on the biased SAW velocity procedure outlined in Section 4.5.3 for although the modelling framework can simulate higher-order temperature behaviour, no derivative sets exist to utilise this. The measurement of higher-order parameters is an active research topic [186], however, and such temperature derivatives may be available in the future.
A.3 Transformation of crystal values

As was discussed in Chapters 2 and 3, the SAW propagation direction has a major impact on device performance, determining $v$ and $K^2$ among other important parameters. The velocity calculation procedure outlined in Section 2.3.3 requires that the stiffness, piezoelectric and dielectric tensors be rotated to the desired propagation direction. SAW substrates come in a variety of cuts (orientations relative to their parent crystal’s axes), and thus a three-dimensional rotation of the tensors is generally required.

Figure A.3 shows the Cartesian quartz symmetry axes $XYZ$ and a particular wafer orientation known as the ST cut $[108]$: some advantages of this orientation are given in Section 3.3.2. This is known as a rotated Y-cut as the surface normal of the wafer is at $42.75^\circ$ to the crystal’s Y axis $[42]$. An Euler angle transformation is used to rotate the original crystal axes to the new wafer orientation through a defined sequence of rotations $[229]$. The initial $XYZ$ axes are rotated by angle $\phi$ about the $Z$ axis to form $X'Y'Z'$; $\phi = 0$ for the ST cut, and thus is not shown in Figure A.3. The $X'Y'Z'$ axes are then rotated by angle $\theta$ about the $X'$ axis to form $X''Y''Z''$. A rotation of this system by angle $\psi$ about the $Z''$ axis forms the final $x_1x_2x_3$ orientation. In this work, the first two rotations are used to set the cut orientation, while the last rotation is used to investigate propagation directions on that cut (e.g., in Figure 2.6). Following the convention in $[34]$, SAW propagation occurs in the $x_1$ direction, while $x_2$ defines the surface normal. The direction cosine matrix of the complete transformation is given by:

$$A = \begin{bmatrix}
\cos \psi \cos \phi - \sin \theta \sin \phi \sin \psi & \cos \psi \sin \phi + \sin \theta \cos \phi \sin \psi & -\sin \psi \cos \theta \\
-\cos \theta \sin \phi & \cos \theta \cos \phi & \sin \theta \\
\sin \psi \cos \phi + \cos \psi \sin \theta \sin \phi & \sin \psi \sin \phi - \cos \psi \sin \theta \cos \phi & \cos \psi \cos \theta
\end{bmatrix}
$$

(A.4)

The relationship between the transformed and original tensor components is thus given by $[45], [221]$:

$$c_{\alpha\beta\gamma\delta\varepsilon\zeta} = A_{i\alpha}A_{j\beta}A_{k\gamma}A_{l\delta}A_{m\varepsilon}A_{n\zeta}c_{ijklmn}
$$

(A.5)
Figure A.3: Sketch of ST-cut quartz wafer orientation (not to scale)
A.3. TRANSFORMATION OF CRYSTAL VALUES

\[ c_{\alpha\beta\gamma\delta} = A_{i\alpha} A_{j\beta} A_{k\gamma} A_{l\delta} c_{ijkl} \]  \hspace{1cm} (A.6)

\[ d_{\alpha\beta\gamma} = A_{i\alpha} A_{j\beta} A_{k\gamma} d_{ijk} \]  \hspace{1cm} (A.7)

\[ \varepsilon_{\alpha\beta} = A_{i\alpha} A_{j\beta} \varepsilon_{ij} \]  \hspace{1cm} (A.8)

where the Greek indices denote the transformed components. \( e_{\alpha\beta\gamma} \) is calculated by first computing \( d_{\alpha\beta\gamma} \) as above and then multiplying by the reduced stiffness matrix (see [221] and the discussion in [24]). It should be noted that tensor summation is still used here (see the Nomenclature), leading to a large number of computations for higher-order tensors. As an example, rotating the quartz tensors to the ST-X orientation (\( \phi = 0, \theta = 42.75^\circ, \psi = 0 \)) produces:

\[ c_E = \begin{bmatrix}
86.74 & -8.60 & 27.49 & 1.05 & 0 & 0 \\
-8.60 & 130.74 & -4.81 & -1.84 & 0 & 0 \\
27.49 & -4.81 & 96.63 & 13.44 & 0 & 0 \\
1.05 & -1.84 & 13.44 & 41.22 & 0 & 0 \\
0 & 0 & 0 & 0 & 67.47 & -7.60 \\
0 & 0 & 0 & 0 & -7.60 & 30.35
\end{bmatrix} \]  \hspace{1cm} (A.9)

\[ e = \begin{bmatrix}
0.171 & -0.133 & -0.038 & -0.082 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.107 & -0.072 \\
0 & 0 & 0 & 0 & -0.099 & 0.067
\end{bmatrix} \]  \hspace{1cm} (A.10)

\[ \varepsilon^S = \begin{bmatrix}
3.921 & 0 & 0 \\
0 & 4.005 & \approx 0 \\
0 & \approx 0 & 4.019
\end{bmatrix} \]  \hspace{1cm} (A.11)

\(^1\)The IEEE Standard on Piezoelectricity [33], while an excellent general reference, contains some serious misprints in its tensor transformation example: mistakes were acknowledged in [230]. The procedure shown here was verified using the example tensors and results given in [231]; additional examples may be found in [184].
# Appendix B

## Sensor configurations

### B.1 Standard die

The following table shows the parameters of each standard die as described in Section 3.3.5. The 0° and 35° columns show the nominal resonant frequency of each device, while the number of IDT finger pairs, reflectors per grating and type of resonator are also tabulated. Figure 3.12 shows the location of each die.

<table>
<thead>
<tr>
<th>Die</th>
<th>Linewidth ($\mu$m)</th>
<th>$0^\circ f_{res}$ (MHz)</th>
<th>$35^\circ f_{res}$ (MHz)</th>
<th>FP</th>
<th>Reflect.</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.82427</td>
<td>432.78</td>
<td>448.81</td>
<td>40</td>
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### APPENDIX B. SENSOR CONFIGURATIONS

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B.2 LARGE DIE

Large Die 1-10 are formed by connecting two of the standard die in series (see Section 3.3.5). Die 11-16 use extreme finger pair, reflector and aperture values: the larger number in each row represents the upper SAWR on the die. Die 17 and 18 are similar to the standard die but have different propagation angles. Die 11-18 all use optimal designs.

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B.2 Large die

Large Die 1-10 are formed by connecting two of the standard die in series (see Section 3.3.5). Die 11-16 use extreme finger pair, reflector and aperture values: the larger number in each row represents the upper SAWR on the die. Die 17 and 18 are similar to the standard die but have different propagation angles. Die 11-18 all use optimal designs.
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element analysis of acceleration-induced frequency change in SAW resonators,” in 

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