Solid State MEMS Resonators in Silicon
by
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Abstract

Two of the greatest challenges in MEMS are those of packaging and integration with CMOS technology. Development of solid state RF MEMS resonators in silicon, resonators that do not require any release etch step, eliminates the necessity for complex encapsulation methods and costly packaging. Such solid state solution could also enable direct integration into front-end-of-line (FEOL) processing in CMOS, making these devices an attractive choice for on-chip signal generation and signal processing.

This thesis discusses the physics, design considerations, and process developments to build such solid state MEMS resonators in silicon, showing a series of incremental stages of the prototyping of such devices. The major challenge of building solid state MEMS resonators lies in maintaining comparable device performance relative to released ones, especially quality factor $Q$. Energy localization structures, such as acoustic Bragg reflectors (ABRs) are implemented for such solid state resonators to maintain high $Q$ and suppress spurious modes. Towards the goal of high aspect-ratio structures that have the capability of direct CMOS integration, deep trench (DT) capacitor based MEMS resonators are studied and demonstrated. This concept enables high $Q$, low loss multi-$GHz$ resonators in a simple, robust manufacturing process.

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Chapter 1

Introduction

Micro-Electro-Mechanical Systems, or MEMS, has become a rich field both in research and application over the past few decades. Since H.C. Nathanson invented the first MEMS device, the Resonant Gate Transistor [1] in 1965, the technology emerged and thrived, expanding across different fields, far beyond the initial terms as when the technology was first developed. The successful commercial products include inkjet head from Hewlett-Packard, pressure sensors from Nova Sensors, digital micro-mirror device (DMD) from Texas Instruments, accelerometers and gyroscopes from Analog Devices, and numerous many other sensors and actuators [2] [3]. In fact, the popular smart phones and health tracking devices nowadays are critically enabled by a series of such MEMS devices that are integrated into the entire system.

As the name indicates, MEMS is a “system” that achieves certain functionality, at the “micro” scale, that is typically seen combining the physics from both “electrical” and “mechanical” domains. Due to this nature of signal conversion between different physical domains, they are typically used as transducers. This includes sensors that convert other signals such as force, deformation, velocity, heat, magnetic filed etc. into electrical signals, and actuators that convert electrical control signals into motions. And in general terms, the transducer application of MEMS extends far beyond just mechanical domains and electrical domains. Applications also include bio-chips, chemical sensors, micro-fluidics devices, optical and IR devices etc.

The methods to build such mechanical functional devices at the micro level are
inherited and expanded from the fabrication processes of microelectronic devices, enriched with bulk micro-machining methods including wafer bonding, KOH etch, DRIE etch, release etch etc. that are unique to MEMS alone [4]. The reason to have these extra processing techniques is that MEMS devices typically have suspended mechanical components, such as bars, beams, cantilevers, membranes etc. This is what distinguishes MEMS devices from standard micro electronic devices, and what makes it complicated to design, fabricate, and industrialize.

A successful MEMS product often faces a few challenges:

- Stiction of suspended structures. This is caused by the surface traction force generated from liquid during the drying process at release step.

- Particle failures. The suspended structures are also susceptible to particles. Trapped particles in MEMS devices can result in short circuit, block of motion, change of mechanical mass etc.

- Packaging challenge. A large portion of cost for MEMS products is from the packaging process. Due to its nature of multi-physics interaction, the transducer surface should be exposed. This makes it challenging to package everything while leaving the interfacing surface intact. A typical packaging process would affect the mechanical behavior of the device itself, such as generating extra initial stress. Careful designs need to be implement to get around such interactions. Moreover, these packaging processes cannot be easily standardized since MEMS devices are rich with varieties and physical domains.

- Integration with circuits. The circuit fabrication process has been standardized, for example, using the CMOS process. Due to its variety nature, the MEMS fabrication processes are significantly different from circuit processes, and therefore, the two cannot be easily integrated. MEMS and circuit are typically fabricated on separate chips and wire bonded afterwards. This compromises on size, weight and power (SWaP) of the system, and reduces the device performances.

From the perspective of one category of MEMS devices, the RF MEMS resonators,
this thesis presents efforts to build MEMS devices and methodologies that are at an attempt to overcome such challenges, looking into a complete solid state solution where the MEMS motional components are fully embedded in the solid medium, and therefore requiring no complex release etch steps, post-processing or special packaging, and such devices can be easily integrated with circuit processes.

1.1 Background and Application of RF MEMS Resonators

1.1.1 Applications

Radio frequency (RF) communications have been a primary technology driver since the invention of AM radio at the beginning of the 20th century. The desire of mobility and miniaturization calls for reduce size, weight and power (SWaP) of the RF electronics. Nowadays, integration has reached a point where RF chips built with pure electrical components can support the most required functionality. The limiting factor for further integration, however, lies in the bulky expensive off-chip passive RF components, such as inductors, capacitors, varactor diodes and ceramic filters [5].

The RF MEMS devices are developed to find a solution to such bottlenecks of traditional RF circuits. Examples of RF MEMS components include switches, high-

\[ Q \]

inductors, variable capacitors, and MEMS resonators and filters. The mechanical traits have enabled such MEMS components to achieve the RF functionality with much smaller size, and functioning on chip, making RF MEMS a critical technology of interest to the wireless design community.

As one branch of the RF MEMS family, RF MEMS resonators offer an attractive alternative to more traditional LC tanks and off-chip Quartz crystals due to their high

\[ Q \]

, small footprint, and capacity for intimate integration with CMOS [5]. This leads to reduced parasitics from on-chip and off-chip routing for high frequency operation, smaller size and weight, and decreased power consumption by alleviating constraints for impedance matching networks. The reason for such benefits is because RF MEMS
resonator is able to harness mechanical resonance, which leads to 4 to 5 orders of reduction in footprint relative to LC tanks.

Most common applications of RF MEMS resonators are to build high Q filters and oscillators, which can be subsequently used in wireless communications and microprocessing.

For wireless communication applications, the crowded spectrum at radio front end requires extreme frequency selectivity. The MEMS resonators can be used as high Q filters, providing channel-select transceivers for sensor networks, or for ad-hoc configurable radios.

Si MEMS resonators also have promising applications in micro-processing. Oscillators built with RF MEMS resonators consume much smaller power, cost less, so it can be used for on-chip clocking. Additionally, it can be potentially used to build a distributed on-chip clocking network. In current processor technology, a lot of power is consumed distributing the clock signal from a low frequency external crystal over the entire processor. Instead, a distributed clock network is called for that provides local clocking throughout the processor through an array of synchronized oscillators. This can be achieved with silicon-based low-power RF MEMS based oscillators, synchronized through mechanical interactions for low skew, low jitter clocking.

1.1.2 Figures of Merit of RF MEMS Resonators

There are several figures of merit that are commonly benchmarked for MEMS resonators. These figures of merit include resonant frequency $f$, quality factor $Q$, $f \cdot Q$ product, electromechanical coupling coefficient $k_{eff}^2$, motional impedance $R_X$, spurious mode suppression, temperature coefficient of frequency (TCF), etc. Their definitions are explained as the following:

- Resonant frequency $f$. The resonant frequency corresponds to one of the eigen-mode frequencies of the mechanical resonant cavity. It is typically the peak frequency. The resonant frequencies can be acquired from solving the mode-shapes, or using finite element eigenfrequency solvers.
The quality factor $Q$. It is a dimensionless parameter that characterizes a resonator's bandwidth relative to its center frequency, defined as

$$Q \triangleq \frac{\omega_0}{\Delta \omega}$$  \hspace{1cm} (1.1)

Additionally, it can also be equivalently defined from the energy perspective. Higher $Q$ indicates a lower rate of energy loss relative to the stored energy inside the resonator. To put into equations

$$Q \triangleq 2\pi \frac{E_{\text{stored}}}{E_{\text{loss per cycle}}} = 2\pi f_0 \frac{E_{\text{stored}}}{P_{\text{loss}}}$$  \hspace{1cm} (1.2)

If represented as a time signal, a resonator with higher $Q$ would die out slower. The envelope of oscillation decays proportional to $e^{-\alpha t}$, in which $\alpha$ is the attenuation rate. In this case, the $Q$ can also be equivalently defined as

$$Q \triangleq \frac{\omega_0}{2\alpha} = \frac{\pi f_0}{\alpha}$$  \hspace{1cm} (1.3)

Typically, the MEMS resonator design would target higher $Q$, meaning an electro-mechanical mode that stores more energy, and suffers lower loss.

Common loss mechanisms for resonator design include squeeze film damping [6], anchor loss [7], thermal elastic damping (TED) [8], phonon-phonon scattering [9] etc.

- $f \cdot Q$ product. It is listed alone because it characterizes how close the resonator is performing to the theoretical limit of $Q$ at different frequencies. Typically the loss factor is larger at higher frequency, resulting in lower $Q$. However, the theoretical limit of $f \cdot Q$ is typically kept at constant. This theoretical limit is only constant at relatively low frequency ranges ($< 1GHz$) in the Akheiser regime [9] where the $f \cdot Q$ product is limited by phonon-phonon scattering instead of anchor loss.

- Electromechanical coupling coefficient $k_i^2$. To characterize the coupling effi-
ciency between mechanical domain and electrical domain, electromechanical coupling coefficient \( k_t^2 \) is commonly used. It is defined as the converted mechanical energy divided over the total input energy.

\[
k_t^2 = \frac{\text{Output Mechanical Energy}}{\text{Input Electrical Energy}} \quad (1.4)
\]

There are also other equivalent definitions for this coefficient [10].

- The motional impedance \( R_X \). It is defined as the input voltage divided by the output current at resonance.

\[
R_X \triangleq \frac{v_{in}}{i_{out}} \quad (1.5)
\]

Typical resonator design would target lower \( R_X \), meaning stronger signal at resonance. If the MEMS resonator is represented as an equivalent circuit, such as a series RLC resonator, the motional impedance would equal the equivalent resistance.

- Spurious modes. The spurious modes refer to the undesired modes around the targeted resonance frequency. For filter and oscillator applications of RF MEMS resonators, it is desirable to have no spurious modes close to the targeted peak. Spurious modes can be very common for a mechanical resonator, because a mechanical cavity (such as a bar or plate) is typically rich with eigenmodes, even when the geometry has no distortions. Therefore, spurious modes suppression is an important task in MEMS resonator design. For MEMS resonators built on a suspended plate, this goal can be achieved by cleverly design the anchors [11].

- Temperature fluctuation affects material properties, including Young’s modulus, density etc., which consequently shifts the resonant frequency of the MEMS resonator. This effect is characterized by the temperature coefficient of frequency (TCF), which is defined as the following:

\[
TCF = \frac{1}{f} \frac{\partial f}{\partial T} \quad (1.6)
\]
The nature of mechanical vibration makes it possible for MEMS resonators to generate $Q$ that is several orders of magnitude larger than electrical LC resonators. Expressed in the terms of equivalent circuits, it is able to provide equivalent inductance and capacitance orders of magnitude larger than that from integrated circuits. And typically they consume footprint at only the scale of tens of microns. This is the fundamental reason why MEMS resonators can outperform their electrical counterparts.

The extra energy transduction between the electrical domain and mechanical domain, however, require high efficiency transduction mechanisms that can couple energy conversion between two domains. Capacitive (electrostatic) and piezoelectric mechanisms are the most extensively explored transduction mechanisms for MEMS resonators due to their benefits of easy fabrication and high performances. The capacitive transduction provides large quality factor and the best mode purity, while the piezoelectric transduction offers excellent coupling efficiency and low motional impedance [12].

At high frequency ranges, mechanisms with less parasitics, such as the Field Effect Transistor (FET) mechanism can be implemented for sensing instead of either capacitive or piezoelectric effects.

1.1.3 Examples of RF MEMS Resonators

Except classifying RF MEMS resonators into electrostatic and piezoelectric through transduction mechanisms, RF MEMS resonators can also be classified by its variety of structures. In this section, we discuss some examples of RF MEMS resonators that will be relevant to the resonators discussed in this thesis.

The Comb-Drive Resonator

The most classic and well-known electrostatic MEMS resonator would be the comb-drive resonator, invented by Bill Tang and Roger Howe in 1989 [13] (Figure 1-1). It relies on an array of lateral “comb shaped” capacitors to drive and sense mechanical
motion. The structure is suspended by long slender beams anchored to the substrate, and the suspended silicon bulk structure (H shape in the center) works as the lumped mass, together with all the damping mechanisms such as air-damping, this system behaves exactly like the classic mass-spring-damper (KMb system).

Depending on the required aspect-ratio, the structure can be fabricated either through bulk micro-machining or surface micro-machining. The first prototype is based on a polySi based surface micro-machining process.

On the driving side, the force is generated from the attraction force between two capacitor electrodes. This leads to the change of overlapping area of the capacitor, while the gap size is kept at constant. The AC voltage generates periodic capacitive force, which drives the structure into motion. If the frequency of such force matches the natural resonant frequency of the structure, it will be driven into resonance and outputs maximum vibration amplitude.

On the sensing side, the motion is sensed using the symmetric lateral capacitors as well. In this prototype, the motion is detected by applying a carrier frequency and observe through the spectrum analyzer. In matured comb-drive resonator technologies, such motion can be sensed on the symmetric combs through applying a DC bias voltage. This leads to an AC current generated from the change of capacitance.
resulting from the mechanical motion.

Surface Acoustic Wave (SAW) Resonators

Surface Acoustic Wave (SAW) is an acoustic wave travelling along the surface of a material. The energy only propagates along the surface, and it only has an evanescent tail into the depth direction that carries no energy propagation. This is an effect that was first explained by Lord Rayleigh in 1885 and named after him.

Since the energy is confined on the surface, if designed correctly, it can be used to build resonators [15]. Typically, it is built on top of a piezoelectric material, using an array of inter-digitated-transducer (IDT) metal electrodes to generate such surface travelling waves (Figure 1-2). The acoustic wave is generated through piezoelectric effect. On the sensing end, another array of IDT metal electrodes of the same pitch size is used to pick up the acoustic effect. The cavity length should match the SAW wavelength for maximum $Q$ of such resonator, and the SAW wavelength is twice the pitch size of the IDT.

One advantage of the SAW technology is its simplicity of processing—it only requires one photo-mask to fabricate. SAW devices can be used to build electronic circuits, such as filters, oscillators and transformers. SAW filters are used in mobile phones, providing significant advantage in performance, cost and size over older technologies such as quartz crystals and electrical LC filters.
Figure 1-3: Schematics of (a) the Film Bulk-Acoustic-Resonator (FBAR) and (b) the Solidly Mounted Resonators (SMR) [19].

**Bulk Acoustic Wave (BAW) Resonators**

In contrast to SAW resonators, Bulk Acoustic Wave (BAW) resonators are based on bulk longitudinal wave to form resonance. Classic examples of BAW resonators would be FBARs and SMRs (Figure 1-3) [16] [17] [18] [19]. The core of the resonator is a bulk of piezoelectric material that is sandwiched between two electrodes. It is driven into mechanical resonance by applying a voltage across the two electrodes. This piezoelectric material is created by deposition onto the substrate, and it is a thickness mode. To form boundaries for acoustic confinement, the bottom can either be etched open, or isolated with a series of thin films forming a Bragg reflector.

Compared with SAW devices, unit area of electrode of BAW resonators drives a smaller volume, so the transduction efficiency is larger. But the process is wave more complicated, which involves either a release etch step, or deposition of multiple layers of materials. And another disadvantage is that since the resonance frequency is defined by thickness, it cannot be controlled by photo-lithography, so there can only be one frequency option per batch of fabrication.

SAW devices are well suited up to around $1.5 \, GHz$, but above this frequency, FBARs and SMRs deliver compelling performance advantages. Since the resonance frequency is inversely proportional to resonator size, BAW resonators reduce in size with higher frequencies, making them ideal of multi-GHz applications. Additionally, compared with SAW devices, BAW resonators are far less sensitive to temperature
Figure 1-4: Examples of the contour mode resonator, (a) SiBAR resonator [21] and (b) AlN contour mode resonator [22]

variations, and delivers low loss and steep filter performance.

BAW resonator can also be designed to achieve lithographically defined frequency, and the transduction mechanism can be either piezoelectric or electrostatic. These BAW resonators in which the resonance mode is defined in the plane of photolithography are also named as contour-mode resonators. Examples of such resonators would include the disk resonator [20], the silicon bulk acoustic resonator (SiBAR) [21] (Figure 1-4a), the AlN contour-mode resonator [22] (Figure 1-4b), etc. Both the disk resonator and SiBAR are based on air-gap electrostatic transduction, in which the driving force is aligned with the resonating direction of the modeshape. The AlN contour-mode resonator, however, is based on the $d_{31}$ piezoelectric coefficient, and the direction of the modeshape is perpendicular to the direction of the driving force.

Since these devices are built with bulk longitudinal wave, instead of surface wave, or even flexural wave, the transduction efficiency is much higher, and it is less affected by the loss mechanisms such as thermal elastic damping (TED). Therefore, these resonators can achieve high $Q$ and they are lithographically defined so that multiple resonators targeting different frequencies can be fabricated from one batch of fabrication. This capability is significant when it involves integrating a resonator bank for filter applications on the same chip.

On the other hand, all of these devices are suspended structures, and require
a release step at the very end of the fabrication process, making the fabrication complicated and costly. And since it would require vacuum for high $Q$ operation for such resonators, the packaging process can be challenging and expensive as well.

**Air-Gap Transduction vs. Dielectric Transduction**

In the comb-drive resonator, the mechanical spring and mechanical mass are distinctively separated. This is not the case for most MEMS resonators. In fact, in all the BAW resonators discussed previously, there is no distinct boundary between mass and spring, and it is just a "modeshape" inside the resonant cavity, solved from the wave propagation PDE. All it requires to design a MEMS resonator is to find such bounded mechanical mode with high $Q$. And in the end, correct excitation at the natural frequency of such high $Q$ modeshape will lead to maximum amplitude of resonance. The frequency response is exactly the same as the 2nd order KMb system, therefore, it can be equivalently expressed as a KMb system. The equivalent mass $M_{eff}$ and equivalent spring constant $K_{eff}$ can be derived if necessary.

In the comb-drive example, the electrostatic force is generated by laterally changing the overlapping area of the capacitance, on the other hand, the electrostatic force can also be generated by changing the gap size, such as the SiBAR mentioned above [21]. In this second transduction method, the movement will be perpendicular to the capacitance surface. Since these structures are based on capacitors using air gap as the dielectric, this method is called air gap transduction.

To increase driving efficiency and reduce the motional impedance for air-gap resonators, direct methods would be to increase the driving area and reduce the gap. However, the gap cannot be too small due to limit of the aspect ratio of DRIE etching. To address this issue, it is necessary to introduce dielectrically filled resonators.

Dielectric capacitive transduction has several benefits over common air-gap transduction:

- In dielectric transduction, the capacitor gap is created by thin film deposition instead of etching. As a result, the gap can be much smaller, which increases driving efficiency.
Figure 1-5: (a) Schematic of dielectrically transduced free-free longitudinal bulk-mode resonator. The dielectric films are incorporated into the resonator, driving and sensing electrostatically. (b) Cross section of bar resonator. A bias voltage $V_{DC}$ is applied to the resonator. An ac voltage $v_{in}$ on one end drives the resonance, while an output current $i_{out}$ is measured at the other. The normalized amplitudes of the third and ninth longitudinal-mode harmonics are displayed. [23]

- The dielectrically filled gaps eliminate drawbacks of air-gaps such as stiction and electrical pull-in.

- The driving force is further enhanced due to the increase of dielectric constant.

An example of the dielectrically transduced resonator is the Internal Dielectrically Transduced resonator [23], as displayed in Figure 1-5. To optimize the performance of this type of resonator, direct analogy from air-gap resonators is incorrect. Instead of sensing at the point of maximum displacement, the internal dielectrically transduced resonator senses at the point of maximum strain. As shown in Figure 1-5b, the dielectrics are placed at the nodes of displacement modeshape, which are the places for maximum strain. In addition, for dielectrically transduced resonators, both capacitor plates are part of the resonant cavity. And this is exactly the reason why it is called the “internal” dielectric transduction.

The internally dielectrically transduced resonators have yielded the highest acoustic resonant frequencies (up to 4.5 GHz) and among the highest frequency-quality factor products (up to $5.1 \times 10^{13}$) published to date in silicon [24], [23]. In addition, these dielectrically transduced resonators demonstrate improved efficiency as frequency is scaled up, providing a means of scaling MEMS resonators to previ-
ously unattainable frequencies. However, as the frequency is further scaled up above 10 GHz frequency or even into the mm-wave frequency range (> 30 GHz), the parasitics through driving and sensing capacitors become inevitable. This imperfection motivates new sensing mechanisms.

The Resonant Body Transistor

FET sensing is by nature applicable for high frequency operation, due to its excellent isolation between input and output which results from the gate-oxide-channel structure. Furthermore, this sensing mechanism can take advantage of industrial transistor development, and therefore make use of high cut-off frequency and small scales of transistors for superior performance in MEMS resonators.

The application of FET sensing for MEMS resonators can be traced back to 1967, when Nathanson demonstrated the Resonant Gate Transistor (RGT) [1], driving resonance in a conductive cantilever with an air-gap capacitive electrode, and sensing by the resonance-modulated current in the FET channel.

In contrast, the Resonant Body Transistor (RBT) is a recently-demonstrated MEMS resonator that forms resonance inside the body of the transistor rather than the gate [25]. It inherits the geometry of the internal dielectrically filled resonator, with the addition of the FET channel inside the fin (Figure 1-6, grey region) for sensing instead of capacitor sensing. The RBT can also be seen as a sensing transistor directly integrated in the resonator body, and its geometry is very similar to that of an Independent-Gate FinFET [26]. The FinFET is a candidate for the next-generation transistor in CMOS. This similarity in geometry indicates the potential for RBT to be integrated in CMOS.

As a result of the benefits of FET sensing, the RBT can amplify the mechanical signal prior to any feed-through parasitics, pushing operating frequencies to previously inaccessible ranges in silicon, demonstrating the highest resonant frequency in silicon to date [27].

Figure 1-6 shows a top-view schematic of the RBT principle of operation. In the vertical dimension, it is the structure of an internal dielectrically filled resonator,
except that one of the capacitors (dielectric near $G_2$) is now not used to generate capacitive current, but acts as the gate to drive FET sensing in the channel $S - D$.

The region in light grey represents the undoped active area of the FET, while the blue region is highly doped. The active area near the drive electrode $G_1$ is biased into accumulation (red), so that a capacitive force acts across the thin dielectric film (yellow) driving longitudinal waves in the fin. A DC gate voltage is applied to $G_2$, generating an inversion channel (blue) which results in a DC drain current. At resonance, elastic waves modulate the drain current by the piezoresistive effect. The gain of the transistor reduces the output impedance of the device, providing high transduction efficiency at RF and mm-wave frequencies.

1.2 CMOS Integration of MEMS Resonators

1.2.1 The Challenge of CMOS-MEMS Integration

Two of the greatest challenges currently faced by MEMS are those of packaging and integration with CMOS technology. There are two main approaches to integrate MEMS with circuits: to include the electronics and MEMS functionalities on separate chips that are packaged together into a multichip system, or to monolithically integrate the
electronics and MEMS functionalities onto a single chip. The motivation for monolithic integration includes enhanced signal transduction, reduced footprint, improved immunity from parasitics and electromagnetic interference, robustness to harsh environments, and potentially lower cost compared to multichip systems. However, monolithic integration introduces challenges. Methods for MEMS-CMOS cofabrication have focused on modular MEMS-first [28] [29] or MEMS-last [30] processes in which the MEMS devices are created in one set of process steps and the electronics are created in a second set of process steps, or vice versa. However, these MEMS-first and MEMS-last processes require an increased number of masks, which decreases yield and increases cost due to added complexity. Moreover, the constraints on the process sequence, thermal budget, and materials require a compromise between the MEMS and electronic devices and lead to reduced performance [5] [31]. Non-modular MEMS-CMOS processing in which the MEMS and CMOS devices share process steps has also been demonstrated using the Back-End-of-Line (BEOL) CMOS stack. This approach reduces mask count but limits the MEMS materials to metals and dielectrics. This method also requires a post-processing release step to suspend the structure [32] [33].

The need for direct integration of MEMS devices with CMOS is critical for successful implementation of high frequency active MEMS resonators. Monolithic integration of these devices can provide basic RF and mm-wave building blocks with high quality factor ($Q$), small footprint, and low power for use in wireless communication, microprocessor clocking, navigation and sensing applications. Nevertheless, the majority of MEMS resonators require a release step to freely suspend the moving structures. The released structures necessitate complex encapsulation and packaging, restricting fabrication to MEMS-last or BEOL processing of large-scale devices.

To overcome these obstacles, it is worth investigating this novel type of RF MEMS resonator—the unreleased solid state MEMS resonator. The unreleased solid state resonator refer to micro-electromechanical resonators that are fabricated without any released step. They are solidly embedded between the substrate and the capping medium. The invention of such solid state resonators directly addresses the
issues of monolithic integration and packaging. By fabricating resonators side by side with transistors using exactly the same process, MEMS resonators can be directly integrated into the Front-End-of-Line (FEOL) CMOS processing. This provides RF and microwave CMOS circuit designers with on-chip MEMS building blocks with few if any additional mask steps, making these devices an attractive choice for low power clock generation and high-\(Q\) tank circuits (Figure 1-7).

Development of solid state resonators is not limited to application in CMOS processes, and can be implemented in applications where a minimal or no-packaging solution is needed.

1.2.2 Energy Confinement Methods

Solid state MEMS resonator provides numerous benefit at the system integration level, however, the major challenge of making such resonators is to maintain equal device level metrics compared with regular released ones. This is especially true for maintaining the quality factor \(Q\). With this solid design, there will be no gaps between the resonator and the surrounding. As a result, a straight-forward implementation by just “removing” the release step would not provide good performance, since the acoustic energy can leak through wave paths into the surrounding medium. The performance of an solid state resonator can therefore be degraded relative to
its released counterpart. Nevertheless, this energy loss into the surrounding medium can be mitigated, or even perfectly eliminated, by adding acoustic energy localization structures, achieving $Q$-enhancement for solid state resonators, and providing performances comparable to or even superior than the released ones.

The energy localization methods can be transferred and inspired from some methods used in designing released RF MEMS resonators, and nano-photonics research. For regular suspended resonators, two categories of structures have been proposed for the localization of acoustic vibrations in place of $\lambda/4$ suspension beams: the acoustic Bragg reflector (ABR) and the phononic crystal (PnC). Both of them can be analogously used in the context of solid state resonators.

**Acoustic Bragg Reflectors**

Similar structures named distributed Bragg reflectors have been used in optical devices [34]. Its acoustics analogue, the acoustic Bragg reflector (ABR), works in similar principles, for elastic waves. The ABR is composed of periodic layers of two materials of low and high acoustic impedance. This periodicity induces bandgaps for acoustic waves. At each layer interface of the ABR, a fraction of the acoustic wave energy is reflected. To form coherent superposition of these reflected waves, these layers can be optimized at odd multiples of one quarter wavelength, resulting in an overall reflectivity identical to that of free or rigid boundary conditions.

In 1965, W. E. Newell introduced the idea of applying ABRs to thickness mode piezoelectric resonators for wireless applications in high frequency integrated circuits [35]. This work was further developed in fully integrated surface micromachining technology for solidly mounted resonators (SMRs), as introduced in Section 1.1.3. These ABRs are composed of multiple depositions of alternating materials, resulting in isolation in one dimension at a single frequency per wafer. In-plane isolation can be achieved using lithographically defined ABRs, as demonstrated in a suspended plate [36]. This configuration enables resonators of multiple frequencies to be fabricated side by side on the same chip.
Phononic Crystals

An alternative to the ABR for acoustic energy localization is the phononic crystal (PnC), which is mostly lithographically defined. They have been recently explored by several groups for microscale applications, including acoustic mirrors for resonators in suspended plates [37], acoustic waveguides, and filters [38].

Like the ABR, the phononic crystal is also a periodic structure, with periodicity in 2D or even 3D. It is analogous to photonic crystals, or even to atoms in a crystal lattice. And similar to the ABR, this periodicity induces a bandgap that can reject waves over a range of frequencies.

Figure 1-8 shows the most commonly seen PnC resonator design. It is composed of a silicon plate etched with periodic holes through microprocessing. A wave is excited on the very left and transmitted and sensed to the very right. Resonance occurs inside the cavity defined by the absence of phononic crystal. This PnC resonator works exactly like a Fabry-Pérot interferometer in optics.

Typically, air holes are etched as scattering elements in a silicon slab (or slab made of another material) to form a PnC structure. There are also solid scattering approaches to fill these holes with materials with acoustic impedance that is distinct from that of the slab [38]. This type of solid scattering design can be borrowed for solid state resonator energy localization.
Both types of structures can be borrowed for the design of unreleased solid state MEMS resonators, however, the major difference lies in that the bottom and top of the solid state resonator will be wrapped around by solid materials, as shown in Figure 1-9. This brings significant change to mode design. With these adjacent solid materials, the modeshape extends beyond the resonator-ABR slab, so the design process should consider the entire structure, instead of just optimizing the design of the resonator cavity and the ABR. The methodology is very similar to what is used in photonic waveguides [39]. The details of such difference and design methodology will covered in the following chapters.

1.3 Previous Work

This section recapitulates the key results from the work of the master’s that are relevant to the work discussed here in this thesis. Previous work includes the demonstration of the first fully unreleased solid state MEMS resonators, and some key results from the COMSOL simulations of the solid state MEMS resonator enhanced with acoustic Bragg reflectors (ABRs). This experimental demonstration of solid state resonators gives $f \cdot Q$ products comparable to that of the released ones. And COMSOL simulations show that enhanced with ABRs, it is able to maintain high $Q$, and suppress spurious modes.
1.3.1 The First Solid State MEMS Resonator

To demonstrate the concept and feasibility of solid state resonators, the first fully unreleased solid state MEMS resonator without energy localization structures is demonstrated [40]. It is based on the platform of the Resonant Body Transistor (RBT) [25], fabricated with exactly the same steps except the end released etch.

As stated in Section 1.1.3, and shown in the schematic of Figure 1-10a, the RBT has the structure that is very similar to the independent-gate FinFET. The working mechanism for the RBT is discussed in Section 1.1.3. Such solid state RBT is bounded on all sides by a thick $SiO_2$ layer, including the bottom, where the buried oxide layer (BOX) is not etched away. An SEM of the solid state RBT (before metallization) is found in Figure 1-10b, showing the field oxide (FOX) layer on top of the device with silicided holes for electrical contact to the silicon device layer underneath. The inset of Figure 1-10b depicts the device with oxide cladding removed to show the underlying RBT.

These solid state RBTs were tested in a standard two-port configuration at room temperature in a vacuum probe station (Figure 1-11). Vacuum measurement was only necessary to prevent oxidation of the Ni metallization (metal conducting lines
Figure 1-11: Schematic of two-port measurement for frequency characterization of RBT. The drive and sense gates of the RBT are biased into accumulation and inversion, respectively. An AC excitation is superimposed on the drive gate, while the piezoresistive modulation of the drain current is detected at the output.

to the resonator), and does not affect device performance.

The measured frequency response of the solid state RBT is given in Figure 1-12. The DC bias of the inversion gate $V_{G2}$ was set at 3 $V$, 4 $V$, and 4.3 $V$ successively, with a DC accumulation gate voltage $V_{G1}$ of −1.12 $V$, drain voltage $V_D$ of 4.31 $V$, and an input RF power of −13 $dBm$. The device exhibits one peak at 39 $GHz$ and a spurious mode at 41 $GHz$. The $Q$ of 129 at 39 $GHz$ ($f \cdot Q$ product of $5 \times 10^{12}$) is $4 \times$ lower than that of its released counterpart [27].

The signal increases with sensing gate voltage. This effect strongly validates that the signal originates from mechanical resonance. With the increase of $V_{G2}$ from 3 $V$ to 4.3 $V$, the resonance frequency shifts by 0.1 $GHz$ and 0.2 $GHz$ for 39 $GHz$ and 41 $GHz$ peaks respectively. The observed frequency shift results from local resistive heating due to increased DC drain current at higher gate voltage, which alters the Young's modulus of silicon.

This result was the first time that these or any other resonators have been demonstrated in a fully-unreleased solid state. By removing the final release step, the fabrication process of the solid state RBT becomes exactly the same as that of the independent-gate FinFET. Accordingly, this solid state RBT demonstrates the feasi-
Figure 1-12: Measured frequency response of the solid state RBT after standard short-open de-embedding

bility of direct integration into FEOL CMOS processing, providing RF and microwave CMOS circuit designers with on-chip MEMS building blocks, making these devices an attractive choice for low power clock generation and high-\(Q\) tank circuits.

### 1.3.2 Acoustic Bragg Reflectors for \(Q\) Enhancement

**Design Principles**

The performance of the solid state resonator can be improved by adding energy localization structures. One method is adding the one-dimensional periodic structure like the ABR. Based on the commonly used SOI process for MEMS resonators, the schematic of one design of solid state resonators enhanced with ABR was shown in Figure 1-9b.

Here the solid state resonator is fully embedded in oxide, composed of the buried oxide (BOX) from the SOI wafer at the bottom and the field oxide (FOX) at the top. And the ABR is also composed solely of CMOS materials—\(Si\) and \(SiO_2\). In this configuration, the length of each of ABR layer, and the length of the resonant cavity are all lithographically defined. This one-mask design enables resonator banks of various frequencies on the same chip, providing multiple degrees of freedom in the
Figure 1-13: Frequency sweep in COMSOL for cross-section views of free bar (a), released resonator-ABR plate (b), solid state resonator-ABR structure embedded in oxide (c), and simple embedded resonator embedded in oxide (d). The curves plot average strain of the resonators against the excitation frequency, and the resonators used are of thickness-length ratio of 6.5 and ABR number of 7; the characteristic contour plots describe the $x$ component of the strain tensor at resonators of aspect ratio of 3.5 and ABR number of 3.

ABR design. These design aspects all align with the goal of solid state design for easy fabrication and packaging, and capability of direct FEOL CMOS integration.

The characteristics of these solid state structures are compared with freely suspended resonators, released resonators isolated with lithographically defined ABRs, and simply embedded resonators without any energy localization methods. The COMSOL simulation results of such comparison is in Figure 1-13.

In this comparison, the side view cross-section is used to construct the 2D solid mechanics simulation. The center rectangle represents the resonator body, which is designed for the 1st harmonic longitudinal vibration at 1 GHz. A pair of equal and
opposite line forces are applied on the left and right boundaries to drive the structure, and the integration of strain component $\varepsilon_{xx}$ over the entire resonant body is used as the signal output. The driving forces are scanned across frequency to get the frequency response of the structure. Free boundary conditions are used for released resonators, or just surfaces exposed to air/vacuum. And Perfectly Matched Layers (PMLs) are used for boundaries that allow wave to radiate without reflection, such as the boundaries that are enclosed by the bulk silicon substrate.

From the mode shapes and frequency responses from Figure 1-13, it can be seen that the released bar provides the sharpest peak, but it is also rich with spurious modes. These spurious modes are originated from the standing wave pattern from the second dimension. On the other extreme, the simply embedded resonator in oxide provides almost no peak at all, due to homogeneous energy dissipation into the surrounding medium. The resonator-ABR structure on a released plate exhibits fewer and weaker spurious modes, but also lower $Q$. Of all configurations, the solid state resonator-ABR structure provides the purest mode due to damping of undesired plate modes in the non-resonant direction. Moreover, the solid state resonator has higher thickness uniformity of the mode present in the resonator cavity, providing a larger effective area for sensing. On the other hand, this out-of-plane damping also contributes to a reduced $Q$ of the targeted mode. But this reduction in $Q$ can be mitigated by using higher aspect ratio, since $Q$, being defined as energy stored over energy lost, depends on the ratio of the bulk size storing energy at resonance to the area size exposed to radiation loss [41].

This is intuitive because the higher the aspect ratio, the larger the reflecting area and the less the leakage for acoustic energy. This also leads to the result that the 3rd harmonic has a better performance [41]. For higher harmonics, same thickness fits in more wavelengths, therefore the equivalent reflection area is even larger.

With these approaches, the solid state design is able to match the performance of released resonator-ABR structure with extra advantage in spurious mode suppression.
Figure 1-14: Acoustic bandgap comparison between phononic crystal and acoustic Bragg reflectors. The ABR provides a wider bandgap with no eigenmodes beyond the bandgap, and it requires a smaller footprint. The inset shows a 2 × 2 unit cell for the PnC used in this analysis. The contour plots show the topview of the transmission line structure, with amplitude of displacement decreasing with penetration depth.

**Acoustic Bragg Reflectors vs. Phononic Crystals**

As discussed in Section 1.2.2, ABR is a 1D special case of the phononic crystal (PnC). PnCs are widely studied and applied as a method to localize acoustic energy, including released resonators [37] [38]. When it comes to designs of solid state resonators, it is important to compare the performance of the two in the context of longitudinal mode resonators that are lithographically defined.

As one way to study the bandgap, a transmission line configuration is investigated in COMSOL 2D solid mechanics module (Figure 1-14), with the wave being launched on the very left by a pair of line forces, and sensed on the right by averaging the strain. It is a finite structure, so the shape of the curve would only reflect the position
and strength of bandgap, but not represent the bandgap itself, since the bandgap is defined for infinite periodicities. PMLs are used to create radiation boundaries that does not generate wave reflection. To created the equivalence of infinitely wide structure, periodic boundary conditions are added on top and bottom. This way it is translational symmetric in the $y$ direction, and the transmission property only depends on the cell structure in the $x$ direction. Based on the figure, the simulation results shows that the ABR has several advantages over the PnC:

- ABRs provide a much wider bandgap than that of PnCs for given impedance contrast of materials and for the same footprint.
- To achieve a near-perfect bandgap, it requires many fewer layers for the ABR compared to the PnC, requiring a smaller footprint.
- At frequencies beyond the bandgap, there exist spurious eigenmodes for the PnC, which result in undesired strong resonance. On the other hand, the ABR provides a perfect bandgap without introducing spurious modes.

To make the comparison more intuitive and straightforward, we can simulate the entire structure, sandwiching the resonator cavity by two reflector arrays on each side (Figure 1-15a). A pair of equal an opposite line forces are applied at the boundaries of the resonator, exciting longitudinal waves in the $x$ direction. PMLs are used at both ends of the entire structure to absorb waves that propagate into infinity. The intention of the simulation is to account for variation in the $x$ direction only, so periodic boundary conditions are applied in the $y$ direction. This can be approximated by very wide structures in real design. The simulations results show that for the same footprint and material set, the ABR offers clear benefits, with a $9 \times$ higher $Q$, $20 \times$ larger signal output, and suppression of spurious modes at both low and high frequency (Figure 1-15b).

These results can be intuitively understood from symmetry argument. To cause less spurious modes and better efficiency, the mode needs to be as uniform in the $y$ direction (non-resonant direction) as possible. This requires the reflector and resonant
Figure 1-15: Comparison of performance of solid state resonator embedded in PnC and ABR. The contour plot is a topview simulation result in COMSOL with periodic boundary condition added to top and bottom. A pair of equal and opposite forces is applied on both edges of the resonator.
cavity to have the same type of symmetry in the $y$ direction. The shape of the resonator is predefined, which has translational symmetry of arbitrary step size. The ABR structure maintains exactly the same type of symmetry, but the PnC only has translational symmetry of the multiples of the cell size. This discrepancy between the PnC and resonant cavity itself causes extra reflections at the matching boundary, generating spurious modes, reducing the effectiveness of reflection. As a result, in the case of this longitudinal 1D mode, the ABR would perform better than PnCs. However, it is worth noting that if the resonator targets some complicated plate modes that do not have translational symmetry of arbitrary step size in the $y$ direction, the PnC may turn out to work better after design optimization. In the end, the key of the design is to match the symmetry of the reflector to the symmetry of the mode shape.

And note that even in the released case when targeting the 1D longitudinal contour mode, people commonly use PnC like structure instead of the ABR. This is because it is impossible to use ABR since everything is on a suspended plate, etching ABR would break the geometry into separate parts, whereas etching holes to define PnC is possible. This makes it another unique feature for unreleased solid state resonators—everything is solidly filled so even the non-realistic ABR structure in the case of released can be fabricated conveniently.

1.4 Thesis Outline

In previous works, the first solid state MEMS resonator is demonstrated without any energy confinement methods. It exhibits two resonances at 39 $GHz$ and 41 $GHz$, with quality factor ($Q$) of 129 at 39 $GHz$ is $4\times$ lower than that of its released counterpart. It is a CMOS compatible technology that paves the way for Front-End-of-Line (FEOL) integration of MEMS resonators. To better confine acoustic energy, basic design rules for ABR used in solid state resonators are studied using COMSOL. Results show that from simply applying ABRs next to the resonant cavity, the solid state resonators are able to provide comparable $Q$ to released ones, when the structure is of high aspect
ratio. And in addition, the solid state resonator has great advantage in spurious mode suppression, since the ABR only acts as a reflector for the targeted mode. For a high-aspect ratio 1D cavity, using ABR is preferred compared with the PnC, since using ABR preserved the translational symmetry in the width direction. Simulations shows that using ABR for solid state resonator is able to provide $10\times$ in $Q$ under the same footprint.

In this thesis, the ultimate goal is to implement the concept of solid state MEMS resonators that require no post-processing and special hermetic packaging, with device performance such as quality factor $Q$, spurious mode selection that are comparable or even superior than the released ones. These will be contour mode resonators, so that the critical resonance dimensions are lithographically defined, enabling integration of a resonator bank on the same chip. And because they require no release etch step, and the materials are CMOS based, they would have the capability of direct Front-End-of-Line (FEOL) integration.

Towards this goal, this thesis covers the following topics:

- Chapter 2 discusses the modeling of electrostatically transduced resonators, comparing the performance of air-gap transduction and dielectric transduction, and shows the modeling and study of acoustic Bragg reflectors (ABR).

- Chapter 3 discusses the first CMOS-based solid state RBTs that are demonstrated in IBM’s 32SOI process with resonance frequencies above $11\ GHz$, $Q$'s of $24-30$, footprint of less than $5\ \mu m \times 3\ \mu m$ and TCF of less than $\pm 5\ ppm/K$. These are solid state MEMS resonators that are implemented with ABRs to confine acoustic energy. They are fabricated at the transistor level of the CMOS stack and are realized without the need for any post-processing or packaging.

- To further improve $Q$, Chapter 4 demonstrates the prototype of the deep trench (DT) based solid state MEMS resonator, functioning at $3.3\ GHz$ with a $Q$ of $2057$ and $R_x$ of $1.2\ k\Omega$. DTs were implemented both as electrostatic transducers and as ABRs to localize vibrations in the solid state resonator. Such $Si$-poly$Si$
combination creates a weak bandgap based reflector that can cause minimum scattering and form a high $Q$ design for solid state MEMS resonators.

- To further improve device performance, and deal with the issues associated with weak bandgap designs such as large footprint, design complexity, sensitivity to fabrication variations etc., Chapter 5 introduces the design of dual trench DT based solid state MEMS resonators. The unit cell of such structure is based on two trenches, using one trench for electrical transduction, and the other for bandgap modulation. In addition, such design provides robustness to periodic fabrication variations, and tunable bandgap that can be adjusted to a “moderately” weak bandgap size. This new type of structure also applies design principles such as array transduction, GRIN transition region to enhance the performance.
Chapter 2

Theory and Modeling

2.1 Mechanical Properties of MEMS Materials

The analysis and device modeling in this thesis are based on material properties provided in Table 2.1. These MEMS material properties are acquired from numbers from COMSOL material library and [42] [43].

Note that the $c$ matrix structure is discussed in Appendix A.2.3, and Young's modulus $E$ and Poisson's ratio $\nu$ are only applicable to isotropic materials. The $c$ matrix of $<110>$Si is derived from $<100>$Si using axis rotation relation provided in (A.32) and (A.33).

Table 2.1: Basic Mechanical Properties of MEMS Materials

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<th>$\nu$</th>
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<th>Symmetry</th>
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<th>( E ) (GPa)</th>
<th>( v )</th>
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0 & 0 & 0 & 0 & 101.6 & 0 \\
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\end{bmatrix}
\] |
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51.5 & 51.5 & 182.7 & 0 & 0 & 0 \\
0 & 0 & 0 & 65.6 & 0 & 0 \\
0 & 0 & 0 & 0 & 65.6 & 0 \\
0 & 0 & 0 & 0 & 0 & 65.6
\end{bmatrix}
\] |
| Al | Isotropic | 2700 | 70 | 0.35 | \[
\begin{bmatrix}
112.3 & 60.5 & 60.5 & 0 & 0 & 0 \\
60.5 & 112.3 & 60.5 & 0 & 0 & 0 \\
60.5 & 60.5 & 112.3 & 0 & 0 & 0 \\
0 & 0 & 0 & 25.9 & 0 & 0 \\
0 & 0 & 0 & 0 & 25.9 & 0 \\
0 & 0 & 0 & 0 & 0 & 25.9
\end{bmatrix}
\] |

2.2  Modeling of Electrostatically Transduced Resonators

Both RLC resonance from electrical circuits and KMb resonance from mechanical systems are 2\(^{nd}\) order systems, as a result, there is an equivalent representation between the two systems. Take the mechanical KMb system for example, if the input is the driving force \( F \), and the output is the vibration amplitude \( U \), the frequency
response is

\[ U(\omega) = \frac{U_{\text{static}}}{1 - \frac{\omega^2}{\omega_0^2} + i \frac{\omega}{Q \omega_0}} \]  \hspace{1cm} (2.1)

in which \( U_{\text{static}} \) is the amplitude under static force, \( Q \) is the resonance quality factor, and \( \omega_0 \) is the natural resonance frequency (pole) of this 2\(^{nd} \) order system. These terms are expressed as

\[
\begin{align*}
U_{\text{static}} &= \frac{F_{\text{static}}}{K} \\
\omega_0 &= \sqrt{K/M}
\end{align*}
\]

As discussed previously, most MEMS resonators are not isolated mass-spring-damper system. But such lumped parameters can be extracted as equivalent values from the modeshape, based on the fundamental physics. Therefore, an equivalent circuit can be drawn for the MEMS resonator.

This section discusses such methods, and the common models used to analyze electrostatically transduced MEMS resonators.

### 2.2.1 Air-Gap Resonator Modeling

To illustrate the general process, a simple example is used. As shown in Figure 2-1a, the resonator has a longitudinal modeshape, with the driving electrode on the left, and the sensing electrode on the right. The amplitude of such modeshape is mapped right under the geometry. Assuming we are only targeting odd number of harmonics (anti-symmetric), and the bar is suspended at the middle so the anchor does not affect such modeshapes. And note here the capacitive force is based on the change of gap size, not area. The transduction process can be derived as the following [44].

On the driving side, an AC voltage is applied on top of a DC bias voltage. This DC+AC driving mechanism enables the primary driving force to be at the same frequency as the AC voltage. Calculate the attraction force using the energy method:

\[ F = \frac{1}{2} (V_{DC} + v_{ac} e^{i\omega t})^2 \frac{\partial C}{\partial x} = V_{DC}^2 \frac{\epsilon_0 A_{cap}}{2g^2} + V_{DC}v_{ac} \frac{\epsilon_0 A_{cap}}{g^2} e^{i\omega t} + v_{ac}^2 \frac{\epsilon_0 A_{cap}}{2g^2} e^{i2\omega t} \]  \hspace{1cm} (2.2)

in which \( V_{DC} \) and \( v_{ac} \) are the DC and AC bias voltages respectively, \( \epsilon_0 \) is the dielectric
Figure 2.1: (a) Schematic of an air-gap resonator. The signal is sensed at the point of max displacement on the edge, and one of the capacitor plates is not part of the resonant cavity. (b) Schematic of an internal dielectrically filled resonator [23]. The signal is sensed at the point of max strain, and the capacitors are part of the resonant cavity. Both of these device form longitudinal resonance, and the 3rd harmonic is exhibited for both devices for comparison. In both of these structures, the geometry is assumed to be very wide in the dimension that is perpendicular to the mode, so that the mode can be treated as 1D.

constant, $A_{cap}$ is the capacitor area, and $g$ is the gap size of the capacitor. In this formula, the 1st term is the static DC bias force, which does not contribute to resonance; the 3rd term is at double the frequency, and is small considering $v_{ac} << V_{DC}$; the 2nd term represents the driving force for resonance, and its frequency equals the frequency of the AC voltage. So the combined voltages generate a DC bias force, a first order force at the driving frequency, and a negligible second order force at double the frequency. Therefore, in first order, the driving force can be taken simply as

$$f_{ac} = V_{DC} v_{ac} \frac{\epsilon_0 A_{cap}}{g^2} e^{i \omega t}$$  \hspace{1cm} (2.3)

To express the excitation force in general terms, it can be written as a function of both space and time (driving only on the left)

$$\frac{\partial f_{ac}(x, t)}{\partial x} = -V_{DC} v_{ac} \frac{\epsilon_0 A_{cap}}{g^2} e^{i \omega t} \delta(x - L/2)$$  \hspace{1cm} (2.4)

Assuming the resonant cavity to be a one-dimensional bar of length $L$, at reso-
nance, the general modeshape can be analytically expressed as:

\[
u(x, t) = U_0 \sin\left(\frac{n\pi}{L} x\right)e^{i\omega_n t}\tag{2.5}\]

in which \(x\) is the coordinate with the origin being the center of the bar, \(n\) is an odd integer dictating the mode number, \(U_0\) is the amplitude, and \(\omega_n\) is the eigenfrequency of the modeshape. Note here \(U_0\) is unknown and is to be calculated based on the driving force. The modeshape is simply a 1D longitudinal standing wave inside the cavity. The expression of \(\omega_n\) is

\[
\omega_n = 2\pi f_n = \frac{n\pi}{L} \sqrt{\frac{c_{11}}{\rho}}\tag{2.6}
\]

In particular, the 1st eigenmode can be expressed as:

\[
u(x, t) = U_0 \sin\left(\frac{\pi}{L} x\right)e^{i\omega_1 t}\tag{2.7}\]

And its frequency is

\[
\omega_1 = 2\pi f_1 = \frac{\pi}{L} \sqrt{\frac{c_{11}}{\rho}}\tag{2.8}
\]

in which \(c_{11}\) is the elastic constant for longitudinal waves (details on such constants will be discussed in Appendix A), \(\rho\) is the density.

Under the excitation force expressed in (2.4), all the eigenmodes in (2.5) will be excited. And the amplitude \(U_0\) of each eigenmode can be derived using the beam equation, which is the 1D case for elastic wave with internal damping [45]. The beam equation is derived from Newton’s second law on an infinitesimal element.

\[
\rho \frac{\partial^2 u(x, t)}{\partial t^2} - \eta_{11} \frac{\partial^3 u(x, t)}{\partial t \partial x^2} - c_{11} \frac{\partial^2 u(x, t)}{\partial x^2} = \frac{\partial \sigma_0(x, t)}{\partial x}\tag{2.9}
\]

in which \(\eta_{11}\) is the damping factor for longitudinal wave (details in Appendix A), \(c_{11}\) is the elastic constant for longitudinal wave, \(\rho\) is material density, and \(\sigma_0(x, t) = f_{ac}/A_{cap}\) is the excitation force per area. Based on the general response of a 2nd order system
(2.1), the damping factor for the \( n \)th harmonic can be related to \( Q \) as

\[
Q = \frac{\sqrt{c_{11}}}{\eta_{11} k_n}
\]  

(2.10)

in which \( k_n = n\pi/L \) is the wave number for the \( n \)th harmonic.

By substituting (2.4) and (2.5) into (2.9), the mode amplitude \( U_0 \) of each harmonics can be extracted by decomposing the force delta function to get the corresponding Fourier component. The end result for \( U_0 \) for the \( n \)th harmonic is (using (2.10) to substitute \( \eta_{11} \) for \( Q \))

\[
U_0 = \frac{2\epsilon_0 Q L}{n^2 \pi^2 c_{11} g^2} V_{DC} v_{ac}
\]  

(2.11)

On the sensing side, this maximum displacement at resonance modeshape is detected as the change of capacitance. A DC voltage bias is applied, and an AC current will be detected resulting from the sinusoidal motion at the end of the bar.

\[
\frac{dQ}{dt} = V_{DC} \frac{dC}{dg} \frac{dg}{dt} = V_{DC} \frac{\epsilon_0 A_{cap}}{g^2} \omega_n U_0 e^{i\omega_n t}
\]

(2.12)

in which \( Q \) is the total charge, \( g \) is the gap size, \( \omega_n \) is the angular frequency for the \( n \)th harmonic, and \( U_0 \) is the resonance amplitude at resonance, derived in (2.11).

With the relations (2.6), (2.11) and (2.12), the motional impedance \( R_X \) of the resonator can be derived as

\[
R_X = \frac{v_{ac}}{i_{out}} = \frac{n \pi g^4 \sqrt{c_{11}}}{2 \epsilon_0^2 Q A_{cap} V_{DC}^2}
\]  

(2.13)

### 2.2.2 Dielectric Resonator Modeling

As a direct comparison, the structure of the dielectrically transduced resonator is shown in Figure 2-1b. As seen from the plot, when the airgap is replaced with dielectric, the modeshape extends to all the solid components and both electrodes become part of the resonator. To get maximum transduction efficiency, the dielectrics should be placed at points of maximum strain, as to be shown from the derivation.

Assuming the location of the dielectric is at distance \( d \) to the center, and the
equations for air-gap resonator only needs to be modified slightly. The modeshape (2.5) is still the same, except now $L$ is the entirely length including the dielectrics and the end gate materials. The driving force (2.4) should be modified as

$$\frac{\partial f_{ac}(x, t)}{\partial x} = V_{DC}v_{ac} \frac{\epsilon A_{cap}}{g^2} e^{j\omega t}[\delta(x - (d - g/2)) - \delta(x - (d + g/2))]$$  \hfill (2.14)

Note here the changes are with both the dielectric constant, and the locations of the forces. It is now a pair of forces instead of one single force. Substitute both the modeshape (2.5) and the force (2.14) into the beam equation (2.9), there is [23]

$$U_0 = \frac{2\epsilon Q}{n^2\pi^2 c_{11}} \frac{L}{g^2} [\sin(k_n(d - g/2)) - \sin(k_n(d + g/2))] V_{DC}v_{ac}$$  \hfill (2.15)

in which $k_n = n\pi/L$, with $n$ being an positive odd number.

And again using the same expression (2.12) for sensing, there is the $R_X$ expression as

$$R_X = \frac{v_{ac}}{i_{out}} = \frac{n\pi \sqrt{c_{11}\rho}}{2\epsilon^2 Q A_{cap} V_{DC}^2} \frac{g^4}{[\sin(k_n d - k_n g/2) - \sin(k_n d + k_n g/2)]^2}$$  \hfill (2.16)

Note that the expression is similar to air-gap transduction (2.13), except an extra term of sines and cosines. This expression can be further simplified as

$$R_X = \frac{v_{ac}}{i_{out}} = \frac{n\pi \sqrt{c_{11}\rho}}{8\epsilon^2 Q A_{cap} V_{DC}^2 \cos^2(k_n d) \sin^2(k_n g/2)}$$  \hfill (2.17)

From this expression, it can be concluded that the $R_X$ is minimized if $\cos(k_n d) = 1$, meaning the dielectrics are placed at the positions of zero displacement, i.e. max strain. And in addition, the $R_X$ is further reduced by the square of the dielectric constant of the filling material. Furthermore, since $\sin^2(k_n g/2) \simeq (k_n g/2)^2 \sim n^2 g^2$ when the dielectric is very thin, the $R_X$ scales as $1/n$, instead of $n$ for the case of air-gap resonators. As the result, the motional impedance would decay for higher harmonics. This is a unique trait for internal dielectric transduction, making the method applicable to higher harmonics and higher frequency ranges.
2.2.3 Equivalent Circuit Model for Electrostatic MEMS Resonator

The common circuit model for electrostatically transduced MEMS resonator is the Butterworth-van Dyke (BVD) model. It is shown in Figure 2-2. In this equivalent circuit, the mechanical resonance is represented as a series RLC branch, $C_0$ is the electrical capacitor for driving and sensing, and $C_{ft}$ is the feed-through capacitor between the input and output.

The $L_x$, $C_x$ and $R_x$ in the RLC branch are called motional inductance, motional capacitance and motional resistance respectively. For air-gap electrostatic resonators, since the excitation force is external, the structure can be clearly equivalently lumped as a KMb system, extracting effective mass $M_{eff}$ and effective spring constant $K_{eff}$ and damping constant $b$ based on resonance frequency and stored energy. Once such equivalent lumped KMb parameters are found, the equivalent circuit values can be simply listed based on the dual relation between KMb and RLC as the following [4]

\[
\begin{align*}
\eta &= V_{DC} \frac{\varepsilon_0 \varepsilon_{gap}}{g^2} \\
L_x &= \frac{M_{eff}}{\eta^2} \\
C_x &= \frac{\eta^2}{K_{eff}} \\
R_x &= \frac{1}{\eta^2} \frac{\sqrt{M_{eff} K_{eff}}}{Q\eta^2}
\end{align*}
\]
Similar approaches can be taken for the internal dielectric transduction [46].

The simpler way to get equivalent circuit parameters $R$, $L$, and $C$ is solving from these set of equations

\[
\begin{aligned}
R_X &= R \\
Q &= \frac{1}{\omega_0 RC} = \frac{\omega_0 L}{R} \\
\omega_0 &= \frac{1}{\sqrt{LC}}
\end{aligned}
\]  

(2.19)

in which $R_X$ is acquired from (2.17), $\omega_0$ is based on (2.6), and $Q$ is extracted from (2.10).

With these basic relations, the RF MEMS resonator can be conveniently modeled as a circuit, this is especially helpful for design and analysis when the next stage circuitry is built on top of such device.

### 2.3 1D Model for ABR-based Unreleased Resonators

Bragg reflectors have been used for optical fibers, with the device functioning as a Fabry-Pérot cavity [34]. There are also applications for MEMS resonators, such as underneath the FBAR [17]. In both applications, the wave is normal incidence on all the interfaces. This is also true for the application in this thesis where the unreleased resonant cavity is sandwiched by lithographically defined ABRs.

As discussed in Appendix A.5.1, at normal incidence of elastic waves, the incident P wave remains P wave throughout the process, and the analytical method is completely analogous to the optical electromagnetic wave case.

With this normal incidence and primarily 1D structure, a simple 1D model alone can capture a lot physics. This include resonant frequency, bandgap size, $Q$, energy distribution, mode shape etc. In the case of optical Fabry-Pérot resonator, the 1D model can be built using equivalent circuits, treating it like a transmission line [47]. While for acoustic Bragg reflectors, the author has used summation of the infinite series of reflective components in previous works, which is a recursion formula based method [48]. All these methods only give the baseline for numerical solutions, and cannot provide a full-form analytical end result.
Because the multi-reflective method involves a recursion process, which treats each layer individually at an equal level, it becomes hard to implement in programming once the ABR-based structure becomes over complicated. As a result, in this thesis, the author adopts the forward-backward wave analysis method. This method is easy to implement in programming, extendable to multi-layer, multi-cavity analysis, and can even be used to study geometry variations.

2.3.1 Wave Propagation across a Series of Layers

First of all, the method starts from the analysis of the case in which the wave propagates through a series of layers.

If we trace one wave component, as what the recursion method does, the wave quickly splits into too many components after it crosses a few layers, making the analysis cumbersome. However, all these components are at the same frequency, and the same wave number \( k \) if in the same layer. Consequently, in each single layer, irrespective of how many reflectance there is or where they come from, all the forward propagating components can be summed as one, written as \( A e^{-ikz} \), and all the backward propagating components can be summed as one, written as \( B e^{ikz} \) (Figure 2-3). Here \( A \) and \( B \) are amplitude phasors at the reference planes on the left most boundary of each layer, as marked with dashed line in Figure 2-3. In the incidence domain, however, the reference plane is on the right most boundary. Note here in all the discussions, the \( e^{i\omega t} \) terms are dropped since the frequency is always constant for a single mode.

Now at each boundary, the same boundary conditions as (A.70) can be used. And written in the wave components and going through similar derivations as Appendix A.5.1, there is

\[
\begin{align*}
A_i e^{-i\delta_i} + B_i e^{i\delta_i} &= A_{i+1} + B_{i+1} \\
Z_i (A_i e^{-i\delta_i} - B_i e^{i\delta_i}) &= Z_{i+1} (A_{i+1} - B_{i+1})
\end{align*}
\]

in which \( \delta_i = k_i L_i \), which is the phase shift from the reference plane to the boundary.
Define $r_i \triangleq Z_{i+1}/Z_i$, (2.3.1) can be written in matrix form as

$$
\begin{bmatrix}
A_i \\
B_i
\end{bmatrix} =
\begin{bmatrix}
\frac{1+r_i}{2} e^{i\delta_i} & \frac{1-r_i}{2} e^{i\delta_i} \\
\frac{1-r_i}{2} e^{-i\delta_i} & \frac{1+r_i}{2} e^{-i\delta_i}
\end{bmatrix}
\begin{bmatrix}
A_{i+1} \\
B_{i+1}
\end{bmatrix}
$$

(2.20)

With this ABCD matrix relation, the result can be chained over all the layers to relate the first $A_0, B_0$ with the last $A_{n+1}, B_{n+1}$.

Note that the first interface is a special case, because the reference plane is different. It can be separately written as

$$
\begin{cases}
A_0 + B_0 = A_1 + B_1 \\
Z_0(A_0 - B_0) = Z_1(A_1 - B_1)
\end{cases}
$$

(2.21)

which is simplified as

$$
\begin{bmatrix}
A_0 \\
B_0
\end{bmatrix} =
\begin{bmatrix}
\frac{1+r_0}{2} & \frac{1-r_0}{2} \\
\frac{1-r_0}{2} & \frac{1+r_0}{2}
\end{bmatrix}
\begin{bmatrix}
A_1 \\
B_1
\end{bmatrix}
$$

(2.22)

In the last section, there will be no backward propagating component since the wave incidents from the very left and transmits to the right, which gives $B_{n+1} = 0$. 

Figure 2-3: Schematics of the method of forward-backward wave analysis. In each layer that the wave propagates through, all the forward components are summed into one term, so are the backward components. The reference planes for the phases are marked as dashed lines. Except the semi-infinite section for wave incidence, all the layers use the left-most boundary for phase reference.
With these relations, the end result is

$$
\begin{bmatrix}
A_0 \\
B_0
\end{bmatrix} = \begin{bmatrix}
\frac{1+r_0}{2} & \frac{1-r_0}{2} \\
\frac{1-r_0}{2} & \frac{1+r_0}{2}
\end{bmatrix} \prod_{i=1}^{n} \begin{bmatrix}
\frac{1+r_i}{2} e^{i\delta_i} & \frac{1-r_i}{2} e^{i\delta_i} \\
\frac{1-r_i}{2} e^{-i\delta_i} & \frac{1+r_i}{2} e^{-i\delta_i}
\end{bmatrix} \begin{bmatrix}
A_{n+1} \\
0
\end{bmatrix}
$$

(2.23)

And from this, the total reflectivity can be extracted as $R_{\text{tot}} = B_0/A_0$ and the total transmittivity can be extracted as $T_{\text{tot}} = A_{n+1}/A_0$.

Over the course of such derivations, no particular assumptions are made about the properties of each layer, including material, length, etc. This means this method is not limited to analyzing properties of ABRs, but can be extended to any multi-layer structure, including the structure of solid state resonator being sandwiched by ABRs.

All the programming are implemented in MATLAB. To make the program concise and reusable, a material library is defined as an independent file, and loaded every time before running the main program. Each material is defined as a structure type, containing basic mechanical properties including density, Young’s modulus, Poisson’s ratio, and the stiffness matrix. Secondly, to make the program expandable to any types of periodic structures, it is based on a “Unit Cell” mechanism. The unit cell is defined as the minimum periodicity for a periodic structure. For example, for a typical $\lambda/4$ ABR structure, the unit cell is composed of two quarter-wavelength layers. A function file is dedicated for this unit cell to extract its reflectivity for any input of frequency, material set, and geometry set. Lastly, in the main program, these unit cells are chained into an array by calling the unit cell function recursively. This extracts the total reflectivity of the entire structure.

The program is expandable in that for a different periodic structure, the only adjustment to do is to write a new unit cell function, and call this new function in the main program. And if there is a cavity sandwiched in such periodic array, which is typically at a different length, the only adjustment required is to load different length parameter into the unit cell function when the chaining reaches this particular layer. And the hierarchical programming mechanism is enabled due to the structure of the reflectivity relation in (2.20), which is a chaining relation in itself.
2.3.2 Properties of Acoustic Bragg Reflectors

First of all we study the simplest structure—a periodic array of ABRs, with each unit cell composed of two material layers. Ideally if the array is of infinite length, there will be a range of frequencies that the wave is prohibited to pass through. This frequency band is called the bandgap. However, real structures would always have finite length, making the reflectivity smaller than 1.

In this analysis, we use the MATLAB program discussed in Section 2.3.1 that calls the unit cell $n$ times, with $n$ being the number of periodicities. When $n$ is small, the "bandgap" is degraded into just a high reflective region, but when $n$ is large enough, the reflectivity approaches 1. Figure 2-4 illustrates this behavior. And as a benchmark study, the material pair is $Si/SiO_2$, each at $\lambda/4$ with center frequency being 1 GHz.

Figure 2-4: Amplitude (top) and phase (bottom) of the reflectivity of ABR as a function of frequency. Different curves represent structures with different periodicity numbers $n$. Materials are $Si/SiO_2$, and the center frequency is at 1 GHz.
From this we can observe a few things: $n$ should be at an optimum value to balance reflectivity and footprint requirement; and the reflectivity is always the highest in the center of the bandgap. So to get higher reflectivity and therefore higher $Q$ for the resonator, it should operate as close to the bandgap center as possible. There are also cases where we may want to deliberately generate low reflectivity. The method is then to either use fewer cell number, or just operate close to the bandgap edge.

The bandgap size of the structure can be approximately extracted using a very large cell number $n$ (e.g. 100), and extracting the range where the reflectivity is larger than 0.99.

And note that although most of the ABR application seen in literature uses the $\lambda/4$ layers, it is not a compulsory rule. For two-layer ABR unit cell, the wavelength portion of the two layers always sums up to $\lambda/2$. Length assignment that deviates from $\lambda/4$ would generate smaller bandgap size. For example, Figure 2-5a extracts bandgaps for various length combinations that sum up to $\lambda/2$, using method mentioned above. The numbers in the legend are the lengths of the first layer, and the second layer is of the complementary length that adds up to $\lambda/2$.

From this figure, we can see that the bandgap size shrinks as the length combination deviates from the optimum $\lambda/4$ combination. This can be observed from another perspective by plotting the reflectivity as a function of number of cells $n$, as shown in Figure 2-5b. It can be seen from the figure that the larger the bandgap, the smaller number of layers it is required for the reflector, and therefore the smaller the footprint. Another feature of non-$\lambda/4$ reflector is that it generates a phase shift after reflection. Because the $\lambda/4$ reflector generates no phase shift at the center frequency (phase shift still exists for non-center frequencies), it can be conveniently treated as a free or rigid boundary condition when solving for resonator mode shapes at the center frequency. The non-$\lambda/4$ reflectors however, generate phase shift at center frequency. So there is no simplified treatment for mode analysis, and it has to be solved numerically.

Another aspect that affects the performance of the reflectivity of the ABR is the acoustic impedance ratio $r = Z_2/Z_1$. The larger this ratio, the bigger the bandgap and the smaller the footprint. It is very useful to make similar plots as that in
Figure 2-5: Study of the effect of length combinations in each ABR unit cell. (a) Bandgap plot for different length combinations. Colored parts are the frequencies where eigen modes can exist. (b) Reflectivity vs. cell number $n$, with the top being amplitude and the bottom being phase.
Figure 2-6: Study of the effect of acoustic impedance ratio in each ABR unit cell. (a) Bandgap plot for different material pairs. Colored parts are the frequencies where eigen modes can exist. (b) Reflectivity vs. cell number $n$, with the top being amplitude and the bottom being phase.
Figure 2-5a and 2-5b, on various material combinations that will be encountered in this thesis. Such results are shown in Figure 2-6. From this figure, we can see that certain material pairs, such as Si/SiO$_2$, have very large acoustic impedance contrast, and therefore provide very large bandgap and strong isolation, while others, such as Si/polySi, has very small bandgap and weak acoustic isolation.

2.3.3 Unreleased Resonator with ABR Isolation

As discussed in Section 2.3.1, when a resonator cavity is added between two ABR arrays, the program can be tweaked to get the frequency response of the entire structure. The result of such mode analysis is as if launching the wave outside the resonator, to let it work like a Fabry-Pérot cavity. The actual designed unreleased resonator would be different from this, and have the driving force right inside the cavity. Despite such difference, since here is the eigenmode analysis, which is unaffected by the driving force, the key features such as $Q$, frequency, and mode shape extracted from this method is accurate.

In this analysis, the transmitivity $T$ will be extracted. If the structure is just an ABR, a rejection band will appear where the bandgap should be. When there is a resonator cavity embedded between two ABR arrays, resonant peaks will appear inside such rejection band. Figure 2-7a shows such analysis for the Si/SiO$_2$ ABR analyzed in Section 2.3.2. The material of the resonant cavity is Si, of length $\lambda/2$—twice the length of the Si portion of the ABR length in the unit cell. Data fitting shows that with only 15 unit cells, the energy leak across the ABR becomes very small, and the $Q$ of the resonator converted from this energy loss alone can be as large as $7 \times 10^6$. The fitted curve is plotted in red in Figure 2-7a.

With all the reflectivity extracted from such method, the mode shape can be calculated numerically as well, by writing out the amplitude at each coordinate using the piecewise expression in Figure 2-3. The calculated mode shape of such structure is shown in the top part of Figure 2-7b. The red dots indicate the places where the Si/SiO$_2$ interfaces are, and the mode shape is normalized to its maximum. The mode decays exponentially into the ABR structure, which is essentially an evanescent tail.
(a) Frequency Sweep of the ABR Array with Cavity Embedded

(b) Mode Shape and Energy Distribution

Figure 2-7: (a) Frequency response of the unreleased resonator with ABRs. The top part is the total transmittivity amplitude, and the bottom is the total transmittivity phase. The blue is the calculated data, and the red is the fitting curve to extract $Q$. (b) (top) Mode shape plot at the peak frequency in part (a), red dots being interface locations, (bottom) energy distribution plot at the peak frequency in part (a).
that carries little energy. For this $\lambda/2$ cavity and $\lambda/4$ reflector layers, the reflector generates no phase shift and acts like a free boundary condition at mid-bandgap. Such result can be verified by observing the mode shape—it is exactly $\lambda/2$ inside the center resonant cavity, and it is maximum displacement on the edge of the cavity.

With the mode shape, the energy distribution can be extracted as well, using formulas from Section A.4. Such result is plotted in the bottom part of Figure 2-7b. This plot is normalized by its maximum as well. The total energy density is the largest inside the resonant cavity, and decays after each reflection. The strain energy and kinetic energy are the time averaged value, and they are complimentary of each other. Because it is a standing wave, the energy packets do not move in space.

This just gives one example of a typical unreleased resonator and ABR structure, and how this analytical method works. These results can be generalized to non $\lambda/4$- $\lambda/4$ ABRs, and ABR with an arbitrary unit cell structure. ABRs with more complex unit cells will be covered in later chapters.

### 2.3.4 Study of the effect of Process Variation

Previous discussions are based on bandgaps from perfect periodicity. In real cases, the periodicity can get disturbed by process variations. The geometry of the ABR and resonant cavity can get affected by process variations such as lithography, etching etc. The effect of such variations can be studied by tweaking the previously mentioned program using Monte-Carlo simulation. This is set up by making the targeted geometry a Gaussian random variable, and calculating the bandgap multiple times using the same method in Section 2.3.2.

Figure 2-8 gives one such example based on the same $Si/SiO_2$ ABR. Figure 2-8a is based on 5% variation of the etched size into $Si$ substrate (which is filled with $SiO_2$), and the pitch size is kept as a constant. Figure 2-8b is based on 5% variation of the pitch size, and the size of the $SiO_2$ layer is kept as a constant. The $x$ axis is the simulation iterations, which is chosen as 10 times in total. The $y$ axis is the frequencies of the bandgap edge, with the blue marking the maximum range, and red marking the minimum.
Figure 2-8: Study of the effect of process variation. (a) The pitch size of each ABR cell is kept at constant, while the thickness of the oxide layer is a Gaussian random variable with $\sigma = 5\% \mu$. (b) The thickness of the oxide layer is kept at constant, while the pitch size of each ABR cell is a Gaussian random variable with $\sigma = 5\% \mu$. 

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The results show that the bandgap is very robust to the variation of the etch process that defines the sizes of the $SiO_2$ layer thicknesses, but is can get affected much more by the pitch size. The pitch size variation is typically determined by the mask writing process, which is very accurate. As a result, the bandgap, and therefore the frequency of the resonator will be relatively robust against fabrication variations.
Chapter 3

Solid State RBT in IBM’s 32nm SOI CMOS Technology

As discussed in Section 1.3.1, the Resonant Body Transistor has been demonstrated in the solid state form for the first time and showed $Q$ of 129 at 39 GHz. This first solid state demonstration has driven the impetus to bring this design onto the broader platform—the CMOS technology. One tremendous benefit of solid state resonators is their potential to be directly integrated with standard CMOS process, providing on-chip MEMS building blocks for circuit designers, and numerous other benefits as mentioned in Section 1.2. The RBT has a few unique traits that make it an ideal candidate for direct CMOS integration.

First, the materials that build the RBT are completely CMOS materials, and the structure of it is very similar to an independent-gate FinFET, which is one version of CMOS transistor. This similarity clears the barriers for direct CMOS integration design. While for other MEMS resonators using non-CMOS materials such as piezoelectric materials, or using other mechanisms such as flexural modes, this idea of direct CMOS integration would be impossible right at the first step.

Second, the RBT is based on active sensing. Unlike other simpler method such as capacitive sensing, Field Effect Transistor (FET) sensing can effectively isolate the mechanical signal from electrical feed-throughs, giving it the capability of working at multi-GHz ranges.
Third, the key element that determines the RBT performance is the transistor embedded in it. This is exactly what the CMOS industry has been good at, and striving to improve node after node. Such integration would directly harness the benefit of CMOS scaling power, giving the MEMS resonator as great performance as the transistor that the CMOS technology node can provide.

To demonstrate the capability of CMOS integration for the solid state RBT, this idea is first tested in the IBM’s 32nm SOI technology, operating above $11 \text{ GHz}$ with $Q$’s of 24-30 and footprint of $5 \times 3 \mu m$. And to enhance $Q$ and reduce energy loss in such solid state design, ABRs are implemented in the Front-End of Line (FEOL) next to the resonant body.

### 3.1 Introduction

Compared with traditional LC tanks and off-chip Quartz crystals, RF MEMS resonators offer reduced size, weight and power (SWaP), high $Q$, reduced on-chip and off-chip parasitics, and most importantly, the capability of intimate CMOS integration.

Over the past decade, one criterion of interest for RF MEMS resonators is scaling to high frequencies, into the multi-GHz domain. This includes applications of personal navigation (94 GHz) and short distance local area networks (LAN) (60 GHz), imaging, and high-definition video links. A majority of MEMS resonators rely on passive transduction mechanisms such as capacitive and piezoelectric to sense the mechanical resonance signal. This would become more and more inapplicable at multi-GHz domain due to the increase of electric feed-through signal, overwhelming the mechanical peaks. To address these challenges, the RBT uses the method of FET-sensing, which effectively isolate the output from the input electrical feed-through, therefore amplifying the mechanical signal before the presence of electrical parasitics. With active sensing, RBTs have been shown to reach order of magnitude higher frequencies than possible with passive resonators [25], [27].

Another criterion of interest for RF MEMS resonators is CMOS integration. Ef-
forts directed toward monolithic CMOS integration have been motivated primarily by improved SWaP, reduced parasitics from off-chip connections, and relaxed constraints on impedance matching [31]. However, the majority of electromechanical devices require custom fabrication including a release step to freely suspend the moving structures. This requires costly complex encapsulation methods and restricts MEMS-CMOS integration to back end-of-line (BEOL) processing [32]. Methods for monolithic integration of MEMS and CMOS in the past have focused on MEMS-first or MEMS-last processes. However the increased mask count, complexity and constraints on the process sequence, thermal budget and materials in these processes result in compromised performance, higher cost and reduced yield. Such custom MEMS processes cannot keep up with rapidly changing CMOS technology. Development of solid state Si-based MEMS resonators in CMOS can overcome these obstacles, allowing for seamless integration into FEOL processing with no post-processing or special packaging.

Realization of the FET-sensed resonators in CMOS technology combines the benefits of a high efficiency sensing mechanism with high-performance transistors of CMOS technology, with major reduction in parasitic effects due to direct integration with surrounding circuitry.

3.2 Design and Simulations

3.2.1 Structure of the Devices

The solid state RBTs in CMOS demonstrated here consist of longitudinal-mode bars driven electrostatically and sensed using a FET incorporated into the resonant body, as shown in Figure 3-1a. The resonant body is created by modifying a standard FET, keeping the FET channel the same, while doubling the body width to make the other half a MOS capacitor. This capacitor side is used to drive resonance electrostatically (capacitive attraction force), and the FET side is used to sense the mechanical motion on the same Si island. This mechanism is exactly how RBT works, as discussed in
Figure 3-1: (a) Schematics of the CMOS Integrated Solid State RBT excluding ABRs. The resonator is driven capacitively on the left, and sensed as a piezoresistive modulation of the nFET drain current on the right. Details of FET layout and doping layers not shown. (b) SEM of CMOS stack cross section showing resonator body and adjacent ABRs obtained using focused ion beam (FIB). The device is formed in the SOI device layer, defined using Shallow Trench Isolation (STI), and in the polySi gate layer.
Section 1.1.3, except the geometry is very different. The major difference is that the
direction of driving here is perpendicular to the direction of the longitudinal mode,
instead of aligned with. In other words, driving force is applied on the top surface,
and it is coupled into the in-plane direction through the Poisson effect. This is not
as efficient as when the driving force is aligned with the resonance direction, but this
design choice is made out of the constraints from this particular CMOS technology.
The IBM 32nm SOI technology is not a FinFET technology, and there is no high
quality capacitors on the vertical sidewall.

The working principle can be detailed as the following:

On the drive side, elastic waves are launched in the Si bar by superimposing DC
and RF voltages \( V_A + v_{\text{in}} \) across the drive capacitor formed using the Si device layer,
gate oxide, and gate polySi layers of the CMOS process. On the sense side, the FET
is biased into saturation with DC gate and drain voltages, \( V_G \) and \( V_D \), respectively.
The body of the resonator is independently grounded from the source to minimize
electrical feed-through. In-plane longitudinal mechanical resonance is detected in the
Si bar through piezoresistive modulation of the drain current \( i_D = I_D + i_{\text{out}}e^{j\omega t} \). In
Si, this piezoresistive sensing provides \( >10\times \) boost in transduction efficiency relative
to electrostatic sensing. It also decouples the output signal from the input, reducing
the effects of feed-through parasitics which can dominate in the GHz regime.

### 3.2.2 Energy Confinement with Acoustic Bragg Reflectors

The resonant cavity is designed to be of length \( L \) and is formed by the gate stack
consisting of the Si device layer, gate dielectric and gate polySi. It is designed
at effective half acoustic wavelength \( (\lambda/2) \). This resonance energy is confined by
taking advantage of the acoustic impedance mismatch between Si and surrounding
materials to form the acoustic Bragg reflectors (ABRs) in the direction of longitudinal
resonance, right next to the resonator. Such ABRs are formed by alternating Si/SiO\(_2\)
regions at quarter-wavelength \( (\lambda/4) \) intervals for the desired frequency (Figure 3-2),
defined using the Shallow trench isolation (STI) in the FEOL in CMOS. They are
created from a series of “dummy transistors” right next to the RBT.
The relative acoustic impedance between the materials of the ABR is $Z_{rel} = Z_{Si}/Z_{SiO_2} \approx 1.65$ and the reflection coefficient given by $R = (Z_{rel} - 1)/(Z_{rel} + 1)$ asymptotically converges towards 1 with an increase in the number of ABRs. Considering the trade-off of total device footprint vs. acoustic reflectivity (and therefore quality factor), these solid state resonators are designed using 7 pairs of 1D ABRs which provide a reflectivity of 99.4% based on 1D analysis. At resonance, the eigenmode is comprised of a sinusoidal standing wave formed in the resonant cavity which decays exponentially in the ABR region.

3.2.3 Special Design Considerations in CMOS

In the course of design of these resonators, several structural aspects of the foundry-provided nFETs are modified. Standard FET doping layers which define the source/drain and body doping were changed to allow ABRs to be designed as close to the devices as possible. The shapes of the active device region of the SOI process and polySi gate regions were modified to create longitudinal bar like structures for definition of the resonant cavity. The number of metal contacts was reduced to reduce distortion...
of the resonant mode of vibrations.

In the aspect of the reflector design, design rule checking (DRC) restrictions of the CMOS process limited the spacing of the ABRs closest to the resonant cavity. To accommodate this rule, the first Bragg reflector is spaced $3\lambda/4$ away from the resonator, as evident in Figure 3-1b. This results in a reduced solid angle to the ABRs from the structure which reduces reflection and quality factor in the resonator.

Additionally, the metal stack on top of the resonant cavity as seen in Figure 3-1b has a strong impact on the eigenmodes of the resonator. The metal layers seen above the resonator were not designed for but were generated as part of the dummy CMP fill of the CMOS process. The high acoustic mismatch between the dielectric fill and low-level metals (e.g. $Z_{Cu}/Z_{SiO_2} = 2.45$) results in acoustic reflections in the thickness direction. This thickness coupling results in spurious modes near the targeted frequency. The CMP fill can be excluded from the process in localized areas, eliminating this effect in future designs. Alternatively, the metal layers above the resonant structure can be designed to provide 3D ABRs for improved quality factor and reduction of spurious modes.

### 3.2.4 Finite Element Analysis

If we use the simple 1D model developed in Section 2.3 to calculate $Q$, considering wave radiation loss across the ABR structure, it would lead to $Q$ around 7500 for 7 pairs of ABRs. This result is unrealistic given the aspect ratio this CMOS structure can provide.

The small aspect ratio of the STI structures, the tapered angle of the Si etch, and the reflections along the vertical direction, would all de-$Q$ the resonator additionally. In the end, it will not be a pure 1D mode, but a complicated 3D mode that is distorted by the structural details. The 1D model is only useful to provide a first order analysis to find out the resonance frequencies and ABR design parameters etc.

To find out the real resonance mode, and how it gets affected with the structural details in CMOS transistors such as salicide, stress liners, metal contacts etc., a 3D COMSOL simulation is required.
Figure 3-3: 3D Finite element analysis of the solid state RBT showing (a) Symmetric half-plane of the 3D geometry of resonant cavity and ABRs, including the full FEOL stack materials starting with the handle wafer up to the first metal layer. (b) stress plot along the resonance direction and (c) frequency response of simulated RBT derived from the integrated stress at the FET channel.
The 3D model is constructed by Bichoy Bahr [49]. It consists of the handle wafer, buried oxide layer (BOX), the resonant structure capped by the stress liner and the pre-metal dielectric (Figure 3-3a). The simulation shows the acoustic structure cut across the axis of symmetry, including the sensing FET with source/drain contacts, and the contacts to the resonator body and the driving capacitor.

The boundary condition at the top of the structure (above the FET and ABRs) was selected to be a free boundary condition. This is due to the fact that the subsequent layers are made of the low-κ dielectric (SiCOH) [50], which has very low acoustic impedance as compared to the materials in the acoustic cavity: Si ($Z_{Si}/Z_{SiCOH} \approx 10.5$) and SiO$_2$ ($Z_{SiO_2}/Z_{SiCOH} \approx 6$). The boundary condition terminating the handle wafer was selected to be a low reflection boundary condition, to account for the large thickness of the handle wafer. This low reflection boundary condition is similar in function to PMLs in 2D simulations.

A frequency sweep of the structure is carried out by applying a squeezing force on the dielectric between the capacitor plates. Figure 3-3b and Figure 3-3c show the resulting mode shape and stress plot in the longitudinal direction, respectively. The predicted resonance frequency is around 11.5 GHz for a longitudinal mode contained in the resonator and ABRs.

### 3.3 Experimental Results

#### 3.3.1 DC Characterization

For DC measurements, the FET was biased at a gate voltage $V_G = 0.4 \, V$ and a drain voltage $V_D = 0.6 \, V$ to verify that the modified FETs showed characteristic transistor behavior (Figure 3-4). Furthermore, the drive-capacitor voltage $V_A$ does not affect the transistor $I_D - V_D$ curves, verifying no DC feed-through.

Due to the modifications made to the overall FET geometry to create resonant devices, the output drain current was found to be approximately $2 \times$ lower at a given operating point as compared to a foundry-provided FET. The DC power consumed
Figure 3-4: DC response of a sample device showing transistor characteristics and no dependence of drain current $I_D$ on drive capacitor voltage $V_A$.

at the operating point is $35 \mu W$.

### 3.3.2 RF Measurement

To measure the RF response of the devices, standard SOLT calibration is used to de-embed the test setup up to the probe tips. This is followed by open and short structures defined in the CMOS die to de-embed the large probe pads and routing down to the lowest metal layer of each device. RF measurements are taken with $-21.9 \, dBm$ input power, no averaging, and a $30 \, Hz$ IF BW using an Agilent PNA-X N5245A. After de-embedding the probe-pads and routing, the electromechanical transconductance $g_o$ is extracted from the Y-parameters as $g_o = Y_{21} - Y_{12}$.

The frequency response of an $11.1 \, GHz$ resonator is shown in Figure 3-5. The amplitude of the resonance peak changes for different values of the DC drive voltage $V_A$, verifying the mechanical nature of the resonance. The response for the lower FET gate voltage $V_G$ of $0.3 \, V$ corresponds to a small FET amplification factor $g_o$ resulting in an indistinguishable resonance peak with respect to the feed-through. The device
Figure 3-5: Frequency response of an 11.1 GHz nFET-ncap resonator showing transconductance $g_m$ and phase under multiple biasing conditions of the drive voltage ($V_A$) and gate voltage ($V_G$).

exhibits a $Q$ of $\sim 30$ with a total footprint of $3 \, \mu m \times 5 \, \mu m$. The measurement closely matches the predicted resonance frequency from the 3D simulation of the designed structure in Figure 3-3.

3.3.3 Effect of Acoustic Bragg Reflectors

The effect of ABRs on device performance was characterized by comparing the effect of different ABR dimensions on the same cavity length. There are devices on which the ABRs targets 5% higher frequency (ABR 1.05), and 5% lower frequency (ABR 0.95) as compared to the resonance frequency. A comparison of the signals of these 3 types of devices is shown in Figure 3-6. The device with ABRs of correct dimensions shows optimized performance at resonance frequency in terms of suppression of spurious modes.
Figure 3-6: Comparison of three identical resonators with ABRs designed for the resonance frequency (ABR 1), 5% higher frequency (ABR 1.05) and 5% lower frequency (ABR 0.95). The resonator with ABRs designed at the resonance frequency shows best performance for $g_a$ and spurious mode suppression.

### 3.3.4 Fabrication Variations and Yield

The yield of FETs in the process was nearly 100%, which emphasizes the merits of CMOS integration to harness the high yield of standard CMOS for MEMS fabrication. The variation in the resonance frequency of the resonators, designed with identical resonance dimensions, is around 0.1-0.5%, and is attributed to lithographic process variations. On the electrical side, such variations are in the form of the variance in the driving MOS capacitor and FET which affects the drive and sense efficiency, the gain at resonance, and electrical contribution to the total $Q$. On the fabrication side, geometric or material variations from layer misalignments, sidewall slope and roughness, film thickness, stress liners, and variation in material acoustic properties affect the resonance frequency and $Q$.  

<table>
<thead>
<tr>
<th>ABR</th>
<th>$g_a$ (µS)</th>
<th>$\Delta g_{a1}$ (µS)</th>
<th>$\Delta g_{a2}$ (µS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>31.4</td>
<td>5.6</td>
<td>7.9</td>
</tr>
<tr>
<td>1.05</td>
<td>27.4</td>
<td>2.8</td>
<td>3.2</td>
</tr>
<tr>
<td>0.95</td>
<td>31.8</td>
<td>5.6</td>
<td>6.9</td>
</tr>
</tbody>
</table>
3.4 Discussion

The first CMOS-based solid state RBTs are demonstrated in IBM’s 32SOI process with resonance frequencies above 11 GHz, $Q$'s of 24 – 30, footprint of less than $5 \mu m \times 3 \mu m$ and TCF of less than $\pm 5 \text{ ppm}/K$. They are fabricated at the transistor level of the CMOS stack and are realized without the need for any post-processing or packaging. CMOS-integrated RBTs are the first step towards realizing on-chip acoustic frequency sources with reduced size, power consumption, and parasitics in wireless communication, navigation and sensing systems.

Seamless integration into a standard CMOS process obviates the need for complex and costly custom processes for MEMS fabrication. The demonstration of resonators fabricated side-by-side with CMOS circuitry greatly reduces parasitics of off-chip access, constraints of limited IO, and power consumption associated with impedance matching networks. Such benefits can provide increased system speed and dynamic range, particularly at RF and mm-wave frequencies of operation.

It is also notable that as a first generation of design, there are several aspect of the device that needs improvement. Firstly the CMP dummy fills above the device layer is unexpected during design, which reduces the performance instead of enhancing it. With correct design, making it into a phononic crystal structure targeting exactly the same frequency, the $Q$ can be greatly improved [51]. Secondly the STIs in the SOI device layer are of very small aspect ratio, which lead to many wave paths that are unconfined around the resonator and more energy loss. As discussed in Section 1.3.2, the $Q$ of such solid state configuration can be greatly improved by using higher aspect ratio—this leads to searches of high aspect ratio structures in CMOS for such integrated design. This idea will be discussed in more details over the following chapters.
Chapter 4

Deep Trench Capacitor Based Solid State MEMS Resonators

4.1 Introduction

With frequency-quality factor products \((f \cdot Q)\) often exceeding \(10^{13}\), RF MEMS resonators offer a high-\(Q\), small footprint alternative to conventional LC tanks and off-chip crystals for clocking and wireless communication. Over the past three decades, much progress has been made in improving key figures of merit of MEMS resonators including small footprint, high \(Q\), low motional impedance, efficient energy coupling \(k^2_{eff}\). In parallel, efforts have focused on system-level metrics including high yield, low cost, robustness, easy packaging and integration with circuits. The challenge lies in building high performance yet easily manufacturable devices—devices that meet both lines of requirements.

In this context, previous chapter introduces solid state resonator design that are directly embedded into the FEOL in CMOS. This deep integration improves the SWaP, reduces parasitics, harnesses the scaling power of CMOS technology and provides on-chip MEMS components, and most importantly, such direct CMOS integration leads to a MEMS process that requires no post processing and special packaging. Performance wise, these devices are able to work in multi-GHz range due to FET active sensing. Yet there are obvious room for improvements for such class of devices—the
Figure 4-1: Two examples of IBM CMOS processes that contain high aspect ratio structures: (a) The DRAM in IBM 45nm SOI process. The DRAM trench of aspect ratio \(-30\) in Si is filled with polySi (figure from [52]). (b) The Deep Trench Isolation process in IBM 8HP process. The trenches are used to isolate electrical signal between adjacent islands.

\(Q\) is too low for significant applications.

Section 1.3.2 discusses ways to improve the \(Q\) of solid state resonators, and if to stay in 1D reflector design, one way is simply increasing the aspect ratio of the entire structure. The Si device layer at FEOL in CMOS is limited in aspect ratio, as the thickness is typically not too much more larger than the FET channel length (e.g. Figure 3-1b). However, in some CMOS processes, there exist structures of very high aspect ratio.

The DRAM technology at IBM uses trench capacitor to store charges (Figure 4-1a) [53] [54]. Such “trench capacitors” are created by etching high aspect ratio trenches into the Si substrate, deposit dielectrics, and fill the trenches with polySi.
This specially developed process enables aspect ratio as large as 30, creating large capacitors that consume tiny footprint, which is an ideal property for memory cells. Apart from DRAM cells, there also exist other structures, such as the Deep Trench Isolation (DTI), used for cutting off the electrical paths between adjacent devices and reduce cross-talk (Figure 4-1b). Both of these processes are initially developed in CMOS for electrical purposes. However, these structures can be re-invented as mechanical components, forming an equivalent acoustic Bragg reflector (ABR) structure to confine acoustic energy.

As a proof of concept, such type of high aspect-ratio deep trench based devices are developed and demonstrated at the university clean room facility, i.e. Microsystems Technology Laboratories (MTL) at MIT.

4.2 Design and Structure

The SEM and schematics of the fabricated devices are in Figure 4-2a. This first generation of Deep Trench (DT) based devices are developed based on DTs of depth 4.5 μm and length 0.8 μm. All of the DTs are of the same dimension, and only the spacing between DTs is a variable. This is to make the trench etch process uniform and always at the optimum parameters. In this first generation, the etch was not perfect, so the trench side wall is curved, which results in voids in the middle of the trenches after depositing polySi fill.

In this deep trench based RF MEMS resonator, both the resonator cavity length and the ABR dimensions are defined by photolithography, making it possible to integrate resonators of various frequencies on the same chip. The deep trench capacitors are used as both electrostatic transducers and ABRs, with all the critical dimensions defined in the same mask, and self-aligned, making the process easy to implement(Figure 4-2b). The structure can also simply be viewed as replicating the same DT at different spacing. The spacing for the ABR determines the reflective frequency band, while the spacings inside the cavity are specifically chosen to place the two transducer DTs at the nodes of the targeted mode shape. As a name of reference,
Figure 4-2: Scanning electron micrographs (SEMs) (a) and 3D model (b) of solid state Deep Trench (DT) MEMS resonator. Acoustic Bragg reflectors (ABRs) formed from periodically spaced DTs define a high-\(Q\) resonant cavity in the center of the device. DT capacitors inside the resonant cavity form electrostatic drive and sense transducers.
we call the DTs used to form ABRs as “reflector DTs”, and the DTs placed inside the resonant cavity as “transducer DTs”.

The ABRs provide a boundary condition that is similar to free or rigid boundary conditions as in the case of released resonators. If we view the reflector DTs as ABRs that provide near perfect reflection, with or without phase shift, such DT resonator turns out to function very similar as the Internal Dielectric Transducers [23]. The difference lies in that it is an solid state resonator that is fully embedded in the substrate, and that each transducer DT has two dielectric layers, providing twice the driving or sensing capacity, if the wavelength is much longer than the length of the DT.

The SEM (Figure 4-2a) shows that the device has a footprint of 50 \( \mu m \times 70 \mu m \), and the cross-section image shows only the device with one transducer DT inside the resonant cavity (1-port device). And it is interesting to note that the center transducer DT is charged differently under the SEM and shows a different color. This is because only the transducer DTs are electrically connected, while the others are just mechanical structures alone.

4.3 Device Fabrication

4.3.1 Process flow

As mentioned previously, the devices are fabricated at MTL in MIT, using bulk Si wafer. The schematics in Figure 4-2b gives enough details about the geometry and materials for each component of the DT resonator. The 3D fabrication process outline for this first generation of DT RF MEMS resonator is provided in Figure 4-3. The detailed step-by-step process parameters are listed in Appendix B.

And such process flow is described as the following:

- 1 \( \mu m \) PECVD \( SiO_2 \) is deposited onto the fresh low resistivity bulk \( Si \) wafer. And such PECVD oxide is patterned to form 0.8 \( \mu m \) wide DT arrays using stepper photo-lithography. Under such hard mask, the 4.5 \( \mu m \) deep trenches
Figure 4-3: Fabrication process flow of deep trench based solid state MEMS resonator. The DT is formed by etching into single crystalline silicon (SCS) and filled with polySi.
are etched in $Cl_2/HBr$ using ICP RIE.

- The hard oxide mask is re-patterned into field oxide layer I (FOX I) to reduce capacitance from the subsequent electrical paths. It is patterned through photoresist mask and wet 7:1 buffered HF (BHF) etch.

- After RCA clean, the trenches are lined with 15 $nm$ Si$_3$N$_4$ and filled with n-type doped polySi. Such polySi is subsequently patterned into electrical paths for the top electrode of the DT capacitor. This also opens the contact area for substrate grounding.

- Then the solid state structure is capped with 1.5 $\mu m$ field oxide II (FOX II) to reduce scattering of elastic wave from the top free surface, and to reduce pad and routing parasitics.

- The FOX II is patterned for metal contact to the transducer DT and substrate.

- Finally, a Ti/Al metal layer is sputtered, patterned by $Cl_2/BCl_3$ RIE, and sintered at 450$^\circ$C in $H_2/N_2$ gases.

To get such DT based resonator with great performance, there are a few key requirements for fabrication:

- Mechanical wise, the trenches should be straight, with smooth sidewalls, and solidly filled. The straight sidewalls would make the geometries as close to designed as possible, and the smooth sidewalls would reduce scattering and improve $Q$ of the resonator. In addition, the polySi deposition should solidly fill the trenches to form the entire structure, without leaving any voids behind.

- Electrical wise, the substrate and the polySi, which electrically connect to the capacitor, should be conductive enough to reduce RC delay. And in BEOL metal stack, the two electrical routing layers (polySi and Ti/Al metal layer) should be well isolated from each other, but in good Ohmic contact wherever contact holes are opened.
Table 4.1: Design Parameter Values for the DT Resonator

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frequency ((f))</td>
<td>3 GHz</td>
</tr>
<tr>
<td>Trench depth (h_{DT})</td>
<td>4.5 μm</td>
</tr>
<tr>
<td>Trench width (w_{DT})</td>
<td>0.8 μm</td>
</tr>
<tr>
<td>Device width (w)</td>
<td>50 μm</td>
</tr>
<tr>
<td>FOX 1 thickness (t_{FOX1})</td>
<td>0.3 μm</td>
</tr>
<tr>
<td>FOX 2 thickness (t_{FOX2})</td>
<td>1.5 μm</td>
</tr>
<tr>
<td>(Si_3N_4) thickness (t_{die1})</td>
<td>15 nm</td>
</tr>
<tr>
<td>polySi thickness (t_{poly})</td>
<td>0.7 μm</td>
</tr>
<tr>
<td>Ti thickness (t_{Ti})</td>
<td>0.1 μm</td>
</tr>
<tr>
<td>Al thickness (t_{Al})</td>
<td>1 μm</td>
</tr>
<tr>
<td>Cavity length (L_{trans})</td>
<td>variable, e.g. 7.5 μm</td>
</tr>
<tr>
<td>ABR pitch (L_{ref})</td>
<td>1.7 μm</td>
</tr>
</tbody>
</table>

And Table 4.1 lists the key parameter values for such DT based resonator.

As seen from the SEM in Figure 4-2a, the fabricated structure from the first generation of devices is far from perfect. The following sections discuss these fabrication challenges and solutions in a bit more detail.

### 4.3.2 Deep Trench Etch

Etching of the deep trenches is the most important step in defining the mechanical structure of the device. A good etch provides high aspect-ratio structure, smooth sidewalls, and uniform etch results across the entire device. The sidewalls should better be slightly angled into a “V” shape to facilitate the trench fill through polySi deposition.

Figure 4-4 provides a few cross-section SEMs during the first few rounds of process development. It is based on hard mask \((SiO_2\) as mask instead of photoresist) etch, using one-step etch recipes in which only the reactive plasma is used. As a result, the etch depth is limited, because bowing of the sidewall will occur once the aspect ratio grows large. Even with the aspect ratio controlled to such smaller value, as seen from the figures, the sidewall is still sometimes non-ideal.

The first etch recipe is the one used for devices in Chapter 4.3 (Figure 4-4a). It is based on \(Cl_2\) and \(HBr\), which generates bowing sidewall, and therefore causes the deposited polySi to form voids inside the DT structure. The etched surface is smooth.
on the sidewall, but the bottom of the trench is very rough due to micro-masking.

After switching to $SF_6$ and $C_4H_8$ gases (Figure 4-4b), and fine tuning the etch parameters including gas concentration, pressure and RF power, the etch profile gets improved, providing smooth sidewall and bottom. However, the trench sidewall is slightly bowed, leaving voids after the polySi deposition as a result. Sometimes the process is able to generate straight sidewalls and provide void-free fills (Figure 4-4c), but this result is not robust enough to generate repeatable results.

![Figure 4-4: DT one-step etch process development. These are SEMs on the cross-section of the wafer after the fabrication process is complete. (a) Etch using gases $Cl_2$ and $HBr$. (b) Etch using gases $SF_6$ and $C_4H_8$. DTs have voids in the middle due to sidewall bowing. (c) Etch using gases $SF_6$ and $C_4H_8$. The polySi fill in this example is void-free.](image-url)
Figure 4-5: SEMs showing steps to get straight, smooth and high aspect-ratio deep trenches. (a) Result from direct DRIE recipe. The roughness on the sidewall is clearly visible. (b) PolySi deposition on top of the trenches from (a), which leads to voids due to the sidewall roughness. (c) Result after the entire treatment of DRIE + HF dip + one-step etch. This results in perfect DT structure. (d) The profile on trenches of various width from such optimized recipe.
Due to the limitations of the one-step etch, it is worth looking into other etching methods that provide higher aspect ratio. High aspect-ratio etch is readily available in micro fabrication, which is the DRIE etch (Figure 4-5a). Such etch process is based on alternating steps of etch and passivation. The disadvantage of this process is that such alternating steps generate scalloping sidewalls, which scatter off waves, and generate tiny voids after polySi deposition (Figure 4-5a, b).

The one-step recipes are beneficial in that the sidewall is very smooth, so an ideal process is one that integrates the benefits of the two. The end recipe after multiple trial and error is based on these following steps:

- Regular DRIE etch, which provides high aspect-ratio structure (Figure 4-5a).
- Short buffered HF (BHF) dip, which etches away part of the oxide mask, making the opening bigger (Figure 4-5a, c).
- Short one-step etch to attack the roughness on the sidewall, which produces straight and smooth end result (Figure 4-5c, d).

With these special treatment for fabrication, it is able to provide straight, high aspect-ratio deep trenches with minimal surface roughness, as illustrated in Figure 4-5c, d.

### 4.3.3 Electrical Considerations

Based on the design of the device, the DT should be able to function as both a mechanical structure and a capacitor. As a result, apart from the etch improvements to get better mechanical structures, the electrical properties of the DTs should also be treated carefully.

In order for the trench capacitors to function at multi-GHz range, the RC delay should be small. In other words, the voltage should drop uniformly across the entire capacitor dielectric layer after propagating through the distributed RC network, which is consisted of the polySi resistor and the polySi-Si$_3$N$_4$-Si capacitor. The measured polySi resistivity is only around 0.003 $\Omega cm$, but the resistance of the polySi routing is
made large by its relatively narrow geometry, defined by the trench width of 700 nm – 1 μm. The capacitor also has a large area due to the etch depth and width designed to form a high aspect-ratio 1D structure. As a result, the capacitance of a single deep trench is at the order of magnitude of 100 fF. All of these factors have made the RC delay a realistic concern.

To address this issue, both the Si substrate grounding and the polySi top layer are made to be sufficiently conductive. During device fabrication, the Si substrate is doped by ion implantation, followed by anneal, and the polySi layer is lined with a 500 nm thick Al layer to reduce RC delay. The electrical properties of such structure can be studied in COMSOL AC/DC module, as illustrated in Figure 4-6.

In such simulations, the focus is on the resistor, made of polySi (red) and top Al (grey), and the capacitor, formed by the dielectric Si₃N₄ (yellow) (Figure 4-6a). Since the polySi fills into the deep trench, its shape is a thin vertical wall that is around 1 μm thick and 8 μm deep, and its width is either 50 μm or 100 μm depending on the design. Apart from the component that fills into the trench, there is also a tether part that leads to the trench fill, which is formed from the same polySi deposition process, with thickness of 800 nm. The Al deposition on top is 500 nm in this study. The input voltage is 1 V, applied from the very left end of the structure into the tether, and the entire out surface of the 10 nm thick Si₃N₄ film coating the polySi is grounded.

After applying a frequency signal from the drive end, the voltage distribution is displayed as in Figure 4-6b, with red being voltage of 1 V and blue being 0. From the simulation result, we can see that beyond certain critical frequency, the voltage distribution starts to become ununiform, and such transition happens at a lower frequency for a wider structure. For example, for width of 50 μm, the voltage distribution is very uniform across the entire DT at 3 GHz, and it starts to become a bit ununiform at 5 GHz. In comparison, such transition frequency becomes much lower for the 100 μm wide structure, for which the voltage distribution becomes ununiform beyond 2 GHz.

And these are only the results for 500 nm thick Al. If it turns out that we need
Figure 4-6: (a) Schematic of the 3D structure used for COMSOL simulation of RC delay. Grey color marks the 500 nm thick Al on top. Red is the polySi deposition that fills the trench, and forms the lead to the fill. And the 10 nm Si$_3$N$_4$ wrapping the polySi inside the trench is marked in yellow. Input voltage of 1 V is applied on the very left end, and the entire out surface of Si$_3$N$_4$ is grounded. (b) Simulations of voltage distribution at various frequencies, for structures of width of 50 μm or 100 μm. For the structure of width 50 μm, driving frequency at 3 GHz is able to generate uniform voltage distribution, while at 5 GHz, the voltage drop starts to become ununiform. While for a very wide structure such as width of 100 μm, such transition happens beyond 2 GHz. This transition frequency can be increased by depositing thicker Al layer on the top surface.
Figure 4-7: SEM of one DT resonator after optimized fabrication. This is one device with two resonant cavities. The trenches are etched using the optimized etch process, providing straight, smooth, high aspect-ratio sidewalls. This leads to solid polySi fill after 800 nm deposition. A 500 nm Al layer is visible on top of the polySi layer, followed by thick field oxide for electrical isolation and mechanical mode confinement. The metal pad routing is also visible on top, which leads to the center transducer DT being charged at a different scale under the SEM.

the 100 μm structure to function well beyond 2 GHz, the solution is to increase the Al layer thickness.

With all these fabrication improvements both on the mechanical side and electrical side, the final device is shown in Figure 4-7. This image is acquired by cleaving the Si wafer after the fabrication process is completed, and doing an SEM on the cross-section at the tilted view angle. Since the device is very small, there is no control on where the cut is landed. So here it is only able to provide the example of the DT based MEMS resonator with two resonant cavities. The devices with single resonant cavities would exhibit similar process results, since they are based on DTs of the same dimension. As seen from the SEM, the optimized fabrication is able to provide
straight, smooth sidewalls, and high aspect-ratio trench structures. And the electrical connection to the transducer DT is good as well, seen from the deeper color under the SEM.

4.4 Working Principles and Simulations

In the case of released resonators, resonant eigenmodes can be calculated readily using the free boundary conditions at the edges of the resonant cavity. With these free boundaries, the eigenmodes can be solved analytically using well developed theories in solid mechanics [55].

For the solid state resonators, complexity arises in that the ABR boundary may induce phase change, and its reflectivity is a function of frequency. This prevents an obvious eigenmode decomposition inside the resonator; although the reflectivity amplitude converges to 1 as the number of ABR layers increase, it cannot be treated simply as a free surface. For solid state resonators bounded with ABRs, two methods are used in this analysis:

- The ABR is treated numerically by the forward-backward wave analysis method to extract its reflectivity as a function of frequency, as discussed in Section 2.3.1. Next, the resonator eigenmode is calculated based on this extracted numerical library of complex-valued reflectivity.

- The eigenmode of the resonator-ABR composite structure is directly calculated through finite element simulation in COMSOL, using PMLs on the boundaries where the waves propagate into infinity.

4.4.1 Numerical Analysis

The analysis method is the same as that described in Section 2.3.2. The unit cell function for the program is based on a two-layer structure, Si and polySi. It should be noted that Si₃N₄ lines the trenches to form the transduction capacitors (shown in yellow in Figure 4-8a), but its acoustic effect is negligible since the fractional
wavelength in it at operating frequency is far smaller than that in the Si and polySi layers, so it is not included in this analysis.

Typically, ABRs are designed with alternating materials at quarter wavelength λ/4 of the targeted reflector frequency, and the resonant cavity is at integer multiples of half-wavelengths nλ/2 [17] (e.g. Figure 4-8a, Design A). This design provides optimal performance and zero phase change as seen at the resonator-ABR interface. However, for a DT resonator the priority in design is effective fabrication, i.e. fixing the trench length δ_{DT} for uniform etch rates and optimal trench fill. Consequently, the only design parameter is the spacing between DTs for modification of the reflective frequency. The pitch size is chosen to be the value to make the two layers sum up to λ/2 at the targeted frequency. The Si layer thickness is therefore set as the complementary part that makes the two layer sum up to λ/2. With this design, both the lengths of the Si and SiO_2 layers will deviate from quarter wavelength, resulting in the narrowing of DT ABR bandgap and degradation of reflectivity (Figure 4-8).

This result is the same as what is discussed in Section 2.3.2—if each layer of the ABR deviates from the λ/4 optimum length, the bandgap will be smaller, and more layers/footprint will be required.

How the bandgap shifts and shrinks in size is presented in Figure 4-8a. From the figure, it can be observed that as the pitch size gets bigger while the trench width kept at constant, the bandgap center frequency shifts to a lower value. This can be qualitatively explained by the formula \( c = \lambda f \). Since the wave speed \( c \), determined by material properties, is kept constant, and that \( \lambda \) is determined by the pitch size (pitch size approximately equals λ/2), therefore, the larger the pitch size, the smaller the frequency. And the bandgap size shrinks because the ABR layers are offset from the optimum λ/4 more and more as the pitch gets longer.

The curves of reflectivity vs. cell number \( n \) is plotted in Figure 4-8b. Again, the bandgap size is equivalently represented as the convergence rate—the bigger bandgap provides faster convergence rate. And also note that geometries apart from λ/4 combinations will induce a phase shift upon reflection. This phase implies that the standing wave inside the resonant cavity is no longer an integer multiple of half-
Figure 4-8: (a) Simulated band structure of DT ABRs formed by alternating layers of Si and polySi. Unit cells of 4 different DT ABRs are shown with various ratios of Si and polySi. This ratio determines the width of the bandgap generated by the ABR. As the pitch size increases, the bandgap shifts down in frequency. Design B corresponds to the design demonstrated experimentally. (b) Reflectivity of DT ABRs as a function of ABR pair number plotted at the center of the bandgap. The more $\delta_{DT}$ and $\delta_{SCS}$ deviate from $\lambda/4$, the larger the phase shift of reflectivity.
wavelength $\lambda/2$, but is rather controlled by a combination of the cavity length and the ABR reflectivity phase.

This new phenomenon makes the DT resonator design challenging: frequency cannot be calculated from the "as-seen" cavity length. A better approach is work backwards—instead of designing resonators and matching boundaries, one can design boundaries and match the resonant cavity.

- DT length $\delta_{DT}$ is selected based on optimum process parameters for trench etch and fill.

- DT spacing $\delta_{SCS}$ is chosen according to the targeted resonator frequency by numerical calculation. The DT ABR determines the frequency range where high-Q resonance can be sustained.

- With fixed DT length and spacing, the cavity length is varied to find the resonance inside the bandgap (Figure 4-9).
Figure 4-10: COMSOL simulation of an solid state DT resonator where drive DT is centered in the resonant cavity. Red and blue indicate peak and trough of displacement in the x direction $u_x$. The inset shows the influence of non-zero phase at the resonator-ABR interface on the resonance mode.

The example of Figure 4-9 shows that the resonance peaks appear at different locations inside the bandgap, determined by the cavity length. In this particular analysis, cavity length of 7.5 $\mu$m is the best value. Note that this is no longer integer multiples of half wavelength ($\lambda/2 = 3.4 \, \mu$m).

### 4.4.2 COMSOL Simulations

To get better mode uniformity and higher $Q$, the in-depth dimension, which is perpendicular to the direction of longitudinal resonance, can be designed to minimize acoustic reflections. To achieve such goal, the 1D model of numerical analysis in MATLAB is no longer sufficient. COMSOL simulations can provide 2D analysis on the entire resonator-ABR cross-section. The frequency response simulation in the solid mechanics module is able to capture the wave propagation in this 2nd dimension. Figure 4-10 gives one such example of the type of device with one transducer DT inside the resonant cavity. In this mode shape plot, the top surface is free boundary, while the other 3 surfaces are bounded with PMLs.
The capping $SiO_2$ is chosen to be thick in order to acoustically match to the resonant cavity, and reduce spurious modes. As seen from the simulation, with 1.5 $\mu m$ thick oxide, there will be some thickness mode in the oxide, but the mode inside the resonator-ABR structure is kept as almost a 1D mode. The inset of Figure 4-10 shows the comparison of such mode against mode in a free bar in the resonant cavity. Due to the phase shift from the DT ABR reflection, the amplitude of the solid state mode is not at maximum on the edge, and therefore it is not integer multiples of $\lambda/2$ inside the cavity either.

As the comparison in Figure 2-6 indicates, the $Si$-poly$Si$ pair has the narrowest bandgap. This weakest reflector pair is chosen, instead of the stronger ones, because weaker reflectors turn out to achieve higher $Q$ for the solid state resonator. This is counter-intuitive to the design case of surface mounted FBARs [17], where stronger reflectors are preferred. In the design case of FBAR, 5 out of the 6 surfaces of the resonator are still free surface, and the only energy leakage path is through the ABR, so the better the reflector, the stronger the $Q$. While for the case of fully unreleased resonators, all the resonator surfaces are not free surfaces, so the surfaces interact with each other through wave scattering. This idea of “weaker reflector for better $Q$” can be elaborated through a set of COMSOL simulations, shown in Figure 4-11.

Figure 4-11a shows the simulation structure and mode shape of the DT resonator with $SiO_2$ filled trenches, while Figure 4-11c shows those of the poly$Si$ filled trenches. In both of these figures, blue color indicates $SiO_2$, red indicates poly$Si$, and grey region is $Si$. The dimensions of the geometry are kept constant, which are exactly the same as the values from fabrication results. The number of ABR cells is the study variable. Figure 4-11b shows that the quality factor $Q$ of such resonator increases with the variable of reflector number $n$. And the $Si$-poly$Si$ ABR is able to provide larger value of $Q$.

Base on the results in Figure 2-6 from Section 2.3.2, we know that the $Si$-$SiO_2$ combination provides a much stronger bandgap than that of $Si$-poly$Si$. However, from Figure 4-11b, we can see that the poly$Si$ filled DT resonators provide a much higher $Q$ than the $SiO_2$ filled ones. 1D theory predicts that without consideration
Figure 4-11: Structure schematics, and mode shape plots, with the color plot being stress $x (\sigma_x)$, and the arrows being displacement field. (a) Mode shape of Si-SiO$_2$ ABR based DT resonator. (b) $Q$ as a function of cell number $n$ for SiO$_2$ based DT resonator and polySi based resonator. (c) Mode shape of Si-polySi ABR based DT resonator. (d) Mode shape of polySi based DT resonator with voids in the top oxide layer (left), and SEM of such fabricated real structure (right).
of material damping, as the number of ABR cells increases, the $Q$ goes to infinity. However, the 2D simulation shows that the $Q$ converges to a fixed value. This value is determined by wave scattering in the vertical dimension.

In the pure 1D model, the only energy leakage path is through the ABRs, so the stronger the reflector, the better the $Q$. However, once the effect of this second dimension is taken into account, the design also needs to consider energy loss into the substrate. The ideal high-$Q$ mode should have a localized standing wave in the in-plane ABR direction, and an evanescent tail into the substrate. For such a pure mode to form, the wave scattering of the ABR should be designed to a minimum. Stronger reflectors will generate stronger scattering into the substrate direction, and in the end de-$Q$ the resonator, so the $Q$ will stop increasing beyond certain cell number $n$. This wave scattering effect can be observed from the mode shape in Figure 4-11a, in which the red arrows are the local displacement vectors, and the color coating indicates stress $x$ component $\sigma_{xx}$. The figure shows that inside the center resonant cavity, the displacement vectors are not purely horizontal. Instead, there are large $y$ components indicating that the wave gets scattered by the strong $Si-SiO_2$ reflectors. On the other hand, weaker reflectors will “absorb” the mode into the top ABR layer better, and result in better confinement as the cell number $n$ increases. As seen in Figure 4-11c, the mode for such $Si$-poly$Si$ ABR indeed extends very deep into the reflector, and the evanescent tail into the bottom $Si$ substrate is uniform as well. Zooming in to observe the displacement vectors, we can see that the $y$ components of the displacement vectors are very small. This low scattering generated from weaker reflectors leads to higher $Q$ of the entire structure.

Obviously, the trade-off in such design is that it will require a larger ABR array, therefore consuming a larger footprint, so the design process should involve the balance between $Q$ and footprint.

Another reason of using poly$Si$ is to meet the requirement of forming DT units that can be used as both a mechanical structure and capacitors. To achieve such functionality, the filling material should be very conductive, and insulators such as $SiO_2$ and $Si_3N_4$ do not meet such requirement.
Another interesting fact to note is that the device will inevitably have fabrication non-idealities. Apart from possible voids mentioned previously, there can be defects close to the surface. For example, the SEM in Figure 4-11d shows the voids formed after deposition of passivation oxide. This oxide layer is created by fast PECVD process, which grows much faster on the top surface than on the step sidewall. As a result, a small notch on the surface before the deposition will lead to a void after the process. Such voids can be sources of scattering, as displayed in the mode shape. For exactly the same geometry as that in the case of Si-polySi DT, existence of such surface defects can reduce the $Q$ by almost a half. Methods to overcome such fabrication non-idealities will be discussed in the following chapter.

4.5 Experimental Setup and Results

Devices were tested in air at room temperature in an RF probe station using a pseudo-differential measurement as shown in Figure 4-12 to cancel parasitic capacitance of both pads ($C_{pad} = 300 \text{ fF}$) and device ($C_0 = 440 \text{ fF}$). No on-chip de-embedding is necessary.

![Figure 4-12: Measurement setup for pseudo-differential testing of DT resonator. An identical dummy resonator which is not driven (no DC voltage applied) provides differential cancellation of the pad and device capacitance.](image)

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Figure 4-13: Measured frequency response of DT resonators with 7.2 μm long resonant cavity, DT length of 950 nm, and 1.7 μm DT pitch in the ABRs. Devices with 20 ABRs and 50 ABRs are shown, with higher Q and lower loss in the latter. Wide frequency sweeps show no spurious modes in the multi-GHz range.
performed.

The frequency response of two solid state DT resonators is shown in Figure 4-13. Since zero bias voltage is applied across the transducers of the dummy resonator, it does not contribute to the differential output $S_{dc21}$. Therefore, the resonator’s motional impedance $R_X = \frac{v_{in}}{i_{out}}$ can be extracted directly from $S_{dc21}$ as [56]

$$S_{dc21} = 20 \log\left(\frac{Z_0}{R_x + Z_0}\right)(dB) \tag{4.1}$$

Applying an RF signal of $-5$ dBm and varying DC bias on the input and output transducers, the devices show clear resonance at 3.2 GHz for a device with 20 ABRs, and 3.3 GHz for a device with 50 ABRs. Wide frequency sweeps showed no spurious modes in the multi-GHz range around resonance. The 50 ABR resonator exhibits a $Q$ of 2057 and $R_X$ of 1.2 kΩ. This translates to an $f \cdot Q$ product of $6.8 \times 10^{12}$, and $k_{eff}^2$ of $5.4 \times 10^{-5}$. This coupling coefficient can be dramatically improved by scaling the dielectric.

As expected, the 50 ABR resonator shows improved performance of both $Q$ and $R_X$ relative to the 20 ABR resonator. This result is in agreement with the theory of DT bandgaps, which predicts $\sim 10\%$ improvement in ABR reflectivity between 20 and 50 ABRs (Figure 4-8b). An identical resonator with only 1 ABR exhibited no measurable resonance. The 0.1 GHz frequency shift with the increase of ABR number is caused by the phase change of reflectivity as the ABR number increases. This frequency shift from an increased ABR number is also observed in COMSOL simulation.

4.6 Discussion

A 3.3 GHz solid state resonator with Deep Trench dielectric drive and sense was demonstrated with performance rivaling that of freely-suspended Si resonators in the same frequency range. Deep Trenches were implemented both as electrostatic transducers and as Acoustic Bragg Reflectors to localize vibrations in the solid state.
Figure 4-14: SEM of the DT resonator implemented in IBM's 45nm SOI process. The metal layer is thinned down by mechanical polishing, followed by a focused ion beam (FIB) process to carve out the device cross-section.

This new concept enables high $Q$, low loss multi-GHz resonators in a simple, robust manufacturing process.

As previously discussed, such devices have high similarity with the DRAM structure in the IBM CMOS process, therefore, it can be implemented in CMOS, as shown in the focused ion beam (FIB) image in Figure 4-14. As the DRAM structure is very high aspect-ratio and deep down into the substrate, the BEOL metal stack on top has to be thinned down before the FIB. The figure shows that the DRAMs are spaced in the same way as the device implemented in-house, designed to be used as electrical transducers and mechanical ABRs at the same time. The dummy CMP fills are cleared in layout design above the resonator area to reduce spurious reflections.

Despite the replication of geometry, this non-customized fabrication faces a few challenges:

- The DRAMs is not optimized for mechanical application, so voids are visible from the FIB image, which lead to scattering and cut-off of the mechanical mode.
• The DRAM poly fill aspect ratio is very large, therefore the resistance of polySi becomes significant at multi-GHz range, which leads to RC delay that reduces signal coupling between electrical domain and mechanical domain.
Chapter 5

Dual Trench Solid State DT MEMS Resonators

5.1 Introduction

Chapter 4 discussed design, development, and measurement of deep trench (DT) based MEMS resonators. These are high aspect-ratio resonators that are solidly embedded, and requires no release step and minimal packaging. The frequency of such resonator is lithographically defined, with the cavity and reflectors fabricated in the same mask and self-aligned. Such neat design is enabled by using the deep trench capacitor that is very similar to the DRAM in IBM's CMOS process, which can function as both a mechanical reflector and an electrical capacitor.

For such DT based MEMS resonators, polySi is chosen to be the filling material inside the trenches. This generates a DT ABR structure formed by material pair of Si-polySi. Apart from the electrical conductivity reason to choose polySi, another purpose is to form a “week reflector” that traps the standing wave inside the ABR layer, instead of scattering if off into the substrate, as discussed in detail in Section 4.4.2. Although this method is able to enhance $Q$, the extremely weak reflector formed by $Si$-poly$Si$ also leads to a few issues.

- The required footprint to generate such high $Q$ is very large. As discussed
in Chapter 2, weaker bandgap calls for more layers to reach the same level of reflectivity than the stronger ones. Figure 4-11b shows that although the ultimate $Q$ for the weaker reflector is much better than that of the stronger ones, the required number of cells is much bigger. Even with 70 cells, the $Q$ still has not converged to its maximum. In practice, only 50 cells are used to balance between $Q$ and footprint.

- The size of the resonant cavity is hard to determine during layout design. The narrow bandgap of the reflector requires precise position of the resonator frequency. This in turn requires the size of the resonator cavity to be almost spot-on. However, the actual bandgap frequency range may vary from the one predicted from calculation, since the exact material properties are unknown. This is especially true for polySi, whose material properties are determined by the deposition conditions during micro-fabrication. This bandgap variation does not affect the design of resonators using the ABR with a large bandgap, which would accommodate for such variations. Whereas for weak bandgaps, such variation would lead to misalignment between the cavity frequency and the ABR bandgap frequencies. In practice, this issue is solved by laying out an array of DT resonators with identical ABRs, but a series of resonator cavity sizes that tightly sweep around the targeted length. However, this leads to a waste of layout area, and also results in low yield.

- The extremely weak bandgap easily gets affected by defects from fabrication. Non-periodic defects such as random voids inside the DT, or occasional surface dents, would cause a shrink-down of the effective bandgap size. The reasoning for such effect is analogous to the bandgap variation study provided in Section 2.3.4. With the initial bandgap already being very narrow, introduction of defects would further reduce the bandgap size and in turn call for an even larger footprint to compensate such reduction. Moreover, such larger structure would make itself more likely to be affected by fabrication variations.

Due to these disadvantages of the extremely weak bandgap size from Si-polySi,
the fabrication yield is very low, and the result gets non-reproducible. Another feature to note in previous designs is that only one DT is used for driving and only one DT is used for sensing. It will be discussed in this chapter that the $Q$ can be improved by replacing such one DT design with array transduction.

To address the issues of fabrication yield and sensitivity to fabrication non-idealities, this chapter introduces a new design of deep trench based unreleased solid state MEMS resonator, named the “Dual Trench” DT MEMS resonator. Such design is able to utilize the benefit of weak bandgap structure, yet get the bandgap size controllable through fabrication so that it does not get too weak to cause issues mentioned above. The details are discussed in the following sections.

5.2 New methods and Design Improvements on DT MEMS Resonators

5.2.1 A Different Perspective—Waveguide Analysis

As discussed in Section 4.4.2, 1D analysis provides useful insights and guideline, but to get accurate and comprehensive understanding, 2D COMSOL simulation is a must. However, previous simulations are based on methods that build the entire parametric structure, and then sweep the key design variables such as pitch size, resonator cavity length etc. to find the best combination, or more efficiently, to run optimization programs on such key variables to find out the best design values. Although these methods can provide results, they turn out be very cumbersome, computationally heavy, and time-consuming, since each iteration of design is a frequency sweep study itself, which contains hundreds of single simulations at each individual frequency. And moreover, what are provided at the very end of the sweeping process are only results on which design is better, or some rough trend on directions to change the parameters, rather than insights on why and how the parameters are chosen that way.

A better analysis method is to use techniques adopted in photonics waveguide research [57] [39] [58]. Typical waveguides have closed bounds along the propaga-
tion direction, which provide free or rigid boundary conditions that generate total reflection. However, there are also open waveguides that guide the wave by mismatch of the impedance, which generates total reflection beyond the critical angle. The purpose of waveguide design is to get the energy contained inside the guiding material, leaving little or no energy inside the wrapping material. What enters the wrapping material should at best be just an evanescent tail that carries no energy propagation. To analyze a waveguide, the method is typically cutting off one slice of the waveguide, and analyze the property of this single slice, either analytically, or numerically. The method is legitimate since the structure has translational symmetry, therefore, proper analysis of a single slice would unveil property of the entire waveguide. With this “sliced” analysis that focuses on a much smaller geometry, only very little computational power is required.

The DT ABR structure can be treated as a waveguide with half open boundaries (the bottom of the DT ABR layer is open to the substrate). The end goal of mode design is to let the wave energy get constrained inside the DT ABR top layer, instead of inside the substrate. This is exactly what the waveguide does. The notion to treat the DT ABR as a waveguide when its true purpose is to reflect waves is a bit counter-intuitive, but this will get clearer as the discussion digs deeper.

If we were to analyze the DT ABR structure alone, and ignore the resonant cavity for the time being, it will be a near-perfect periodic structure with translational symmetry (finite length). This translational symmetry is a bit different from that of the uniform waveguide, in that the symmetry operator works only with discrete values that are integer multiples of the pitch size $L$, instead of any real values. The wave function solution to the elastic wave equation in such structure with discrete translational symmetry satisfies the Bloch’s theorem

$$u(x) = e^{ikx}u_0(x)$$

in which $u(x)$ is the displacement field solved from the wave equation, $k$ is the wave number, $x$ is the spatial coordinate, and $u_0(x)$ is a periodic function with the same
periodicity as the waveguide, which is simply $L$ for such 1D periodic structure. This theorem leads to the result that for any two cross-sections spaced at $L$ along the direction of periodicity, there is the relation of

$$u(x + L) = e^{ikL}u(x)$$

(5.2)

Because of the translational symmetry at periodicity $L$, only this one slice is sufficient for analysis. Such model can be built in COMSOL solid mechanics module, with the schematic of the simulation geometry shown in the top-left corner of Figure 5-1a. Based on Equation (5.2), Bloch boundary conditions are applied between the left and right boundaries. The top surface is simply a free boundary, while the bottom is a bit tricky, since it is a direction where the wave can propagate freely. To achieve such effect, the bottom section that represents the Si substrate is simply made extremely thick, 10 times the thickness of the top slab in this particular simulation (which is not shown in the figure). Now with these simulation settings, if we were to extract the eigenmodes that can exist in such waveguide, all we need to do is to run the eigenmode solver on such sliced geometry. And of course the eigenmodes will depend on the predetermined $k$ value. As a result, to get the complete picture, the eigenmode solver is run for each $k$, while the $k$ needs to exhaust the space between 0 and $2\pi/L$, which is the size of the first Brillouin zone. If we were to plot the values of such eigen frequencies against the wave number $k$ values, we obtain the dispersion curves that are typically seen in solid state physics when analyzing electron waves in an atomic lattice [59], or nanophotonics when analyzing optical waveguides [58] [39]. Since the unit cell has mirror symmetry at the center line, such dispersion relation will be symmetric along $k = \pi/L$, so only $k$ scan up to $\pi/L$ will be sufficient.

Figure 5-1a gives the result of such dispersion curves for the DT ABR structure. Blue dots are data points from simulation, which are chosen to be denser close to the $k$ of interest, $\pi/L$. The two inclined lines mark the wave speed of P wave (longitudinal, upper) and SV wave (one type of shear, lower) in the $<110>$ direction in single-crystalline Si. Analogous to the terms used on photonics, the area above such lines
Figure 5-1: (a) $k - \omega$ dispersion curves for the DT ABR, in which the $k$ axis is normalized to $k_0 = \pi/L$ and the frequency axis has unit GHz. The inset on top-left shows the geometry used in COMSOL simulation to generate such curves. Bloch boundary conditions are applied between the left boundary and the right boundary, and the bottom $Si$ is set 10 times the thickness of the top DT ABR layer to capture the fact that the wave can propagate freely in that direction (not shown in the inset). Blue dots are the eigenmode frequencies corresponding to each $k$, the yellow zone marks the area between the shear wave sound cone and the longitudinal wave sound cone, and the green zone marks the longitudinal wave sound cone. (b) The waveguide eigenmodes at $k = \pi/L$. The modes map to the numbers marked in the dispersion curves in (a). The first 3 are SAW modes, and the remaining 3 are bulk longitudinal modes. Mode (4) is the target for DT MEMS resonator design.
can be named as the “sound cone”. It is named as “cone” because this is typically plotted for $k$ vector in 2D, in which a cone shape is formed along the frequency axis. The “sound cone” line separates the modes that can propagate freely in $<110>$ $Si$, from the ones that cannot. From Snell’s law, the $k$ of the waveguide equals the $x$ component of $k$ inside $Si$, so if the wave were to propagate freely inside $Si$, there will be an inequality of $k_{\text{waveguide}} \leq k_{Si}$, which generates the phase velocity $c$ relation of

$$c_{\text{waveguide}} = \frac{\omega}{k_{\text{waveguide}}} \geq \frac{\omega}{k_{Si}} = c_{Si}$$  \hspace{1cm} (5.3)

This means all the waveguide modes above the sound cone line will be able to propagate freely inside the substrate material $Si$. What about the modes that appear below the sound cone line? From Snell’s law, $k_x$ in $Si$ will be equal to the $k$ of the waveguide, but now with the dot below the $Si$ sound cone line, this $k_x$ is larger than the maximum $k$ that can be sustained for free waves. From wave propagation theory, this means the wave will simply be evanescent inside $Si$, with the evanescent tail wave number being

$$k_e = \sqrt{k_z^2 - k^2}$$

And these types of modes are the preferred ones since with wave being evanescent in $Si$, the energy will be fully localized or “guided” inside the top DT ABR region.

Note that different from what is typically seen for such waveguide dispersion relations, there are two sound cone lines instead of one, so there will be 3 types of modes: the ones that are fully confined from both shear and longitudinal free waves in $Si$, the ones that are only fully confined from longitudinal free waves, and the ones that are not confined at all for either types of waves. These 3 regions are marked as white, yellow, and green respectively in Figure 5-1a.

Direct raw simulation data would display dense piles of eigenmodes above both sound cone lines (yellow and green regions). The ones displayed in Figure 5-1a are extracted from such raw data, showing only modes for which the energy is concentrated in the DT ABR layer. The 3 branches below the shear wave sound cone line (white zone) are the surface acoustic wave (SAW) modes, with the polarization primarily
in the $y$ direction, as shown in (1), (2), and (3) in Figure 5-1b. And the 4 branches above the shear wave sound cone line but under the longitudinal wave sound cone line (yellow zone) are longitudinal modes, with the primary polarization in the $x$ direction. These modes are shown as (4), (5), and (6) in Figure 5-1b. In each of these eigenmode plots, the plot on the left shows the displacement field, and the heat plot on the right shows the energy density. The displacement field plot displays the magnitude of local displacements in rainbow color, and the displacement vectors in red arrows. Seen from both the displacement fields and energy heat plot, it is obvious that the first 3 modes are SAW modes for which the energy is concentrated on the top surface, and the remaining 3 modes are longitudinal modes for which the energy concentrates in the entire DT ABR layer. Mode (4) is the pure longitudinal mode that we are interested in, and the one that we used for the resonator design in Chapter 4. Such mode is chosen because it is a bulk acoustic wave (BAW) mode that covers more volume than the SAW mode, and the displacement field couples directly to the driving forces across the dielectrics. All of these factors increase the electro-mechanical coupling efficiency $k_{eff}^2$ of the resonator designed using this waveguide structure.

Here we should clarify how a structure used to guide waves can be used as an ABR to reflect waves. Based on the dispersion curves, the waveguide only guides waves when it operates on such dispersion curves, or inside the sound cone. Therefore, if we were to excite waves away from such “guiding zones”, the waves would not be able to propagate freely inside the waveguide. In other words, it will be an evanescent mode, and the wave that hits the structure end boundary will get total reflection, leaving only an evanescent tail inside the structure. And the farther it operates away from such mode curves, the shorter the evanescent tail. These are exactly the operation zones that transform a waveguide into a reflector.

Note that in Chapter 4, the wave is launched only on a single DT capacitor. This gives control of the $k$ of the waves being driven. In fact, since it is driven at a single dot in space like a delta function $\delta(x)$, the $k$ packet, derived from the Fourier transform of spacial distribution, would be uniformly distributed in the entire $k$ space. Therefore, wherever the wave is launched in frequency, it will always excite the modes
with all the possible $k$’s uniformly, including the $k$’s that fall inside the sound cone and are low $Q$. On the other hand, if we were able to control the $k$ through a certain driving pattern so as to make it concentrate around $k = \pi/L$, the driving forces would couple merely to a single $k$ mode, that is outside of the sound cone, and therefore high $Q$. This gives the rationale of why array transduction can provide higher $Q$: array transduction generates a $f = \text{sinc}(k - \pi/L)$ like packet that is concentrated around $k = \pi/L$ and out of the lossy sound cone, providing a much more efficient transduction.

With this idea, the resonator design now becomes the process of mismatching two DT ABR waveguides. Assuming the two DT ABR waveguides are just slightly different from each other—this could be a slight variation in surface geometry or material, or just simply variation in the pitch size. If we were to concatenate these two waveguides and operate at the same frequency $\omega$ and wave number $k$, since now the dispersion branches are not aligned with each other after such structural variation, only one waveguide would be able to guide wave, depending on which frequency it operates. Now the targeted resonator mode would be a mode that can propagate freely inside the waveguide that forms the “resonator”, but unable to propagate, or evanescent in the waveguides that form the “reflectors”. Since our choice of the waveguide modes are the ones outside of the sound cone, the energy would be constrained solely inside the waveguide segment that forms the resonator, leaving only evanescent tails inside the reflector waveguide, and the substrate. This chain of reasoning leads to a natural way of building a DT ABR based resonator, and this process does not require brute-force simulation of the entire resonator structure, all it needs is to find out the dispersion curves of two single waveguide unit cells (one for the resonator cell and one for the reflector cell).

Up to this point, the idea of solid state resonator design is refreshed by this new perspective of waveguide dispersion analysis. The following sections will frequently adopt this method when it comes to designs of other DT based resonators, and this method can be applied to any types of solid state resonators as well.

In addition, there are a few key points to note.
Firstly, as mentioned, the waveguide modes outside the sound cone is preferred, since the energy would be confined for such modes. On the other hand, if it is a mode inside the sound cone, the wave would be able to propagate freely inside the substrate material $Si$, making the energy not confined, and any resonators built with it low $Q$. Note that the modes between the two sound cone lines (yellow region) would be well isolated from the longitudinal free modes, but not isolated against the shear free modes. These modes will tend to have lower $Q$ if designed incorrectly, but since the waves launched from squeezing the capacitor dielectric are primarily longitudinal components, it couples much more easily to these longitudinal eigenmodes rather than the shear eigenmodes at the same frequency range.

Secondly, the filling material should be of lower acoustic impedance than the substrate. This is essential for such out-of-the-sound-cone modes to exist. The intuitive explanation is the analogy to simple wave guiding: the top material should be of lower impedance than the substrate material for a guided mode to exist. For example, the Love wave in a uniform layer that is mounted on top of a substrate would need such requirement [45]. Based on this argument, the average acoustic impedance of the top DT ABR layer should be smaller than that of the substrate material, which can be equivalently stated as the filling material should have lower impedance than the substrate.

And lastly, there are a few technical details to note for such simulations.

- The direct eigenmode solution would include much more modes than the ones shown in Figure 5-1a. The raw data is trimmed by eliminating the junk modes including the free propagation modes inside $Si$, surface modes on the bottom surface, etc. The method for such data extraction is to select the modes for which the energy is concentrated on the top DT ABR slab, using an energy ratio probe. COMSOL has the function to extract energy integrated over certain geometry, and such energy ratio probe can be defined using a global variable that divide the two integrated energy parameters.

- The thickness of the $Si$ substrate layer should be chosen carefully. The goal is to
reveal the longitudinal modes that are submerged inside the shear wave sound cone, but not to introduce too much mode distortion. Too thick a substrate layer would emphasize the free propagating shear modes and lose the longitudinal modes, while too thin a substrate layer would introduce distortion due to the reflection from the bottom free surface. Through trial and error, it is found that the optimal substrate thickness should be 10 times the thickness of the top DT ABR layer.

5.2.2 Design Improvements

The study of dispersion relation \((k - \omega)\) plots provides insights and direct guidelines into designing of solid state resonators with high \(Q\) mode shape. These can help reduce simulation workload, and reduce learning cycles. A few key results from such method are discussed in the previous section.

Once the waveguide mode is targeted, work still needs to be done to extract resonator figures of merit such as the quality factor \(Q\), motional impedance etc. This process would inevitably require building the complete model of the resonator, and run frequency sweep in finite element tools, such as COMSOL. This section would use some results from such types of simulations to clarify the key points about the design principles for solid state DT MEMS resonators. But before discussing the results, here we state the methods and techniques used to run simulations/studies more efficiently.

- The COMSOL geometric model is build in a completely structural way. The DT based resonator geometric model is typically a parametrized model that consists of dozens of DT structures. And in the study process, it would require such parameters, or even the fundamental DT geometry to be able to vary according to the study goal. If we were to draw the entire geometry in a flat structure, it would be very difficult to make modifications, so instead, the geometry is constructed in a hierachical scheme, in which each waveguide cell is built as a parametrized substructure that is called by the main program to lay out into
an array. With such hierachical geometry, it becomes very convenient to make modifications on the geometry, and to study the performance out of various geometry variations.

- Asymptotic wave expansion (AWE) is used to reduce the simulation time for each frequency sweep study. Such AWE is a build-in feature in COMSOL, which runs local expansions over intervals to reduce the actually required runs of simulations.

- Method of rational function fitting [60] is used to extract the $Q$ after acquiring direct frequency sweep simulation data. Such fitting is much more accurate, and requires fewer data points, compared with regular non-linear curve fitting methods.

The key design rules for high $Q$ longitudinal mode solid state DT resonator are listed in the following:

**Array Transduction**

Figure 5-2 shows the comparative simulation results of such complete COMSOL model, in which part (a) is the one-DT structure used in Chapter 4, and part (b) is the structure using array transduction. Both figures zoom in at the very center of the complete solid state resonator structure to show a clearer view of the modeshape. The complete structure is composed of 50 DTs on each side of the resonant cavity. The color marks the intensity of $\epsilon_{zz}$, and PMLs are used to absorb waves on the edges where the wave propagates into infinity.

Figure 5-2a illustrates how one slice can be cut out of the ABR structure, and used for dispersion relation study mentioned in the previous section. Figure 5-2b demonstrates the idea of array transduction, in which the transducer array has a different surface structure and pitch size than the reflector array. And this simulation geometry is built using the hierachical structure mentioned above, which is composed of an array of instances of unit cells. As previously discussed, such resonator design can be simply viewed as matching two types of waveguides. Since the geometries of
the unit cells are only slightly different, the dispersion curves are slightly offset from each other, and therefore, the reflection on the DT ABR boundary is comparatively weak and the evanescent tail into the DT ABR is very long. This comparatively weak reflector would help to enhance $Q$. It is notable that since array transduction fixes $k$ as well as $\omega$, the mode is cleaner, leading to larger $Q$ as well. To drive such transducer array, one scheme is to apply the same DC biases on all DTs, and apply positive and negative ac voltages alternatively over such arrays. In this way, the targeted wavelength will twice the length of the pitch size, making the driving wave number to be $k = 2\pi/(2L) = \pi/L$, which is the wave number for which the ABR structure becomes reflective.
Figure 5-3: (a) Schematics showing “index guiding” in a simple structure. The top layer has to have lower acoustic impedance than the substrate to form a guided mode. (b) Illustration of the resonator mode formed by $<110>$Si–polySi vs. the mode formed by $<100>$Si–polySi. The transducer array is marked in the middle.

**Low Impedance Guiding**

Figure 5-3 illustrates the idea of acoustic impedance selection for the materials inside the DT ABR layer. Analogous to optical wave guiding, it would require the top material to have lower acoustic impedance than the substrate for a confined guided mode to form (Figure 5-3a). For the DT ABR structure, this can be equivalently expressed as that the average acoustic impedance of the top layer should be smaller than that of the substrate. Take Si substrate for example, the acoustic impedance for longitudinal waves varies as a function of crystal orientation. If the filling material is chosen as polySi, the mode would only be high $Q$ in the $<110>$ direction, as illustrated in Figure 5-3b. This is because the longitudinal acoustic impedance lists in increasing order as $<100>$Si, polySi, and $<110>$Si. Only the $<110>$Si–polySi
combination meets the impedance requirement for "index guiding". Even though any two materials with impedance contrast can form an ABR for released resonators, this does not automatically translate to the design of solid state resonators. As shown in the bottom part of Figure 5-3b, once the impedance of the top material becomes larger than that of the substrate, the DT ABR structure no longer functions as a closed waveguide, and most of the energy leaks into the substrate, leading to a very low $Q$ mode.

**Maintaining Translational Symmetry**

Assuming to construct the array transduction mechanism, only the pitch size is slightly offset between the two waveguide eigenmodes. If such offset is small, the operating mode inside the transducer array would nearly be able to propagate inside the reflector array. Therefore, the reflector array functions like a "weak reflector", allowing large wave penetration depth (long evanescent tail) into the reflector, and consuming large footprint in order to reach high reflectivity. Weak reflector also means that there is little scattering at each reflection when the wave crosses an interface.

Even though we are targeting a longitudinal mode, due to the existence of top free surfaces, surface geometries and slightly slanted trench sidewalls (to facilitate trench fill process), the waves experience oblique incidence on the interfaces almost all the time. Every time at such oblique incidence, it splits out a tiny component of shear waves. Since the longitudinal mode operates inside the shear wave sound cone, these scattered shear wave components make it possible for this longitudinal mode to couple to the leaky shear modes close to it. This process reduces the $Q$ of the resonator. And the stronger such scattering is, the lower the $Q$.

Analogous to the operation of weak bandgap ABRs, weak reflectors have many challenges including footprint, and sensitivity to fabrication variations. In fact, the essence to reduce such wave scattering is not by forming weak reflectors, but by forming reflectors that are similar to transducers. Even when the difference between the two pitch sizes is relatively large (therefore being a strong reflector), this similarity can be achieved using a transition region that slowly varies the pitch size from the
transducer zone to the reflector zone [61]. One type of structure that has been used in optics for such purpose is the gradient indexing structure (GRIN) [58]. In order to reduce wave scattering, it requires the transition function to have smooth gradients [62]. For example, the following function is infinitely derivable, and the derivatives are 0 on both ends, which smoothly transits to the constant zone for both the transducer array and the reflector array.

\[ L_i = L_2 + (L_1 - L_2) \exp\left(-\frac{1}{(1 - \frac{r^2}{a^2})}\right)/\exp(-1) \]  

(5.4)

Figure 5-4a illustrates one design of DT resonator based on such GRIN transition idea. The GRIN function is plotted in 5-4b. The transition pitch sizes are sampled from such GRIN function, which is not a continuous function of space. As a result, there will still be scattering, but this effect will reduce as more layers are used for the GRIN region.

The intuitive explanation of why such GRIN structure would help to reduce wave scattering and enhance \( Q \) is because it helps to maintain the translational symmetry of the structure as much as possible. From the perspective of symmetry analysis, scattering is introduced whenever such translational symmetry is broken [62].

It is worth noting that how dramatically the mindset has changed for the design of solid state resonators. In Chapter 4, the DT ABR is simply treated as a reflective
boundary condition that is similar to a free boundary, and the design goal is to find the correct cavity size that matches such boundary condition—the resonator and the reflector are treated separately. While in this section, after introducing array transduction, and GRIN structure for maintaining translational symmetry, the hard boundaries between the resonator and its reflectors are removed. There is no need to clarify which is the resonator and which is the reflector. The essence of the mode design for the solid state resonator is to maintain translational symmetry as much as possible, and localized the mode in the guiding layer.

5.3 Dual Trench Solid State DT Resonator

The structure of solid state DT resonator from Chapter 4 has unit cell of only one DT. This single DT is used as both an electrical capacitor and a mechanical structure at the same time, making it an elegant design that reduces footprint and fabrication complexity. On the other hand, it also adds limitations to the device capabilities. For example, the bandgap size is tiny due to the small acoustic impedance mismatch between $Si$ and poly$Si$. This bandgap can be tuned smaller by varying the pitch size, but it cannot be made bigger using the same material set.

However, the bandgap can be increased if we were to use a different filling material. But since the filling material needs to be conductive for capacitor purpose, it cannot be materials such as dielectrics. Metal fill could be an option, but the internal loss of most metals are very large and would reduce the $Q$ of the mechanical mode, and plus, depositing metal uniformly on the sidewall and fill the trenches could be a challenge in terms of fabrication [63] [64]. Such limits of trench filling materials make the bandgap uncontrollable, making the devices susceptible to the disadvantages of weak bandgap structures as mentioned at the beginning of the chapter.

One intuitive solution is to use different types of trenches for the transducer DTs and reflector DTs, as shown in Figure 5-5a. The transducer array is made of poly$Si$ filled DTs, making it able to function as capacitors, and the reflector DTs are made of $SiO_2$ filled DTs, forming a large bandgap structure. However, simulation shows such
Figure 5-5: (a) Structure using polySi filled trenches to drive and sense, and using SiO₂ filled trenches to form reflectors. (b) Structure using a mixed trench layout, in which both polySi filled trenches and SiO₂ filled trenches are distributed in the transducer zone and reflector zones.

structure can not provide $Q$ beyond 100. The reason is the translational symmetry is broken, and the wave gets scattered into the substrate direction badly after hitting the oxide DT ABR boundary.

The correct design based on such idea of mixed trenches is shown in Figure 5-5b. Even though the polySi now distributes everywhere, still only the center portion is used for transduction. This new design maintains translational symmetry, and is therefore able to provide much higher $Q$. Comparing with Figure 5-4a, it can be seen that the array pattern is the same, and the difference lies in the structure of the unit cell.

Figure 5-6a shows the structure of the unit cell. Now the unit cell consists of two DTs, instead of one. The first DT (DT 1) is filled with polySi after dielectric deposition, and it can function as an electrical capacitor, while the second DT (DT 2)
Figure 5-6: (a) Unit cell of the dual trench resonator. DT 1 acts as the electrical component, and DT 2 functions to modulate the bandgap size. DT 2 is fully filled with $SiO_2$. (b) Unit cell of the dual trench resonator in which DT 2 is only partially filled with $SiO_2$, and the remaining gap is filled with polySi in the same polySi deposition step that fills DT 1.

is filled with $SiO_2$, and its purpose is to modulate the bandgap size of the mechanical structure formed by an array of such dual DTs. Due to such characteristics of the unit cell, the solid state DT based resonator built with such cell is named as the “Dual Trench” DT MEMS resonator.

And note that DT 2 does not necessarily have to be fully filled with $SiO_2$, the oxide deposition can only cover a certain thickness, leaving the remaining gap to be filled by polySi during the step of polySi deposition that fills all the trenches. Due to such flexibility, and since the thickness of the deposited $SiO_2$ layer can be controlled during device fabrication, such dual trench unit cell has the capability to make the bandgap size tunable. This tunability is based on staying with the same material set ($Si$, polySi and $SiO_2$), since switching to different material sets may cause fabrication challenges such as trench fill difficulty.

In summary of the design parameters, there are 3 parameters that primarily affect the bandgap size and position: pitch $L$, trench width $w_{DT}$, and deposited oxide thickness $t_{ox}$. Among these 3 parameters, the trench width $w_{DT}$ is fixed due to
fabrication constraint on the trench fill step, but the pitch size $L$ is used to position the center frequency of the bandgap, and oxide thickness $t_{ox}$ can be used to tune the width of the bandgap.

5.4 Fabrication Process

The fabrication process for dual trench DT MEMS resonator has a few more steps than the simple DT resonator from Chapter 4. Whether the oxide filled trenches are fully filled or partially filled does not affect the process flow. The dual trench DT resonator process are illustrated in Figure 5-7 (fully filled) and Figure 5-8 (partially filled).

In descriptive words, the fabrication process is as the following:

- 1 $\mu m$ PECVD $SiO_2$ is deposited onto the fresh low resistivity bulk n type $Si$ wafer. Afterwards, such PECVD oxide is patterned to form 0.8 $\mu m$ wide DT arrays using stepper photo-lithography. With such hard mask, the 8 $\mu m$ deep trenches are etched with the etch recipe described in Section 4.3.2.

- The hard oxide mask is re-patterned into field oxide layer I (FOX I) to reduce capacitance from the subsequent electrical paths. It is patterned through photore sist mask and wet 7:1 buffered HF (BHF) etch. This mask is also used as the ion implantation mask afterwards.

- The Si wafer is ion implanted with phosphorous twice, each at tilt angle of 8°. These tilt avoids the channeling effect, and achieves implantation on the trench sidewall as well.

- After growing CVD oxide, it is pattered into the alternating geometry through photo-lithography and wet etch in BHF. The oxide deposition can either fully fill the trench if possible, or just partially fill the trenches.

- After RCA clean, the trenches are lined with 10 $nm$ $SiO_2$ and filled with n-type doped poly$Si$. The poly$Si$ grows uniformly on top surfaces and sidewalls,
Figure 5-7: Fabrication process flow for dual trench DT MEMS resonator. (a) DTs are etched into Si substrate using oxide hard mask. (b) Oxide hard mask is patterned into a window for ion implantation into the substrate. (c) After ion implantation, oxide is deposited uniformly and patterned by wet etch. (d) After depositing thin dielectric layer, n type polySi is deposited and patterned to fill inside the remaining DTs. (e) Field oxide layer is deposited on top of such structure for electrical isolation and acoustic confinement. (f) Electrical contact holes are etched through field oxide. (g) Ti–Al metallization stack is deposited and patterned.
Figure 5-8: Fabrication process flow for partially filled dual trench DT MEMS resonator. (a) DTs are etched into Si substrate using oxide hard mask. (b) Oxide hard mask is patterned into a window for ion implantation into the substrate. (c) After ion implantation, oxide is deposited uniformly. This partially filled oxide is covered by photoresist and patterned into the alternating geometry. (d) After depositing thin dielectric layer, n type polySi is deposited and patterned to fill inside the remaining DTs. (e) Field oxide layer is deposited on top of such structure for electrical isolation and acoustic confinement. (f) Electrical contact holes are etched through field oxide. (g) Ti-Al metallization stack is deposited and patterned.

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Table 5.1: Design Parameter Values for the Dual Trench DT Resonator

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frequency (f)</td>
<td>1.3 GHz</td>
</tr>
<tr>
<td>Trench depth (hDT)</td>
<td>8 μm</td>
</tr>
<tr>
<td>Trench width (WDT)</td>
<td>0.8 μm</td>
</tr>
<tr>
<td>Device width (w)</td>
<td>60 μm, 100 μm</td>
</tr>
<tr>
<td>FOX 1 thickness (tFOX1)</td>
<td>0.6 μm</td>
</tr>
<tr>
<td>FOX 2 thickness (tFOX2)</td>
<td>0.5 μm</td>
</tr>
<tr>
<td>Dielectric thickness (tdiel)</td>
<td>10 nm</td>
</tr>
<tr>
<td>polySi thickness (tpoly)</td>
<td>0.8 μm</td>
</tr>
<tr>
<td>Ti thickness (tTi)</td>
<td>0.1 μm</td>
</tr>
<tr>
<td>Al thickness (tAl)</td>
<td>1 μm</td>
</tr>
<tr>
<td>Fill SiO2 thickness (tOX)</td>
<td>0.15 μm</td>
</tr>
<tr>
<td>Transducer DT pitch (Ltrans)</td>
<td>3.4 μm</td>
</tr>
<tr>
<td>Reflector DT pitch (Lref)</td>
<td>variable, e.g. 3.8 μm</td>
</tr>
</tbody>
</table>

filling all the trenches, including the ones that are partially filled with SiO2 if the oxide DTs are indeed partially filled. Such polySi is lined with a thin layer of Al to reduce RC delay, and these layers are subsequently patterned into electrical paths for the top electrode of the DT capacitor. This same step also opens the contact area for substrate grounding.

- The solid state structure is capped with 500 nm field oxide II (FOX II) to reduce scattering of elastic wave from the top free surface, and to isolate the electrical signal between metal layers.

- The FOX II is patterned for metal contact to the transducer DTs and substrate.

- Finally, a Ti/Al metal layer is sputtered, patterned by Cl2/BCl3 RIE, and sintered at 450°C in H2/N2 gases.

Table 5.1 lists the key parameter values for the dual trench DT resonator.

5.5 Numerical Simulations

5.5.1 Reflectivity of Dual Trench ABR

As discussed in Section 5.3, the unit cell of the dual trench DT resonator consists of two DTs, with one DT used for electrical transduction, and the other DT used
Figure 5-9: Absolute values of reflectivity as a function of frequency, for various cell numbers, for (a) 0.1 µm thick oxide, (b) 0.15 µm thick oxide, (c) 0.25 µm thick oxide, and (d) fully filled oxide. (e) Extracted peak reflectivity vs. number of cells. (f) Extracted peak frequency vs. number of cells.
to modulate the mechanical bandgap size. Using the numerical method developed in Section 2.3, the reflectivity of such dual DT structure can be extracted using MATLAB, as shown in Figure 5-9. Figure 5-9a–d shows the reflectivity for oxide thickness of 0.1 \( \mu m \), 0.15 \( \mu m \), 0.25 \( \mu m \) and fully filled respectively. In each of these plots, it displays the absolute reflectivity as a function of frequency, for 5 cells, 10 cells, and 30 cells respectively. As observed from these figures, the bandgap size (length of the segment where the reflectivity is close to 1) increases as the deposited oxide thickness increases, with the maximum bandgap ratio being around 30% when the trench is fully filled with SiO\(_2\). By adjusting the oxide thickness, this bandgap size can only be tuned smaller, not bigger. But since 30% is already a big bandgap ratio, this provides enough range for bandgap tuning.

One interesting fact to notice is that the high reflectivity band shifts in frequency as the number of cells increases. Such peak reflectivity and center frequencies can be extracted as well, plotted in Figure 5-9c, d. As seen from such figures, the bandgap center frequency gets stable when the number of cells increases beyond 10. And in consistent with results from previous chapters, wider bandgap would cause the reflectivity to converge to 1 faster.

5.5.2 Dispersion Relations

The dispersion analysis method introduced in Section 5.2.1 can be used to analyze the dual trench unit cell as well. Figure 5-10 and 5-11 show the results from such analysis. Figure 5-10 is the dispersion relation study based on the fully filled dual trench unit cell, while Figure 5-11 is the dispersion relation study based on the partially filled dual trench unit cell in which the SiO\(_2\) thickness on the trench sidewall is 0.15 \( \mu m \).

Unlike Figure 5-1, here dispersion curves from two structures are overlaid in one plot for comparison. Take Figure 5-10 as an example, the unit cell geometry used in COMSOL simulation is shown in the inset of Figure 5-10a. To represent the inherent mirror symmetry in this unit cell, the bandgap tuning trench is cut in half, leaving one half on each side. This does not affect the analysis result since the Bloch boundary condition is applied. In this particular example, the trench used for bandgap tuning
Figure 5-10: (a) $k - \omega$ dispersion curves for the dual trench DT unit cell, in which the $k$ axis is normalized to $k_0 = \pi / L$ and the frequency axis has unit GHz. The inset on top-left shows the geometry used in COMSOL simulation to generate such curves. Bloch boundary conditions are applied between the left boundary and the right boundary, and the bottom $Si$ is set 10 times the thickness of the top DT ABR layer (not shown in the inset). Blue and red dots are the engenmodes, the yellow zone marks the area between the shear wave sound cone and the longitudinal wave sound cone, and the green zone marks the longitudinal wave sound cone. (b) The waveguide engenmodes at $k = \pi / L$. The modes map to the numbers marked in the dispersion curves in (a). The first 2 are shear dominant modes, and the remaining 2 are bulk longitudinal modes. Mode (4) is the target for resonator design.
Figure 5-11: (a) $k - \omega$ dispersion curves for the partially filled dual trench DT unit cell, in which the $k$ axis is normalized to $k_0 = \pi / L$ and the frequency axis has unit GHz. The inset on top-left shows the geometry used in COMSOL simulation to generate such curves. The oxide thickness is 0.15 $\mu$m on the trench sidewall. Bloch boundary conditions are applied between the left boundary and the right boundary, and the bottom $Si$ is set 10 times the thickness of the top DT ABR layer (not shown in the inset). Blue and red dots are the engenmodes, the yellow zone marks the area between the shear wave sound cone and the longitudinal wave sound cone, and the green zone marks the longitudinal wave sound cone. (b) The waveguide engenmodes at $k = \pi / L$. The modes map to the numbers marked in the dispersion curves in (a). The first 2 are shear dominant modes, and the remaining 2 are bulk longitudinal modes. Mode (4) is the target for resonator design.
is fully filled with $SiO_2$. The pitch size is the only study variable, while all the other parameters including trench width, depth, thickness of each materials etc., are kept as constants.

In the dispersion plot Figure 5-10, the red dots are from pitch size of 3.5 $\mu m$, and the blue dots are from pitch size of 3.58 $\mu m$. The $k_0$ used to normalize both sets of curves is chosen to be $k_0 = \pi/(3.5 \ \mu m)$. As a result, to put both plots on the same scale of $k$, the dispersion curves for pitch size of 3.58 $\mu m$ will only reach $k_{norm} = 3.5/3.58 = 0.98$ (blue dashed line in Figure 5-10a) after $k$ scaling, and the curves beyond that are just symmetric mirror image. The shear and longitudinal sound cones are similar as what is described for Figure 5-1. And selected eigen modes are plotted in Figure 5-10b, with the first 2 being shear dominant modes, and the remaining 2 being longitudinal dominant modes. From the displacement rainbow plot on the left and the energy heat plot on the right, it is obvious that mode (4) has the cleanest longitudinal mode, and it is therefore the mode the design is targeting at.

From overlaying the two sets of dispersion curves, we can see how the modes shift after perturbing the pitch size. If, for example, the pitch size of the transducer DTs is 3.5 $\mu m$, and the pitch size of the reflector DTs is 3.58 $\mu m$, the wave will be able to propagate when operating on the red curves, but this same mode will be evanescent after reaching the reflector since it is not on the blue curves. Even if we use array transduction to operate at $k/k_0 = 1$, since the array size can never be infinite, the $k$ will always span a certain width around the targeted value. Therefore, to construct high $Q$ resonators, such modes should be as far away from the sound cone as possible, and the two modes should be separated as far as possible at both the targeted $k$ value and its vicinity. For example, mode (4) of both pitch sizes are well separated over the entire plotted range of $k$, and the mode is almost pure longitudinal, which couples perfectly to the driving forces. The disadvantage is that it operates closer to the sound cone than the other modes, but this sound cone coupling effect can be reduced by using larger transduction arrays (which leads to purer $k$ value).

Figure 5-11 can be analyzed in a similar way. It plots pitch size of 3.4 $\mu m$ against 3.5 $\mu m$. Here since the longitudinal bandgap is smaller (as shown in the comparison
in Figure 5-9), mode (3) and mode (4) are closer to each other (the separation of these two branches can be viewed as the bandgap in such context). But still if we make the transducer DTs at pitch size 3.4 μm, and reflector DTs at pitch size 3.5 μm, the mode will again be able to propagate on one waveguide but isolated on the other, forming an solid state resonator under array transduction.

5.5.3 Resonator Eigenmodes and Q Enhancement Approaches

Resonator Eigenmodes

As discussed in Section 5.2.2, to study the full frequency response of the entire structure and extract resonator properties such as the Q, the fully model has to be built in COMSOL. Apart from the techniques mentioned in Section 5.2.2, a MATLAB optimizer was built controlling the COMSOL finite element solver at each iteration to find the optimal solution that generates the best Q. For example, the best design variables searched by this optimizing program can be chosen as just the transducer array pitch size (L_{trans}) and the reflector array pitch size (L_{ref}), while all the other parameters can be kept at constants.

This same numerical simulation procedure can be applied on both types of dual trench DT resonator structures, with the bandgap tuning trench fully filled, or partially filled. The optimized frequency response results are shown in Figure 5-12. Figure 5-12a shows the schematic of the structure, in which the bandgap tuning trench is fully filled. As introduced previously, the structure is based on matching two dual trench DT waveguides with different pitch sizes, using GRIN as the transition region to keep better translational symmetry. The transducer array is divided into 3 segments, in which the 1st and the 3rd segments are used as driving arrays, and the 2nd segment is used as the sensing array. This setting is depicted in Figure 5-12b, with the function of each region marked on top of the simulation geometry schematic. In each driving array, it is driven with positive voltage and negative voltage alternatively, similarly, the sensing array is also sensed in such differential way. This differential driving/sensing mechanism is able to drive the structure efficiently, while reducing the
Figure 5-12: Comparison of the optimized eigenmodes from fully filled and partially filled dual trench DT resonators. (a) 3D Schematic of a fully filled dual trench DT resonator structure. (b) Geometry used in COMSOL Simulation to extract resonance modeshape. (c) Modeshapes from both structures, with red and blue being peak and trough of the wave pattern of the $\sigma_{xx}$ distribution. (d) Comparison of frequency response of both structures. The dots are data points from simulation, and the curves are data fitting results using rational functions.
electrical feedthrough floor. The simulated modeshapes for both types of structures are shown in Figure 5-12c, and the corresponding frequency responses are plotted in Figure 5-12d.

Based on these simulations results, it can be concluded that partially filled dual trench structures are able to provide almost twice as better signal level and Q. This result can be explained by the weaker bandgap of the partially filled dual trench structure. As discussed in Section 5.2.2, weak bandgap helps reduce scattering and enhance Q, and this comparison exactly demonstrates this design rule. And note that from results in Figure 5-9, even this “weak bandgap” would have bandgap ratio of around 11%, which is far bigger than the 2% bandgap formed by Si-polySi. As a result, this medium-ranged bandgap would have the Q-enhancement advantage of weak bandgap structures, but not suffer from the bandgap narrow-down effect caused by non-periodic defects. All of these are thanks to the bandgap tuning capability of this particular dual trench framework.

Further Q Enhancement Approaches

The quality factor Q of the dual trench solid state DT resonator can be enhanced by using the GRIN structure, and longer transduction arrays.

The effect of the GRIN structure is to gradually transit the pitch size from the transducer pitch size to the reflector pitch size. This gradual transition reduces waves scattering at each reflection, and therefore improves Q. Figure 5-13 shows one example of the comparison between structures with or without GRINS. The base structure is chosen as dual trench DT structure in which the oxide trenches are fully filled. As seen from the frequency response curves in Figure 5-13c, after introducing GRINS, the Q is increased to almost twice as large. Each curve is obtained from running the optimization algorithm on the corresponding structure, so it is a valid comparison that is based on equal footing. The modeshapes for both structures are shown in Figure 5-13a,b. From the modeshapes, it can be observed that abrupt transition of pitch size leads to more scattering into the substrate direction, which is represented by the heavier evanescent tail in the substrate Si (Figure 5-13b, bottom).
Figure 5-13: Study of the effect of GRINs on Q improvement. (a) The eigenmode at resonance for the dual trench DT resonator without GRINs. The plot on top shows the full structure, and the plot at the bottom shows the view that zooms in on the transducer array only. (b) The eigenmode at resonance for the dual trench DT resonator with GRINs. The plot on top shows the full view, and the plot at the bottom zooms in on the transducer array. (c) The frequency response curves from both structures. The dots are actual data points from simulation, and the curves are from data fitting. The pitch sizes, resonator frequencies and Q’s are listed in the figure.
As mentioned in Section 5.2.2, using longer transduction arrays can better localize the distribution of exited wave numbers in the $k$ space, keeping the excited modes away from the lossy sound cone, and therefore improving $Q$. This effect is deduced from analyzing the dispersion plot, and it can be further verified by running simulation on the full structure. Figure 5-14 shows such comparison of transducer array size of 24, 60 and 90, based on dual trench structure in which the oxide DTs are fully filled. Again, each curve is the best result from each geometry, obtained from running the optimization algorithm. From such result, it can be observed that longer array helps to improve $Q$.

5.5.4 Process Variation Study

As discussed at the beginning of this chapter, the solid state resonator design based on weak bandgap structures is susceptible to fabrication variations. Take one example of
the imperfect surface structure, shown in Figure 4-11, the existence of non-periodic surface defects can cause scattering and distort the modeshape. Since the designs in Chapter 4 are based on matching the cavity size to the reflector bandgap, such fabrication variations will shift the bandgap and cause the design match to fail. The common solution is to include a lot of over-designs in the layout, in order to hit a match even after the bandgap shifts. This method wastes layout area, and could still fail when unforeseen defects happen.

On the other hand, the array transduction design methodology developed in this chapter will be more robust against such process variations. Assuming the process condition is uniform across the DTs in one device, the defects will depend on the designed geometry. Since the designed geometry preserves translational symmetry as much as possible, including all the details on the surface layers, any defects, if they exist at all, would have the same type of translational symmetry as well. The benefit of such periodic defects is that the transducer waveguide mode and the reflector waveguide mode will be shifted together, leaving the gap between these two modes almost unperturbed.

In comparison with Figure 5-10, which is the version of fully filled oxide DT without any defects, the dispersion curves after introducing defects are shown in Figure 5-15 and 5-16. Assuming the design is based on two waveguides that are of slightly different pitch sizes, the goal of mode design is to have a tiny offset between the two mode branches. As seen from such figures, existence of voids would result in a large shift of the dispersion curves, especially for the bulk modes. However, since such voids have the same spacial distribution as the DTs, the dispersion curves of both pitch sizes will be shifted together, and the amount of mode offset will almost be preserved.

As a result, even with the existence of defects, the exact same layout would still be able to generate working devices, as long as the mode still exist outside of the sound cone. This robustness against process variations would make the layout design easier, meaning it does not require a lot of over-designs to compensate various foreseeable or unforeseeable process variations—the devices can automatically adjust to such
Figure 5-15: (a) $k - \omega$ dispersion curves for the dual trench DT unit cell with void inside the trench filled with polySi, in which the $k$ axis is normalized to $k_0 = \pi/L$ and the frequency axis has unit GHz. The inset on top-left shows the geometry used in COMSOL simulation to generate such curves. Bloch boundary conditions are applied between the left boundary and the right boundary, and the bottom Si is set 10 times the thickness of the top DT ABR layer (not shown in the inset). Blue and red dots are the engenmodes, the yellow zone marks the area between the shear wave sound cone and the longitudinal wave sound cone, and the green zone marks the longitudinal wave sound cone. (b) The waveguide engenmodes at $k = \pi/L$. The modes map to the numbers marked in the dispersion curves in (a). The first 2 are shear dominant modes, and the remaining 2 are bulk longitudinal modes. Mode (4) is the target for resonator design.
Figure 5-16: (a) $k - \omega$ dispersion curves for the dual trench DT unit cell with void inside the trench filled with oxide, in which the $k$ axis is normalized to $k_0 = \pi / L$ and the frequency axis has unit GHz. The inset on top-left shows the geometry used in COMSOL simulation to generate such curves. Bloch boundary conditions are applied between the left boundary and the right boundary, and the bottom Si is set 10 times the thickness of the top DT ABR layer (not shown in the inset). Blue and red dots are the engenmodes, the yellow zone marks the area between the shear wave sound cone and the longitudinal wave sound cone, and the green zone marks the longitudinal wave sound cone. (b) The waveguide engenmodes at $k = \pi / L$. The modes map to the numbers marked in the dispersion curves in (a). The first 2 are shear dominant modes, and the remaining 2 are bulk longitudinal modes. Mode (4) is the target for resonator design.
Figure 5-17: (a) COMSOL simulated modeshape of the dual trench DT resonator with voids inside the polySi DT. The plotted wave pattern is $\sigma_{xx}$. (b) COMSOL simulated modeshape of the dual trench DT resonator with voids inside the $SiO_2$ DT. The plotted wave pattern is $\sigma_{xx}$. (c) Frequency response curves from both structures, plotted against the response of the structure with no voids at all. The resonance frequencies and $Q$'s are marked in the figure.
variations to some extent.

And of course the condition for such auto-adjustment to happen is that the mode still exists out of the sound cone. For example, since we are targeting mode (4), in the defect case in Figure 5-15, where the void is in the polySi filled DT, such mode almost disappears. While in Figure 5-16, where the void is in the SiO$_2$ filled DT, such mode still exists, and the device would still work with such defects, under the same layout dimensions.

From the energy heat plot of mode (4), it can be observed that the rule for a defect robust mode is that the defect should not locate at the spot where the energy is concentrated. Placing a defect on a high energy density spot would eliminate such a mode, while placing a defect on a low energy density spot would not cause much perturbation. For example, it can be observed from Figure 5-10, that the acoustic energy is concentrated in the top section of the polySi DT in mode (4). As a result, adding a void in polySi would introduce a lot of disturbance to such mode and push it outside of the sound cone. However, adding a void in SiO$_2$ almost causes no effect to the mode shape at all, as seen in Figure 5-16b, Mode (4) still is a pure longitudinal mode even with the voids.

Such process variation conjectures based on the study of dispersion relations can be verified through the frequency sweep on the complete resonator structure. Figure 5-17 shows such results. As seen from the figures, in consistency with the dispersion mode shape study, the oxide-voided structure shows uniform modeshape. Its $Q$ is reduced compared with the none-voided structure, but the mode still exists under exactly the same layout dimensions. However, the polySi-voided structure would not have the same modeshape anymore, since the mode is scattered by the voids placed exactly on the spots where the energy is supposed to concentrate. And its frequency response also gives $Q$ below 100.
5.6 Conclusions

To address the issues from weak bandgap reflectors used in DT resonators, this chapter discusses the methodology to design and analyze DT based solid state MEMS resonator.

The new perspective of designing DT based resonator is based on concatenating slightly mismatched waveguides. The transducer array and the reflector array share almost the same geometry of the unit cell, except the pitch sizes being different. Such array transduction is able to provide precise control of the driven wave number $k$, fixing the driven mode outside of the sound cone and making it high $Q$. The transduction array is also driven differentially to reduce electrical feed-through.

The key to achieve high $Q$ for such design is to maintain translational symmetry as much as possible. Therefore, GRIN structure is used to gradually transit the pitch size from the transducer array to the reflector array.

To harness the benefits weak bandgap design, the structure should have the capability of bandgap tuning during device fabrication. An ideal bandgap for DT based solid state resonators has a small enough size to provide low reflectivity and trap the waves, yet not too small to get affect by process variations and cause cavity matching problems. The dual trench DT based resonator is developed under this context. Such dual trench unit cell is able to maintain electrostatic transduction capability, yet providing tunable bandgap size during design. Through partially filling one trench with oxide, the bandgap can be tuned to just the right size to support a high $Q$ mode, and at the same time not being too small to get eliminated from process variations.

Such array based dual trench DT solid state resonator design is also able to be relatively robust against unexpected process variations. Periodic defects, such as voids inside the DT, or surface scattering voids generated from material deposition, will be well handled by such design. The reason is that such defects will shift the waveguide modes in both the transducer region and the reflector region together, and in the end preserving the resonance mode. The resonance frequency would still be shifted after the introduction of periodic defects, but the significance lies in that no over-design
is necessary during the layout design stage to protect against such variations. This saves layout space, and increase the yield of such type of devices.
Chapter 6

Conclusions and Future Directions

6.1 Conclusions

This thesis discussed the theoretical analysis, design rules, and performance of solid state RF MEMS resonators, and covered several types of such solid state resonator designs.

The unreleased RBT in IBM’s 32 nm CMOS process demonstrated the capability of CMOS integration for such solid state resonators. Such devices provide resonance frequencies above 11 GHz, Q’s of 24 – 30, footprint of less than 5 \( \mu \text{m} \times 3 \mu \text{m} \) and TCF of less than \( \pm 5 \text{ ppm/K} \). They are directly integrated at the FEOL in CMOS without any necessities for post-processing or MEMS packaging. The disadvantage of such design resides in the small aspect ratio. For the target of such 1D ABR longitudinal mode, structure aspect ratio is the key of improving \( Q \), the limited thickness at the transistor level restricts \( Q \) enhancement of such ABR reflector approach.

To find CMOS compatible approaches to enhance \( Q \), deep trench (DT) structures that are used to function for DRAMs are reinvented to be used as mechanical structures. Such DTs can be laid into an array, functioning both as electrical transducers and mechanical reflectors at the same time. Such simple design provides DT based solid state resonator that generates \( Q \) above 1000, and \( R_X \) at \( k\Omega \) level. The significance of such type of devices is beyond the original motivation of CMOS integration. These solid state resonators with lithographically defined frequency provides a simple
solution that requires no complex release etch processing, or hermetic seal packaging, yet it is able to provide comparable $Q$ to released resonators. And since the ABR only supports the targeted mode, these devices have much better properties of spurious mode suppression compared with released resonators.

The key of achieving high $Q$ for the design of such type of solid state resonators is using reflectors with weak bandgap to trap the mode inside reflector region. However, the bandgap created by DT structure material set is too weak, so that it requires a lot of over-design during layout design, and the signal can be easily affected by process variations. To further enhance $Q$, and provide a design that is robust against process variations, the dual trench DT solid state MEMS resonator is proposed. This type of DT based resonator relies on array transduction and GRIN transition region for better waveguide mode matching. Since the translational symmetry is only slightly perturbed over the entire structure, the wave scattering is reduced, leading to high $Q$ result. Because of the preservation of translational symmetry, the device is less likely to be affected by process variations that create periodic defects. These dual trench structure has the capability to tune the bandgap size by controlling the film thickness during fabrication process. This makes it possible to generate the weak bandgap of the “just right” bandgap size, achieving $Q$ enhancement and process robustness at the same time.

6.2 Future Directions

6.2.1 Mechanically Coupled Solid State MEMS Resonators

One drawback of electrostatically transduced resonators is the large $R_X$ compared with piezoelectric devices. To reduce $R_X$ and increase signal level, there have been methods of creating an array of mechanically coupled resonators [65]. These mechanically coupled resonators have also been implemented for piezoelectric devices to create band-pass filters [66].

The same mechanically coupled concept can be used for solid state MEMS res-
Figure 6-1: (a) Schematic of solid state DT based MEMS resonator using 5 mechanically coupled cavities. The center cavity is perturbed in size to generate mode localization effect and enhance $Q$. (b) Mode shape comparison between single cavity and 5 cavities, showing that mechanically coupled solid state resonator with mode localization is able to improve $Q$ and reduce $R_X$.

onator as well to reduce $R_X$, or to create a pass band for filter applications. If the cavities are coupled side-by-side, it just effectively increases the device width, so a more interesting study is to couple the mechanical cavities in the direction of the modeshape. Figure 6-1a illustrates one example of such design. The 5 mechanically coupled cavities are separated by ABR couplers, and adjusting the number of layers in such couplers will be able to tune the coupling strength.

There has been work on artificially creating asymmetries between mechanically coupled resonators, to localized the mode shape in one cavity, and thereby enhancing the $Q$ of the total structure [67]. Such concept can be applied to mechanically
coupled solid state resonators to further improve $Q$. Figure 6-1b shows that by using mechanically coupled cavities, and mode localization from asymmetric geometry (the center cavity is slightly larger in size), the performance can be boosted in both $Q$ and $R_X$.

Mechanically coupled solid state MEMS resonators is an interesting direction to explore, both theoretically and experimentally.

6.2.2 Solid State MEMS Resonators Based on Piezoelectric Materials

Another approach of reducing $R_X$ for such devices is the route of using a different set of materials, based on the same structure framework and design method. For example, instead of depositing a thin layer of dielectric material before the polySi deposition, it could be the deposition of piezoelectric material such as AlN. And the polySi can also be replaced with any other conductive material that can perfectly fill such trenches. Figure 6-2 shows such concept by plotting the structure of one unit cell.

![Concept of creating piezoelectric material based DT structure.](image)

This design would create the same type of in-plane ABR structure, so all the design methods used for electrostatic solid state resonator are still valid. In addition,
since piezoelectric material is used for transduction, the transduction efficiency $k_i^2$ and motional impedance $R_X$ can be greatly improved. With the introduction of piezoelectric material, the structure still has benefits of release-free fabrication, and simple package at the system level, and the device metrics can also be greatly improved. But since the materials are not standard CMOS materials, this design cannot be directly integrated with standard CMOS technology. However, there are alternative circuit fabrication platforms that contain piezoelectric material, such as GaN technology for power electronics [68]. These platforms could be potential candidates for such integration.

The challenge to implement such idea lies in micro-fabrication. Effort needs to be made to deposit piezoelectric materials onto the narrow trench sidewalls, and fill the remaining trench with metal or polySi void free. Metal trench fill has been a matured technology in CMOS, and there have been technologies of depositing piezoelectric material such AlN onto the sidewall [69]. However, process still needs to be developed to create uniform deposition of piezoelectric material onto the high aspect-ratio trench side wall.
Appendix A

Fundamentals of Elasticity and Acoustic Waves

A.1 Notation

Here lists the common notations used in this chapter.

<table>
<thead>
<tr>
<th>Notation</th>
<th>Meaning</th>
</tr>
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<tbody>
<tr>
<td>$t$</td>
<td>Time</td>
</tr>
<tr>
<td>$\hat{n}$</td>
<td>Unit normal vector at the surface</td>
</tr>
<tr>
<td>$x$</td>
<td>Cartesian coordinate of each material point after displacement</td>
</tr>
<tr>
<td>$X$</td>
<td>Cartesian coordinate of each material point at relaxed state</td>
</tr>
<tr>
<td>$u$</td>
<td>Displacement vector at each material point</td>
</tr>
<tr>
<td>$v$</td>
<td>Velocity vector at each material point</td>
</tr>
<tr>
<td>$\omega$</td>
<td>Angular velocity axial vector</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>Strain tensor</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Stress tensor</td>
</tr>
<tr>
<td>$C$</td>
<td>Elastic stiffness tensor</td>
</tr>
<tr>
<td>Notation</td>
<td>Meaning</td>
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<tr>
<td>----------</td>
<td>---------</td>
</tr>
<tr>
<td>$S$</td>
<td>Elastic compliance tensor</td>
</tr>
<tr>
<td>$H$</td>
<td>Elastic loss tensor</td>
</tr>
<tr>
<td>$S$</td>
<td>Strain vector in Voigt notation</td>
</tr>
<tr>
<td>$T$</td>
<td>Stress vector in Voigt notation</td>
</tr>
<tr>
<td>$c$</td>
<td>Stiffness matrix in Voigt notation</td>
</tr>
<tr>
<td>$s$</td>
<td>Compliance matrix in Voigt notation</td>
</tr>
<tr>
<td>$\eta$</td>
<td>Loss matrix in Voigt notation</td>
</tr>
<tr>
<td>$\sigma_{ij}$</td>
<td>Stress tensor component in the direction of $i$, of the force vector on the surface $j$</td>
</tr>
<tr>
<td>$a$</td>
<td>Orthogonal transformation matrix</td>
</tr>
<tr>
<td>$M$</td>
<td>Transformation matrix for Voigt stiffness matrix</td>
</tr>
<tr>
<td>$N$</td>
<td>Transformation matrix for Voigt compliance matrix</td>
</tr>
<tr>
<td>$\lambda, \mu$</td>
<td>Lamé constants</td>
</tr>
<tr>
<td>$E$</td>
<td>Young’s modulus</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Poisson’s ratio</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density of material</td>
</tr>
<tr>
<td>$b$</td>
<td>Body force</td>
</tr>
<tr>
<td>$\ddot{u}$</td>
<td>Second time derivative of displacement</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>Christoffel matrix</td>
</tr>
<tr>
<td>$c$</td>
<td>Wave speed</td>
</tr>
<tr>
<td>$k$</td>
<td>Wave number vector</td>
</tr>
<tr>
<td>$A$</td>
<td>Polarization vector for elastic waves</td>
</tr>
<tr>
<td>$Z$</td>
<td>Acoustic impedance</td>
</tr>
<tr>
<td>$R$</td>
<td>Reflectivity</td>
</tr>
<tr>
<td>$T$</td>
<td>Transmitivity</td>
</tr>
<tr>
<td>$\nabla$</td>
<td>Gradient operator</td>
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Table A.1 – Continued from previous page

<table>
<thead>
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<th>Notation</th>
<th>Meaning</th>
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<tbody>
<tr>
<td>(\nabla)</td>
<td>Divergence operator</td>
</tr>
<tr>
<td>(\nabla_s)</td>
<td>Symmetric gradient operator</td>
</tr>
<tr>
<td>(\Delta)</td>
<td>Laplace operator</td>
</tr>
<tr>
<td>(\otimes)</td>
<td>Tensor product operator</td>
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A.2 Basic Linear Elasticity

A.2.1 Strain and Stress

Strain Definition

Below elastic limit, solid materials will return to their original state after deformation. This macroscopic behavior, taking metal as an example, can be explained as atomic lattice restoring to the original low energy state after deformation. Under small deformation assumption, such deformation can be linearized. The intuitive definition of strain in the uniaxial case is the ratio of deformation over initial length. However, for a 3D deformation, this needs to be defined more carefully. To characterize a deformation process, we need to first adopt the configuration of the body as a reference. This is typically taken at the unstressed state, relative to a chosen origin \(o\).

At initial non-strained state, each material point in a solid body is referred by its coordinate \(X\). After deformation over the course of time, its spacial coordinate \(x\) varies as a function of time \(t\).

\[
x = \chi(X, t)
\]

(A.1)

i.e.

\[
x_i = \chi_i(X_1, X_2, X_3, t)
\]

To represent the difference of spacial location between neighbourhood material points,
we can define the deformation gradient tensor

\[ F(X, t) \triangleq \nabla \chi(X, t) = \frac{\partial}{\partial X} \chi(X, t) \quad (A.2) \]

Note that vector gradient is defined as

\[ [\nabla v(x)]_{ij} = [\frac{\partial}{\partial x} v(x)]_{ij} = \frac{\partial v_i(x)}{\partial x_j} \]

To get rid of the factor of translational rigid body movement, we are interested in the displacement \( u \) rather than the absolute coordinate \( x \). The vector

\[ u(X, t) = \chi(X, t) - X \quad (A.3) \]

represents the displacement of material point \( X \) at time \( t \). To study the deformation behaviour, often times we are interested the difference of such displacement between neighbourhood points. For this purpose, the displacement gradient tensor \( H(X, t) \) can be defined as

\[ H(X, t) \triangleq \frac{\partial}{\partial X} u(X, t) = \frac{\partial}{\partial X} \chi(X, t) - 1 = F(X, t) - 1 \quad (A.4) \]

Or represented more intuitively in matrix form as

\[
H(X, t) = \begin{bmatrix}
\frac{\partial u_1(X, t)}{\partial X_1} & \frac{\partial u_1(X, t)}{\partial X_2} & \frac{\partial u_1(X, t)}{\partial X_3} \\
\frac{\partial u_2(X, t)}{\partial X_1} & \frac{\partial u_2(X, t)}{\partial X_2} & \frac{\partial u_2(X, t)}{\partial X_3} \\
\frac{\partial u_3(X, t)}{\partial X_1} & \frac{\partial u_3(X, t)}{\partial X_2} & \frac{\partial u_3(X, t)}{\partial X_3}
\end{bmatrix} = \begin{bmatrix}
\frac{\partial u_1(X, t)}{\partial x} & \frac{\partial u_2(X, t)}{\partial y} & \frac{\partial u_3(X, t)}{\partial z} \\
\frac{\partial u_2(X, t)}{\partial x} & \frac{\partial u_3(X, t)}{\partial y} & \frac{\partial u_1(X, t)}{\partial z} \\
\frac{\partial u_3(X, t)}{\partial x} & \frac{\partial u_1(X, t)}{\partial y} & \frac{\partial u_2(X, t)}{\partial z}
\end{bmatrix} \quad (A.5)
\]

This relative displacement can characterize how much the material is stretched or compressed between neighbourhood points. Note this expression alone is not mechanical strain tensor. The displacement gradient tensor \( H(X, t) \) can be decomposed into a
symmetric component and an anti-symmetric (skew-symmetric) component

\[ H(X, t) = \frac{1}{2}(H(X, t) + H^T(X, t)) + \frac{1}{2}(H(X, t) - H^T(X, t)) \]

\[ = \text{sym}H(X, t) + \text{skew}H(X, t) \quad (A.6) \]

Since for any skew symmetric tensor \( \Omega \), there is a unique axial vector \( \omega \) such that

\[ \Omega u = \omega \times u \quad (A.7) \]

This indicates that the skew symmetric part is a local infinitesimal "rigid body" rotation. Therefore, the elastic strain tensor is represented as

\[ (X, t) = \frac{1}{2}(H(X, t) + H^T(X, t)) \]

\[ = \frac{1}{2}(\nabla u(X, t) + (\nabla u(X, t))^T) = \nabla_s u(X, t) \quad (A.8) \]

Note that by taking derivatives to represent relative stretching or compressing, we have used the assumption of small displacements.

Since this is defined under certain coordinate system, it is worth mentioning the expression after rotation of axes. Assuming a coordinate transformation of the form

\[ x' = ax \quad (A.9) \]

or equivalently

\[ x'_i = a_{ij}x_j \]

in which \( a \) is an orthogonal transformation matrix, and Einstein notion is used (summation over repeated index). The new expression of strain under the transformed coordinate is

\[ \epsilon' = a\epsilon a^T \quad (A.10) \]

or equivalently

\[ \epsilon'_{ij} = a_{ik}\epsilon_{kl}a^T_{lj} = a_{ik}\epsilon_{kl}a_{jl} = a_{ik}a_{jl}\epsilon_{kl} \]
Since $\epsilon$ is symmetric, there are only 6 independent variables instead of 9. It is convenient to introduce the Voigt notation, which will show advantage when we discuss the stress-strain relations. The strain under Voigt notation is defined as $S$

\[
S = \begin{bmatrix}
S_1 \\
S_2 \\
S_3 \\
S_4 \\
S_5 \\
S_6
\end{bmatrix} = \begin{bmatrix}
\frac{\partial}{\partial x}u_x \\
\frac{\partial}{\partial y}u_y \\
\frac{\partial}{\partial z}u_z \\
\frac{\partial}{\partial z}u_y + \frac{\partial}{\partial y}u_z \\
\frac{\partial}{\partial z}u_x + \frac{\partial}{\partial x}u_z \\
\frac{\partial}{\partial y}u_x + \frac{\partial}{\partial x}u_y
\end{bmatrix} = \begin{bmatrix}
\frac{\partial}{\partial x} \\
0 \\
0 \\
0 \\
\frac{\partial}{\partial y} \\
\frac{\partial}{\partial z}
\end{bmatrix} \begin{bmatrix}
u_x \\
u_y \\
u_z
\end{bmatrix} (A.11)
\]

or equivalently

\[
S_I = \nabla_l u_j (A.12)
\]

Compare with the strain definition (A.5) and (A.8), there is mapping of

\[
\epsilon = \begin{bmatrix}
\epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\
\epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\
\epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz}
\end{bmatrix} = \begin{bmatrix}
S_1 & \frac{1}{2}S_6 & \frac{1}{2}S_5 \\
\frac{1}{2}S_6 & S_2 & \frac{1}{2}S_4 \\
\frac{1}{2}S_5 & \frac{1}{2}S_4 & S_3
\end{bmatrix} (A.13)
\]

and the symmetric gradient operator $\nabla_s$ has a matrix representation

\[
\nabla_s \rightarrow \nabla_{lij} = \begin{bmatrix}
\frac{\partial}{\partial x} & 0 & 0 \\
0 & \frac{\partial}{\partial y} & 0 \\
0 & 0 & \frac{\partial}{\partial z} \\
\frac{\partial}{\partial z} & 0 & \frac{\partial}{\partial x} \\
\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0
\end{bmatrix} (A.14)
\]

**Stress Definition**

The common definition for uniaxial stress is force per area. For a 3D material, the definition needs to be handled with care. Considering an infinitesimal solid material element as in Figure A-1, there are 3 pairs of faces, and each face is subject to a force
vector which can be decomposed into 3 elements. Such stress state is represented as a 2nd order tensor \( \sigma \), in which \( \sigma_{ij} \) refers to the stress component in the direction \( i \) of the force on the surface \( j \). And it is also a function of spacial coordinate \( x \) and time \( t \), so similar as the notation for strain, it can be written as \( \sigma(x, t) \). From the analysis of balance of torque for such infinitesimal element, we can prove that the stress tensor \( \sigma \) is also symmetric.

![Figure A-1: Schematic of the stress state for a 3D infinitesimal material element](image)

It is named as a "state" because once the stress is defined in such tensor form at a fixed spacial location \( x \), the traction force vector (stress in an arbitrary direction) is determined. From a simple force balance analysis on such infinitesimal element, we can get the traction force vector (same unit as stress) written as

\[
t(\hat{n}, x, t) = \sigma(x, t)\hat{n}
\]

(A.15)
i.e.

\[
t_i = \sigma_{ij}\hat{n}_j
\]
in which \( t \) is the traction vector, and \( \hat{n} = n_i e_i \) is the unit vector of its direction.

Another convenience from such stress tensor definition is that the equation of motion can be formatted in a compact form

\[
\nabla \cdot \sigma + b = \rho \ddot{u}
\]

(A.16)
in which \( u \) is the displacement, \( b \) is the body force vector, and \( \nabla \cdot \) is divergence. The
The divergence of a 2nd order tensor is defined as
\[
[\nabla \cdot \mathbf{T}]_i = \frac{\partial T_{ij}}{\partial x_j}
\]

Under coordinate transformation, similar as that defined for strain (A.10), the stress in the transformed coordinate system is written as
\[
\mathbf{\sigma}' = a\mathbf{\sigma}a^T
\]

or equivalently
\[
\sigma'_{ij} = a_{ik}a_{jl}\sigma_{kl}
\]

Again, since \( \mathbf{\sigma} \) is a symmetric tensor, it is worth introducing the Voigt notation for stress \( \mathbf{T} \) in the column vector form
\[
\mathbf{T} = \begin{bmatrix} T_1 \\
T_2 \\
T_3 \\
T_4 \\
T_5 \\
T_6 \end{bmatrix}
\]

And the mapping rule with regular stress definition is
\[
\mathbf{\sigma} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\
\sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\
\sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} = \begin{bmatrix} T_1 & T_6 & T_5 \\
T_6 & T_2 & T_4 \\
T_5 & T_4 & T_3 \end{bmatrix}
\]

Note this new definition would make the divergence expression a bit more com-
and the divergence operator has a matrix representation of

\[ \nabla \cdot \mathbf{T} = \begin{bmatrix} \frac{\partial}{\partial x} & 0 & 0 & 0 & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ 0 & \frac{\partial}{\partial y} & 0 & \frac{\partial}{\partial z} & 0 & \frac{\partial}{\partial x} \\ 0 & 0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix} \]  

(A.20)

which turns out to be just the transpose of the symmetric gradient matrix operator \( \nabla_s \) as defined in (A.14)

### A.2.2 Constitutive Equations

Hooke's Law states that the strain is linearly proportional to the stress, or vice versa. This can be written as stress being a linear combination of all the strain components, which are called elastic constitutive equations.

\[ \mathbf{\sigma} = \mathbf{C} : \mathbf{\epsilon} \]  

(A.22)

or

\[ \sigma_{ij} = C_{ijkl} \epsilon_{kl} \]

in which \( \mathbf{C} \) is a 4\(^{th}\) order tensor, and \( C_{ijkl} \) are called elastic stiffness constants. Due to the symmetries of stress and strain, \( \mathbf{C} \) has symmetries as well

\[ C_{ijkl} = C_{jikl} = C_{ijk} = C_{jikl} \]  

(A.23)
And from additional elastic energy analysis [45], there is symmetry of

\[ C_{ijkl} = C_{klij} \]  
(A.24)

So with these symmetries, instead of \(3^4 = 81\) elastic constants, there are only 21 at most.

Similarly, there are \textbf{compliance constants}

\[ \epsilon = S : \sigma \]  
(A.25)

which has the same symmetry properties, and independent constants of 21 at maximum.

The stiffness and compliance constants have coordinate transformation relations as the following

\[ C'_{mnop} = a_{mi}a_{nj}a_{ok}a_{pl}C_{ijkl} \]  
(A.26)

\[ S'_{mnop} = a_{mi}a_{nj}a_{ok}a_{pl}S_{ijkl} \]  
(A.27)

It is hard to express the 4th order tensor \( C \) explicitly. But with the Voigt notations, both stress \( \sigma \) and strain \( \epsilon \) are reduced to vectors \( T \) and \( S \), so the \( C \) constant becomes a matrix \((\text{stiffness matrix})\)

\[
\begin{bmatrix}
  c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\
  c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\
  c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} \\
  c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} \\
  c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} \\
  c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66}
\end{bmatrix}
\]  
(A.28)

It is also symmetric based on (A.24). And the independent constants are indeed 21 counting from this matrix.

And \( S \) also becomes a matrix \((\text{compliance matrix})\), which is the inverse matrix
of c, and therefore has the same form of symmetries.

\[
S = c^{-1} = \begin{bmatrix}
s_{11} & s_{12} & s_{13} & s_{14} & s_{15} & s_{16} \\
s_{12} & s_{22} & s_{23} & s_{24} & s_{25} & s_{26} \\
s_{13} & s_{23} & s_{33} & s_{34} & s_{35} & s_{36} \\
s_{14} & s_{24} & s_{34} & s_{44} & s_{45} & s_{46} \\
s_{15} & s_{25} & s_{35} & s_{45} & s_{55} & s_{56} \\
s_{16} & s_{26} & s_{36} & s_{46} & s_{56} & s_{66}
\end{bmatrix}
\] (A.29)

So from definitions of Voigt stress and strain (A.11), (A.18), equations (A.22) and (A.25) become

\[
T = c : S 
\] (A.30)

\[
S = s : T
\] (A.31)

The only complexity from this Voigt notation lies in the coordinate transformation of the stiffness matrix. By going through cumbersome algebra, we get the equivalence of (A.26) in Voigt notation as the following

\[
c' = M c M^T
\] (A.32)

i.e.

\[
c'_{KL} = M_{KI} M_{LJ} c_{IJ}
\]

in which \( M \) is

\[
\begin{bmatrix}
 a_{xx}^2 & a_{xy}^2 & a_{xz}^2 & 2a_{xy}a_{xz} & 2a_{xx}a_{xx} & 2a_{xx}a_{xy} \\
 a_{yx}^2 & a_{yy}^2 & a_{yz}^2 & 2a_{yy}a_{yz} & 2a_{yx}a_{yx} & 2a_{yx}a_{yy} \\
 a_{zx}^2 & a_{zy}^2 & a_{zz}^2 & 2a_{zy}a_{zz} & 2a_{zx}a_{zx} & 2a_{zx}a_{zy} \\
 a_{xy}a_{xx} & a_{yy}a_{xy} & a_{yz}a_{xz} & a_{yy}a_{xz} + a_{yz}a_{xy} & a_{yx}a_{xx} + a_{yz}a_{yy} & a_{yx}a_{xz} + a_{yx}a_{yy} \\
 a_{zx}a_{xx} & a_{zy}a_{xy} & a_{zz}a_{xz} & a_{xx}a_{xx} + a_{zx}a_{xz} & a_{xx}a_{yy} + a_{zy}a_{yx} & a_{xx}a_{xz} + a_{yx}a_{yy} \\
 a_{xx}a_{yx} & a_{xy}a_{yy} & a_{zz}a_{yz} & a_{xx}a_{yz} + a_{xx}a_{yx} & a_{xx}a_{yy} + a_{xy}a_{yx} & a_{xx}a_{yy} + a_{xy}a_{yy}
\end{bmatrix}
\] (A.33)
Here the orthogonal matrix \( \mathbf{a} \) is defined the same as (A.9) and the compliance matrix has the coordinate transformation of

\[ s' = N s N^T \]

(A.34)

i.e.

\[ s'_{KL} = N_{KJ} N_{LJ} s_{IJ} \]

in which \( N^{-1} = M^T \), and \( N \) is detailed as

\[
\begin{bmatrix}
    a_{xx}^2 & a_{xy}^2 & a_{xz}^2 & a_{xy} a_{xz} & a_{xz} a_{xx} & a_{xx} a_{xy} \\
    a_{yx}^2 & a_{yy}^2 & a_{yz}^2 & a_{yy} a_{yz} & a_{yz} a_{yx} & a_{yx} a_{yy} \\
    a_{zx}^2 & a_{zy}^2 & a_{zz}^2 & a_{zy} a_{zz} & a_{zz} a_{zx} & a_{zx} a_{zy} \\
    2a_{yx} a_{zx} & 2a_{yy} a_{zy} & 2a_{yz} a_{zx} + a_{yz} a_{zy} & a_{yy} a_{zx} + a_{yz} a_{yx} & a_{yz} a_{yx} + a_{yx} a_{yy} \\
    2a_{zx} a_{xy} & 2a_{zy} a_{xy} & 2a_{xy} a_{zx} + a_{xy} a_{yz} & a_{zx} a_{xy} + a_{xy} a_{yz} & a_{xy} a_{yz} + a_{yx} a_{zx} \\
    2a_{xx} a_{yx} & 2a_{xy} a_{yy} & 2a_{zx} a_{yz} + a_{zx} a_{yx} & a_{xx} a_{yz} + a_{xy} a_{yz} & a_{xx} a_{yz} + a_{xy} a_{yx} & a_{xy} a_{yx} + a_{yx} a_{yz}
\end{bmatrix}
\]

(A.35)

By comparing with (A.33), we can see that it is the same as \( M \), except for a shift of the factor 2 from the upper right-hand corner to the lower left-hand corner.

### A.2.3 Crystal Symmetries for Anisotropic Materials

The general form of the compliance and stiffness matrices for the anisotropic material was provided in (A.28) and (A.29). For commonly seen anisotropic materials, these matrices can be further simplified by considering more crystal symmetries. The common method to use crystal symmetry to reduce the number of constants in the compliance and stiffness matrices is applying a symmetry operation and equate the new matrix with the old matrix

\[ \mathbf{c} = \mathbf{M} \mathbf{c} \mathbf{M}^T \]

(A.36)
Since compliance and stiffness matrices have the same form of symmetries for the same anisotropic material, all the derivations in the following will only be on \( c \).

And here only the material symmetries that will be encountered in this thesis are discussed.

**Cubic Symmetry**

For a rotation of angle \( \xi \) about the \( Z \) crystal axis, the coordinate transformation matrix is

\[
\mathbf{a} = \begin{bmatrix}
\cos \xi & \sin \xi & 0 \\
-\sin \xi & \cos \xi & 0 \\
0 & 0 & 1
\end{bmatrix}
\]  
(A.37)

from (A.33), the stress transformation matrix is

\[
\mathbf{M} = \begin{bmatrix}
\cos^2 \xi & \sin^2 \xi & 0 & 0 & 0 & \sin 2\xi \\
\sin^2 \xi & \cos^2 \xi & 0 & 0 & 0 & -\sin 2\xi \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & \cos \xi & -\sin \xi & 0 \\
0 & 0 & 0 & \sin \xi & \cos \xi & 0 \\
-\frac{\sin 2\xi}{2} & \frac{\sin 2\xi}{2} & 0 & 0 & 0 & \cos 2\xi
\end{bmatrix}
\]  
(A.38)

By applying \( \xi = 90^\circ \), substituting into (A.36), and doing similar procedures along the \( X \) and \( Y \) axes, we get the stiffness matrix as

\[
\mathbf{C}_{\text{cube}} = \begin{bmatrix}
c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\
c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\
c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & c_{44}
\end{bmatrix}
\]  
(A.39)

Note that there are 3 independent constants for a material with cubic symmetry.
**Hexagonal Symmetry**

Similarly, we can rotate about crystal $Z$ axis with $\xi = 120^\circ, 240^\circ$, using the same $M$ matrix as in (A.38). By substituting into (A.36), we get

$$c_{\text{hex}} = \begin{bmatrix}
    c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\
    c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\
    c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\
    0 & 0 & 0 & c_{44} & 0 & 0 \\
    0 & 0 & 0 & 0 & c_{44} & 0 \\
    0 & 0 & 0 & 0 & 0 & \frac{c_{11} - c_{12}}{2}
\end{bmatrix}$$

which has 4 independent constants.

And moreover, for materials with hexagonal symmetry, the $c$ matrix is invariant not just under rotations of $\xi = 120^\circ, 240^\circ$ along the $Z$ axis, but for any angle of $\xi$. So for materials with hexagonal symmetry, it is isotropic in the hexagonal plane. This can be proved again by using (A.36).

**Isotropic Symmetry**

The isotropic material would have invariant stiffness matrix under rotation of any angle about any axis. It is the highest symmetry for solid materials. Again, using (A.36), we would get the same expression of (A.39), with additional condition of

$$c_{12} = c_{11} - 2c_{44}$$

With this added constraint, there are only 2 independent constants for isotropic materials. These are often times taken to be the Lamé constants $\lambda$ and $\mu$, defined by

$$\begin{cases}
    c_{12} &= \lambda, \\
    c_{44} &= \mu, \text{ and consequently} \\
    c_{11} &= \lambda + 2\mu
\end{cases}$$
So the stiffness matrix becomes
\[
\mathbf{c}_{\text{iso}} = \begin{bmatrix}
\lambda + 2\mu & \lambda & \lambda & 0 & 0 & 0 \\
\lambda & \lambda + 2\mu & \lambda & 0 & 0 & 0 \\
\lambda & \lambda & \lambda + 2\mu & 0 & 0 & 0 \\
0 & 0 & 0 & \mu & 0 & 0 \\
0 & 0 & 0 & 0 & \mu & 0 \\
0 & 0 & 0 & 0 & 0 & \mu \\
\end{bmatrix}
\] (A.43)

And there is a clean form of tensor notation for the constitutive equation of isotropic materials
\[
\mathbf{\sigma} = \mathbf{C} : \mathbf{\epsilon} = 2\mu \mathbf{\epsilon} + \lambda (tr\mathbf{\epsilon}) \mathbf{1}
\] (A.44)
in which \( tr\mathbf{\epsilon} \) means the trace of the strain tensor.

For an isotropic bar under uniaxial stretch, people intuitively define the constants Young’s modulus \( E \doteq \sigma_{xx}/\epsilon_{xx} \) to characterize the stiffness, and Poisson’s ratio \( \nu \doteq \sigma_{xx}/\epsilon_{yy} \) to characterize change of radius in the non-stretched dimension. It can be easily derived that the Lamé constants are related to \( E \) and \( \nu \) with the following relations
\[
\begin{align*}
\lambda &= \frac{\nu E}{(1+\nu)(1-2\nu)}, \\
\mu &= \frac{E}{2(1+\nu)}
\end{align*}
\] (A.45)

So written as a function of Young’s modulus \( E \) and Poisson’s ratio \( \nu \), the stiffness matrix becomes
\[
\mathbf{c}_{\text{iso}} = \begin{bmatrix}
\frac{(1-\nu)E}{(1+\nu)(1-2\nu)} & \frac{\nu E}{(1+\nu)(1-2\nu)} & \frac{\nu E}{(1+\nu)(1-2\nu)} & 0 & 0 & 0 \\
\frac{\nu E}{(1+\nu)(1-2\nu)} & \frac{(1-\nu)E}{(1+\nu)(1-2\nu)} & \frac{\nu E}{(1+\nu)(1-2\nu)} & 0 & 0 & 0 \\
\frac{\nu E}{(1+\nu)(1-2\nu)} & \frac{\nu E}{(1+\nu)(1-2\nu)} & \frac{(1-\nu)E}{(1+\nu)(1-2\nu)} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{E}{2(1+\nu)} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{E}{2(1+\nu)} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{E}{2(1+\nu)} \\
\end{bmatrix}
\] (A.46)
A.2.4 Damping and Attenuation

The previously mentioned constitutive equation (A.22) does not involve any damping, which is the case for ideal materials, and can be used to approximate for weakly damped materials. Actual materials would have various loss mechanisms, such as thermoelastic damping, phonon-phonon scattering, viscous damping etc. These loss mechanisms can be simply modeled as a loss factor that is proportional to the rate of change of elastic stress.

Based on our current notations, to include the damping factor, the new constitution equation becomes

$$\sigma = C : \epsilon + H : \frac{\partial \epsilon}{\partial t}$$  \hspace{1cm} (A.47)

in which $H$ is a fourth order tensor for loss factors.

Again, this can be re-written as the Voigt notation.

$$T = c : S + \eta : \frac{\partial S}{\partial t}$$  \hspace{1cm} (A.48)

And the $\eta$ matrix has the same type of symmetry as the $c$ matrix.

A.3 Linear Elastic Wave Equation

In the previous section, we have introduced a few key equations, including the strain definition (A.8), equation of motion (A.16), and elastic constitutive equation (A.22) in the case of weak loss. These equations can be collected as the following

$$\begin{aligned}
\epsilon &= \frac{1}{2}(\nabla u + \nabla u^T), \\
\nabla \cdot \sigma + b &= \rho \ddot{u}, \\
\sigma &= C : \epsilon
\end{aligned}$$  \hspace{1cm} (A.49)

These equations can be combined to get the elastic wave equation for solid materials. But since a 4th order tensor $C$ is involved, it is hard to write it in a neat form. For an isotropic material, using the simplified constitutive equation (A.44), the wave
equation can be written as

\[ \mu \Delta u + (\lambda + \mu) \nabla (\nabla \cdot u) = \rho \ddot{u} \quad (A.50) \]

in which \( \Delta = \nabla \cdot \nabla \) is the Laplace operator.

The velocity of the wave can be found by substituting the eigenmode of the form

\[ u(x, t) = A \sin(x \cdot \hat{k} - ct) \quad (A.51) \]

in which \( A \) is the polarization vector, \( \hat{k} \) is the unit vector in the direction of wave propagation, \( c \) is wave velocity, and \( t \) is time. These vector/tensor relations can be derived easily using the Einstein notation

\[
\begin{align*}
\nabla u &= A \otimes \hat{k} \cos(x \cdot \hat{k} - ct), \\
\Delta u &= -A \sin(x \cdot \hat{k} - ct), \\
\nabla (\nabla \cdot u) &= -(A \cdot \hat{k}) \hat{k} \sin(x \cdot \hat{k} - ct), \\
\ddot{u} &= -c^2 A \sin(x \cdot \hat{k} - ct)
\end{align*}
\]

in which \( \otimes \) is the tensor product operator that generates a 2nd order tensor based on two vectors, defined by

\[ (u \otimes v) w = (v \cdot w) u \]

Upon these substitutions, we can get the simplified form of the wave equation

\[ \rho c^2 A = \mu A + (\lambda + \mu)(A \cdot \hat{k}) \hat{k} \quad (A.52) \]

From this, we can see that if the wave is transversal, where \( A \cdot \hat{k} = 0 \), there is

\[ c_t = \sqrt{\frac{\mu}{\rho}} = \sqrt{\frac{E}{2(1 + \nu)\rho}} \quad (A.53) \]
and if the wave is longitudinal, where \((\mathbf{A} \cdot \mathbf{k}) \dot{\mathbf{k}} = \mathbf{A}\), there is

\[
c_l = \sqrt{\frac{\lambda + 2\mu}{\rho}} = \sqrt{\frac{(1 - \nu)E}{(1 + \nu)(1 - 2\nu)\rho}} \tag{A.54}
\]

In the case of anisotropic materials, however, using the tensor notation directly cannot lead to neat results. This is where the Voigt notation again gets useful. By collecting equations of Voigt strain definition (A.11), equation of motion (A.16), Voigt stress definition (A.20), and constitutive equations (A.30), we get

\[
\begin{cases}
S &= \nabla_s \mathbf{u}, \\
\nabla \cdot \mathbf{T} + \mathbf{b} &= \rho \ddot{\mathbf{u}}, \\
\mathbf{T} &= \mathbf{c} : \mathbf{S}
\end{cases} \tag{A.55}
\]

After eliminating \(\mathbf{T}\) and \(\mathbf{S}\), we get

\[
\nabla \cdot (\mathbf{c} \nabla_s \mathbf{u}) + \mathbf{b} = \rho \ddot{\mathbf{u}} \tag{A.56}
\]

written in matrix form with Einstein notation, it is

\[
\nabla_{iK} c_{KL} \nabla_{Lj} u_j = \rho \frac{\partial^2 u_i}{\partial t^2} - b_i \tag{A.57}
\]

Again, here \(\nabla_{iK}\) and \(\nabla_{Lj}\) are defined in (A.14) and (A.21)

Now we can substitute the same eigenmode as that in (A.51), in which unit vector \(\mathbf{k} = (k_x, k_y, k_z)\), and get

\[
(l_{iK} c_{KL} l_{Lj}) u_j = \rho c^2 u_i \tag{A.58}
\]

This is called the Christoffel equation. And the \(3 \times 3\) matrix on the left hand side

\[
\Gamma_{ij} = l_{iK} c_{KL} l_{Lj} \tag{A.59}
\]

is called the Christoffel matrix. And similar to what is defined for \(\nabla_{iK}\) and \(\nabla_{Lj}\),
$l_{IK}$ and $l_{Lj}$ have the matrix form of

$$
l_{IK} \rightarrow \begin{bmatrix}
l_x & 0 & 0 & l_z & l_y \\
0 & l_y & 0 & l_z & 0 \\
0 & 0 & l_z & l_y & l_x
\end{bmatrix}
$$

(A.60)

And

$$
l_{Lj} \rightarrow \begin{bmatrix}
l_x & 0 & 0 \\
0 & l_y & 0 \\
0 & 0 & l_z \\
l_z & 0 & l_x \\
l_y & l_x & 0
\end{bmatrix}
$$

(A.61)

And this result is valid for any type of materials—isotropic or anisotropic alike.

For example, for a cubic symmetric material where the axes are aligned with the material axes, the Christoffel matrix becomes

$$
\Gamma = \begin{bmatrix}
c_{11}l_x^2 + c_{44}(1 - l_x^2) & (c_{12} + c_{44})l_xl_y \\
(c_{12} + c_{44})l_xl_y & c_{11}l_y^2 + c_{44}(1 - l_y^2) \\
(c_{12} + c_{44})l_xl_z & (c_{12} + c_{44})l_yl_z \\
(c_{12} + c_{44})l_z^2 & c_{11}l_z^2 + c_{44}(1 - l_z^2)
\end{bmatrix}
$$

(A.62)

And the wave speed and polarization direction is solved from the eigen equation

$$
\Gamma \mathbf{u} = \rho c^2 \mathbf{u}
$$

(A.63)

in which for a solution to exist, the characteristic determinant must be zero

$$
|\Gamma_{ij}(l_x, l_y, l_z) - \rho c^2 \delta_{ij}| = 0
$$

(A.64)

From (A.64) we can see that the wave speed solution is a function of the propagating direction. If we take the direction to be $(l_x, l_y, l_z) = (1, 0, 0)$ for example, the
Christoffel matrix becomes

\[
\Gamma = \begin{bmatrix}
c_{11} & 0 & 0 \\
0 & c_{44} & 0 \\
0 & 0 & c_{44}
\end{bmatrix}
\]

And the wave speeds are \( c = \sqrt{\frac{c_{11}}{\rho}}, \ \sqrt{\frac{c_{44}}{\rho}}, \ \sqrt{\frac{c_{44}}{\rho}} \) respectively.

However, for arbitrary direction, the analytical form of solution is not that simple. The solution can be obtained numerically by solving a series of matrix eigenvalue problems. Figure A-2a shows solutions for single-crystalline silicon as an example. This is the solution in the plane that is perpendicular to Z axis. We can see that the longitudinal wave speed (red) is always larger than shear wave speeds, and in [100] direction, the two shear wave speeds become degenerate, which is exactly the same as what we found from the simple analytical solution.

Since \( k \) is the wave number vector but \( \omega \) is just a scalar, people like to express in the inverse form, which is called the slowness surface. Here Figure A-2b shows such curves for silicon, which is in fact “slowness curves” in the plane that is perpendicular to Z axis.

The Christoffel equation can also be used to derive the velocities for waves in isotropic materials. The Christoffel matrix will have the same look as (A.62), but
Figure A-3: Example of wave velocities in different directions for isotropic material. Poly-silicon is used as the material here. The two shear wave velocities are always degenerate (overlap in the figure) with an added equation of (A.41). With this added condition, the Christoffel matrix will become invariant under any axis rotation of any angle. This can be illustrated in Figure A-3 using poly-Si as an example. Again, here both the velocity curves and slowness curves are plotted.

And for isotropic material, the Christoffel equation can be simplified to give a neat analytical solution. By going through the algebra, we can find that the results are exactly the same as (A.53) and (A.54) which we got using the tensor notation. Note that we need to use $c_{12} = \lambda$ and $c_{44} = \mu$.

And this Christoffel matrix method can be used to study the velocity surfaces for any other materials as well, including materials with hexagonal symmetry, which will not be detailed here.

### A.4 Power Flow and Energy Balance

For any wave equation, the analysis of power flow and energy balance provides an alternative perspective and useful insights into the physics. The energy conservation relation will interrelate the power supplied by the power sources, the power lost through dissipation, the power flow in the waves, and the kinetic and elastic energy...
stored in the wave fields. The electromagnetic counterpart of this energy relation is the Poynting’s Theorem. For elastic waves, similar relations can be derived.

Velocity \( v = \partial u / \partial t \) is directly tied with power, so \( v \) will be used in the energy expressions instead of \( u \). Again, Voigt notation is used.

Based on (A.55), using the constitutive equation with damping (A.48), and the identity \( \nabla \cdot (v \cdot T) = v \cdot (\nabla \cdot T) + T : \nabla v \), we get the energy conservation relation in integral form as

\[
\int_S (-v \cdot T) \cdot \hat{n} \, dS = -\frac{\partial}{\partial t} \left( \int_V \frac{1}{2} \rho |v|^2 \, dV \right) - \frac{\partial}{\partial t} \left( \int_V \frac{1}{2} S : c : S \, dV \right) \]

\[
- \left( \int_V \frac{\partial S}{\partial t} : \eta : \frac{\partial S}{\partial t} \, dV \right) + \int_V v \cdot b \, dV \quad (A.65)
\]

in which the acoustic Poynting vector \( P \), power dissipation \( P_d \), power supply \( P_s \), kinetic energy density \( E_v \) and strain energy density \( E_S \) are

\[
\begin{align*}
P &= -v \cdot T \\
P_d &= \frac{\partial S}{\partial t} : \eta : \frac{\partial S}{\partial t} \\
P_s &= v \cdot b \\
E_v &= \frac{1}{2} \rho |v|^2 \\
E_S &= \frac{1}{2} S : c : S
\end{align*}
\]

So (A.65) can be re-written in the differential form as

\[
\nabla \cdot P + \frac{\partial (E_v + E_S)}{\partial t} + P_d = P_s \quad (A.67)
\]

For sinusoidal acoustic fields, (A.66) can be written using phasors and their complex conjugates as

\[
\begin{align*}
P &= -\frac{1}{2} v^* \cdot T \\
P_d(\text{average}) &= \frac{\rho^2}{2} S : \eta : S^* \\
P_s &= \frac{1}{2} v^* \cdot b \\
E_v(\text{peak}) &= \frac{1}{2} \rho |v|^2 \\
E_S(\text{peak}) &= \frac{1}{2} S : c : S^*
\end{align*}
\]

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And the energy conservation relation (A.67) can be re-written as

\[ \nabla \cdot P - i\omega (E_S - E_u) + P_d = P_s \]  (A.69)

### A.5 Reflection and Refraction of Elastic Waves

When wave propagates across the boundary between two mediums, due to the mismatch in wave speed, it typically changes the direction of propagation and splits into the back propagating component in the first medium (reflection) and forward propagating component in the second medium (refraction). The propagation angle and wave amplitude of such reflection and refraction can be solved using the match condition at this boundary, which is the equivalence of wave speed/amplitude and balance of stress.

\[
\begin{align*}
    & u_1 = u_2 \\
    & T_1 \cdot \hat{n} = T_2 \cdot \hat{n}
\end{align*}
\]  (A.70)

Such boundary condition is well known for the case of electromagnetic waves in an isotropic medium where the incident wave splits into one reflected wave and one transmitted wave. For elastic wave in solid medium, however, due to the existence of two wave speeds for longitudinal and transversal waves, such boundary condition is much more complicated—the incidence wave can split into multiple components, typically two reflected components and two transmitted components.

There are 3 polarization directions for wave incidence analysis (Figure A-4):

- Horizontally Polarized Shear (SH), where the polarization direction is perpendicular to the incidence plane.
- Vertically Polarized Shear (SV), where the polarization direction is in the incidence plane but perpendicular to the direction of propagation.
- Longitudinal (P), where the polarization direction is aligned with the direction of propagation.

Here briefly discusses a few special cases that will be encountered in this thesis.
Figure A-4: Three types of incidence waves for elastic waves crossing a solid medium boundary

### A.5.1 Normal Incidence

The analysis of normal incidence is the easiest case. During such normal incidence, the SH and SV are equivalent, and for any types of incidence, the wave does not split into other types and only generates one reflected component and one transmitted component.

Take the P wave for example, both the reflected wave and transmitted wave are still P waves. Assuming the incidence wave has the expression of $A_ie^{i(\omega t-kz)}$, since for linear system both the reflected and transmitted waves are still at the same frequency, the reflected wave will be $A_re^{i(\omega t+kx)}$, and the transmitted wave will be $A_te^{i(\omega t-k'x)}$.

Using condition (A.70), there are these expressions at $x = 0$

\[
\begin{cases} 
A_t e^{i(\omega t-kz)} + A_r e^{i(\omega t+kx)} = A_t e^{i(\omega t-k'z)} \\
-kc_{11}A_t e^{i(\omega t-kz)} + kc_{11}A_r e^{i(\omega t+kx)} = -k'c_{11}'A_t e^{i(\omega t-k'z)}
\end{cases}
\]

in which the prime labeled symbols are for medium I, while the non-prime labeled symbols are for medium II. Define reflectivity $R = A_r/A_i$ and transmitivity $T = A_t/A_i$, there are

\[
\begin{cases} 
1 + R = T \\
k_{11} + c_{11}R = -k'c_{11}'T
\end{cases}
\]

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Since $k = \omega/c$, with $c$ being the wave speed, the expression can be re-written as

$$\begin{cases} 
1 + R &= T \\
-c_{11}/c_P + c_{11}/c_P R &= -c'_{11}/c'_P T
\end{cases}$$

The term $c_{11}/c_P$ can be defined as **acoustic impedance**. In general terms, it is

$$Z \triangleq \frac{\text{stiffness component}}{\text{wave speed}}$$

With this definition, the expression is simplified as

$$\begin{cases} 
1 + R &= T \\
-Z_P + Z_P R &= -Z'_P T
\end{cases} \Rightarrow \begin{cases} 
R &= \frac{Z_P - Z'_P}{Z_P + Z'_P} \\
T &= \frac{2Z_P}{Z_P + Z'_P}
\end{cases}$$

And this result can be extended to S waves as well. We have seen that for P wave, the elastic modulus is $c_{11}$, so the acoustic impedance is defined as $Z_P = c_{11}/c_P$. In the case of SH/SV waves, the elastic modulus is $c_{44}$, so the acoustic impedance is defined as $Z_S = c_{44}/c_S$. Here the wave speeds $c_P$ and $c_S$ are solved from the Christoffel equation (A.63). And this result is valid for any types of material symmetries, as long as the stiffness matrix $c$ and wave speed are available.

It is also worth noting that for isotropic materials, for P waves there are

$$\begin{cases} 
c_{11} &= \frac{(1-\nu)E}{(1+\nu)(1-2\nu)} \\
c_P &= \sqrt{\frac{(1-\nu)E}{(1+\nu)(1-2\nu)\rho}} \\
Z_P &= c_{11}/c_P = \sqrt{\frac{(1-\nu)E\rho}{(1+\nu)(1-2\nu)}}
\end{cases}$$

and for S waves there are

$$\begin{cases} 
c_{44} &= \frac{E}{2(1+\nu)} \\
c_S &= \sqrt{\frac{E}{2(1+\nu)\rho}} \\
Z_S &= c_{44}/c_S = \sqrt{\frac{E\rho}{2(1+\nu)}}
\end{cases}$$

With these discussions, the reflectivity and transmittivity from medium I (acoustic
impedance $Z_1$) to medium II (acoustic impedance $Z_2$) can be written simply as

$$\begin{cases} R &= \frac{Z_1 - Z_2}{Z_1 + Z_2} \\ T &= \frac{2Z_1}{Z_1 + Z_2} \end{cases}$$  \hspace{1cm} (A.74)$$

for any types of elastic waves, and material properties.

### A.5.2 Oblique Incidence

Analysis of oblique incidence for elastic waves is much more complicated than that for E&M waves, since there are three types polarizations, at two distinct wave speed, even if the material is isotropic. The methodology is to use Snell’s Law at the boundary to equate the $k_x$ components between the incidence wave, two reflected wave components (longitudinal and shear), and two transmitted components. Vector relations in (A.70) at the boundary will provide 4 equations, and reflectivity and transmitivity for longitudinal and shear waves ($R_l$, $T_l$, $R_s$ and $T_s$) are the 4 unknowns. The result for each reflective component can be solved numerically. Since this thesis will mostly just discuss normal incidence analytically, oblique incidence will not be discussed in detail. When there are indeed oblique incidences, it is taken care of automatically by the finite element numeric solver. The detailed theory on analytical derivation of oblique incidence can be found in [45].
Appendix B

Device Fabrication Process

The table below describes the steps required to fabricate the Deep Trench (DT) MEMS Resonator. The fabrication of dual trench DT resonator requires additional steps, which are marked in the table. Both processes are developed and optimized at Microsystems Technology Laboratories (MTL) at MIT.

Table B.1: DT MEMS Resonator Fabrication Process

<table>
<thead>
<tr>
<th>Section</th>
<th>Steps</th>
<th>Detailed Process Parameters</th>
<th>Tool</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mask 1:</td>
<td>Spin photoresist (PR)</td>
<td>SPR-700 at 2000 rpm, about 1.4 μm thick</td>
<td>coater6</td>
</tr>
<tr>
<td>alignment marks</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Exposure,</td>
<td>soft bake 30 s at 95</td>
<td></td>
<td></td>
</tr>
<tr>
<td>develop and</td>
<td>℃, exposure dose 160 ms,</td>
<td></td>
<td></td>
</tr>
<tr>
<td>bake</td>
<td>post exposure bake</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>30 s at 115 ℃, develop</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>in “MF-CD-26” for 2 min, then hard bake 45 s at 120 ℃</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Etch Si</td>
<td>Etch rate: 4 nm/s, CH A oxide breakthrough first, then etch 100 s</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>in CH B</td>
<td></td>
<td>AME5000</td>
</tr>
<tr>
<td>Strip PR</td>
<td>3 min</td>
<td></td>
<td>asher-ICL</td>
</tr>
<tr>
<td>Piranha clean</td>
<td>10 min</td>
<td></td>
<td>premetal-Piranha</td>
</tr>
</tbody>
</table>

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<thead>
<tr>
<th>Section</th>
<th>Steps</th>
<th>Detailed Process Parameters</th>
<th>Tool</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mask 2: Deep</td>
<td>RCA clean</td>
<td></td>
<td>rca-ICL</td>
</tr>
<tr>
<td>Trench etch</td>
<td>Deposit PECVD oxide as hard mask</td>
<td>1um thick, recipe name “CHA-oxide-1um”</td>
<td>DCVD</td>
</tr>
<tr>
<td></td>
<td>Spin PR</td>
<td>SPR-700 at 2000 rpm, about 1.4 $\mu$m thick</td>
<td>coater6</td>
</tr>
<tr>
<td></td>
<td>Exposure, develop and bake</td>
<td>soft bake 30 s at 95 °C, exposure dose 150 ms, post exposure bake 30 s at 115 °C, develop in “MF-CD-26” for 2 min, then hard bake 45 s at 120 °C</td>
<td>i-stepper</td>
</tr>
<tr>
<td></td>
<td>Etch SiO$_2$</td>
<td>Etch rate: 3 nm/s, etch 325 s</td>
<td>AME5000</td>
</tr>
<tr>
<td></td>
<td>Strip PR</td>
<td>3 min</td>
<td>asher-ICL</td>
</tr>
<tr>
<td></td>
<td>DRIE etch in Si DT</td>
<td>5.5 min DRIE to get 7.5 $\mu$m deep</td>
<td>sts2</td>
</tr>
<tr>
<td></td>
<td>Hard mask recess</td>
<td>wet etch in 7:1 BHF for 50s</td>
<td>Greenflo</td>
</tr>
<tr>
<td></td>
<td>One-step Si etch</td>
<td>2 min using the one-step slow etch rate recipe</td>
<td>sts2</td>
</tr>
<tr>
<td>Mask 3:</td>
<td>Spin PR</td>
<td>SPR-700 at 2000 rpm, about 1.4 $\mu$m thick</td>
<td>coater6</td>
</tr>
<tr>
<td>pattern ion</td>
<td>Exposure, develop</td>
<td>dose 160 ms</td>
<td>i-stepper</td>
</tr>
<tr>
<td>implantation</td>
<td>Hard bake</td>
<td>30 min oven hard bake in the 120 °C oven in TRL</td>
<td>postbake</td>
</tr>
<tr>
<td>mask</td>
<td>Wet etch SiO$_2$</td>
<td>Etch rate: 250 – 300 nm/min, etch 3 min</td>
<td>Greenflo</td>
</tr>
<tr>
<td></td>
<td>Strip PR</td>
<td>3 min</td>
<td>asher-ICL</td>
</tr>
<tr>
<td></td>
<td>Piranha clean</td>
<td>10 min</td>
<td>Greenflo</td>
</tr>
<tr>
<td></td>
<td>RCA clean</td>
<td></td>
<td>rca-TRL</td>
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<tr>
<th>Section</th>
<th>Steps</th>
<th>Detailed Process Parameters</th>
<th>Tool</th>
</tr>
</thead>
<tbody>
<tr>
<td>DRIE polymer removal</td>
<td>Wet oxidation</td>
<td>20 min dry oxidation, 15 min wet oxidation, then 20 min dry oxidation</td>
<td>A2-WetOxBond</td>
</tr>
<tr>
<td></td>
<td>Wet etch</td>
<td>1 min wet etch in 14:1 BHF to remove the thermal oxide</td>
<td>Greenflo</td>
</tr>
<tr>
<td>Ion implantation</td>
<td>RCA clean</td>
<td></td>
<td>rca-TRL</td>
</tr>
<tr>
<td></td>
<td>Dry oxidation</td>
<td>1 h dry oxidation at 850 °C to get 10 nm thermal oxide. This is used as the implantation barrier layer</td>
<td>A2-WetOxBond</td>
</tr>
<tr>
<td></td>
<td>Ion implantation</td>
<td>outsource at Innovion. Energy–50 keV, Dose–4e15 cm^{-2}, tilt–7°, rotation–0° and 180°</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Double piranha clean</td>
<td>10 min &amp; 10 min</td>
<td>Greenflo</td>
</tr>
<tr>
<td></td>
<td>Oxide strip</td>
<td>45 s 14:1 BHF dip to remove implantation oxide</td>
<td>Greenflo</td>
</tr>
<tr>
<td>Mask 4:</td>
<td>RCA clean</td>
<td></td>
<td>rca-TRL</td>
</tr>
<tr>
<td>trench oxide</td>
<td>Oxide trench fill</td>
<td>20 min LPCVD oxide deposition</td>
<td>6C-LTO</td>
</tr>
<tr>
<td>fill (used for dual trench DT</td>
<td>Spin image reversal PR</td>
<td>AZ5214 at 2000 rpm, about 1 μm thick</td>
<td>coater</td>
</tr>
<tr>
<td>resonator only)</td>
<td>Exposure</td>
<td>exposure dose 160 ms</td>
<td>i-stepper</td>
</tr>
<tr>
<td></td>
<td>Post exposure bake</td>
<td>120 °C for 1.5 min on hotplate</td>
<td>postbake</td>
</tr>
<tr>
<td></td>
<td>Flood exposure and develop</td>
<td>1 min flood exposure, then develop in AZ422 for 5 min with ultrasonic, followed by a second round of 1 min flood and 10 min development with ultrasonic to clear resist in the trenches</td>
<td>EV1</td>
</tr>
<tr>
<td>Section</td>
<td>Steps</td>
<td>Detailed Process Parameters</td>
<td>Tool</td>
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</tr>
<tr>
<td>Hardbake</td>
<td>30 min</td>
<td>postbake</td>
<td></td>
</tr>
<tr>
<td>Etch SiO₂</td>
<td>Etch rate: 470 nm/min, wet etch 30 s in 7:1 BHF</td>
<td>Greenflo</td>
<td></td>
</tr>
<tr>
<td>Strip PR</td>
<td>3 min</td>
<td>asher-ICL</td>
<td></td>
</tr>
<tr>
<td>Mask 5: poly-Si fill and etch</td>
<td>Piranha clean 10 min</td>
<td>Greenflo</td>
<td></td>
</tr>
<tr>
<td></td>
<td>RCA clean</td>
<td>rca-TRL</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Dry oxidation 1 h dry oxidation at 850 °C to get 10 nm thermal oxide. This is used as capacitor dielectrics</td>
<td>A2-WetOxBond</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Poly-Si deposition two consecutive depositions, each run takes 100 min to get a total thickness of 800 nm</td>
<td>6A-nPoly</td>
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</tr>
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<td></td>
<td>Anneal</td>
<td>B3-DryOx</td>
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<tr>
<td></td>
<td>Al deposition deposit 750 nm of Al</td>
<td>Endura</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Spin PR SPR-700 at 1200 rpm, about 1.8 μm thick</td>
<td>SPR-700 at 1200 rpm, about 1.8 μm thick</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Exposure, develop and bake</td>
<td>dose 170 ms</td>
<td>i-stepper</td>
</tr>
<tr>
<td></td>
<td>Etch Al and poly-Si</td>
<td>etch 300 s</td>
<td>rainbow</td>
</tr>
<tr>
<td></td>
<td>Strip PR 4 min, extra time is for cleaning</td>
<td>asher-ICL</td>
<td></td>
</tr>
<tr>
<td>Mask 6: field oxide patterning</td>
<td>Deposit PECVD oxide 500 nm thick</td>
<td>concept1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Spin pr spr-700 at 2000 rpm, about 1.4 μm thick</td>
<td>spr-700 at 2000 rpm, about 1.4 μm thick</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Exposure, develop and bake</td>
<td>dose 160 ms</td>
<td>i-stepper</td>
</tr>
</tbody>
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Table B.1 – *Continued from previous page*

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<th>Section</th>
<th>Steps</th>
<th>Detailed Process Parameters</th>
<th>Tool</th>
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</thead>
<tbody>
<tr>
<td>Dry etch SiO₂</td>
<td>etch rate: 200 nm/min, etch 2 min</td>
<td>lam590-ICL</td>
<td></td>
</tr>
<tr>
<td>Strip pr</td>
<td>3 min</td>
<td>asher-ICL</td>
<td></td>
</tr>
<tr>
<td>Mask 7:</td>
<td>HF dip</td>
<td>14:1 BHF, dip 15 s</td>
<td>Greenflo</td>
</tr>
<tr>
<td>Metallization</td>
<td>Deposit metal</td>
<td>100 nm of Ti and 1 um of Al</td>
<td>Endura</td>
</tr>
<tr>
<td></td>
<td>Spin pr</td>
<td>spr-700 at 2000 rpm, about 1.4 µm thick</td>
<td>coater6</td>
</tr>
<tr>
<td></td>
<td>Exposure, develop</td>
<td>dose 140 ms</td>
<td>i-stepper</td>
</tr>
<tr>
<td></td>
<td>and bake</td>
<td></td>
<td></td>
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<td></td>
<td>Dry etch the metal</td>
<td>etch 135 s</td>
<td>rainbow</td>
</tr>
<tr>
<td></td>
<td>stack</td>
<td></td>
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</tr>
<tr>
<td></td>
<td>Strip pr</td>
<td>3 min</td>
<td>asher-ICL</td>
</tr>
<tr>
<td></td>
<td>Sinter</td>
<td>450 °C for 30 min with forming gas (N₂/H₂)</td>
<td>A3-Sinter</td>
</tr>
</tbody>
</table>
Bibliography


[68] Laura C Popa and Dana Weinstein. 1 GHz GaN resonant body transistors with enhanced off-resonance rejection.