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Electrical Engineering

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MODELING AND CHARACTERIZATION OF ELASTIC WAVE
PROPAGATION IN MICRO-SCALE PHONONIC CRYSTALS

BY

YASSER MOHAMED SOLIMAN

B.S., Electrical Engineering, University of Houston, 2005

THESIS
Submitted in Partial Fulfillment of the
Requirements for the Degree of

Master of Science
Electrical Engineering

The University of New Mexico
Albuquerque, New Mexico

May, 2010
 Anyone with the least amount of experience in life profoundly understands that no worthy task can be accomplished without the input, support and help of many others. This work is no different. Here I would like to thank many for their support and help during my graduate career at the University of New Mexico, and the first can never be any being except God. That is because He is the One who I believe blessed me with great people to work with, great parents to spend their entire lives dedicated for my brothers and I, an enormously supportive wife to love, a son who magically melts stressful days with a smile on his face, a great educational institution at which to study, a great national laboratory at which to learn and research, the physical and mental capability to carry out tasks and many more bounties. I can never be thankful enough; truly, all praise is due to God.

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Yasser Soliman
Albuquerque, NM
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ABSTRACT OF THESIS

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ABSTRACT

Micro-scale phononic crystals are micro-electro-mechanical-systems (MEMS) made of one material periodically embedded in another material, leading to periodic changes in elastic properties of the composite structure. Such devices exhibit elastic bandgaps, which are very useful in many commercial applications. Filtering, guiding and mirroring of elastic waves are a few applications in which phononic crystals can be used. In this manuscript, the physical origins of phononic bandgaps were successfully determined using a one-dimensional model to isolate resonances contributing to the creation of phononic bandgaps. Phononic crystals were further modeled using a two-dimensional technique called the Plane Wave Expansion Method. A solution for the convergence problem of the plane wave expansion method, previously believed to be a result of the large elastic impedance difference between the constituent materials, was successfully demonstrated. This new formulation of the plane wave expansion method reduced the computation time from 18 hours, using Fortran running on a Unix environment with eight parallelized processors, to 1 minute using Matlab running on a simple windows machine. The computation time was more than 1000 times faster than that using the conventional plane wave expansion method formulation. Finally, phononic crystal devices
operating in the MHz as well as devices operating at the GHz frequency range were modeled, designed, fabricated, and tested. Good agreement between theoretical and experimental results was observed. In the future, phononic crystal high-Q cavities should be considered, including their fabrication procedure as well as developing a method by which elastic coupling into such cavities is readily achieved.
Table of Contents

Table of Contents .............................................................................................................. vii
List of Figures .................................................................................................................. viii
List of Tables ..................................................................................................................... xi
Chapter 1 – Introduction ..................................................................................................... 1
  1.1 Definition .................................................................................................................. 1
  1.2 Figures of Merit ........................................................................................................ 3
  1.3 Applications .............................................................................................................. 4
  1.4 Parameter and Material Choice ................................................................................. 6
Chapter 2 – Physical Origins of Phononic Bandgaps ....................................................... 15
  2.1 Introduction ............................................................................................................. 15
  2.2 Formulation ............................................................................................................. 16
  2.3 Recursive Reflection Equation ............................................................................... 19
  2.4 Results ..................................................................................................................... 21
  2.5 Modeling the Mie Resonance ................................................................................. 26
Chapter 3 – The Plane-Wave-Expansion Method for Modeling Phononic Crystals ........ 35
  3.1 Overview ................................................................................................................. 35
  3.2 Formulation for 2D Plane Wave Expansion Method .............................................. 36
  3.3 Convergence Comparison for High-Contrast Solid-Solid Phononic Crystals ........ 39
Chapter 4 – Fabricated Phononic Crystal Devices Operating in the MHz and GHz
  Frequency Ranges ............................................................................................................. 47
  4.1 Electro-elastic Transduction ................................................................................... 47
  4.2 Fabrication Process for W-SiO2 Phononic Crystals [52] ........................................ 56
  4.3 Fabrication Challenges in Solid-Solid Phononic Crystals [52] .............................. 59
  4.4 Effect of Release Holes on Micromachined Phononic Crystals [52] ..................... 62
  4.5 Phononic Crystal Devices Operating in the GHz Frequency Range [52] ............... 70
Conclusions ....................................................................................................................... 77
Appendix A ....................................................................................................................... 78
References ......................................................................................................................... 86
List of Figures

Figure 1 – An illustration of a phononic crystal showing the radius of the inclusions, \( r \) (green), in a host material (blue) and the lattice pitch, \( a \) .......................................................... 3

Figure 2 – Normalized bandgap width vs. \( r/a \) ratio for a PnC comprised of W rods in SiO\(_2\) background material. Results were produced using Finite Difference Time Domain (FDTD) simulations [32, 33] ........................................................................................................... 7

Figure 3 – Repeating cell (unit cell) in a phononic crystal ........................................... 8

Figure 4 – Velocity mismatch versus the inclusions radius to lattice pitch, \( r/a \), ratio required for optimum bandgap ................................................................. 10

Figure 5 – Schematic diagram of a 2D square lattice phononic crystal showing the distinct \( \Gamma X \) and \( \Gamma M \) directions of elastic wave propagation inside the crystal, the lattice pitch, \( a \), the lattice filling fraction, \( r/a \), the wavelength of the incident elastic wave \( \lambda \), and the Bragg and Mie resonance conditions necessary for realizing a spectral band gap [35] ........................................................................................................................................... 12

Figure 6 – Gap to mid-gap ratio comparison between the simple cubic, hexagonal and honeycomb arrangement of the W inclusions in the SiO\(_2\) medium, produced using the finite-difference time-domain method [32] ......................................................................................................................... 14

Figure 7 – Tungsten inclusions in SiO\(_2\) host matrix. The planes approximation method uses a number of planes, Plane \( P_1 \), with effective impedance \( (Z_1) \) and effective velocity \( (C_1) \) based on the filling fraction of the material constituents in plane \( P_1 \), and Plane \( P_2 \), with effective impedance \( (Z_2) \) and effective velocity \( (C_2) \) in Plane \( P_2 \) for the \( (a) \) \( \Gamma X \) and \( (b) \) \( \Gamma M \) directions in a square lattice to determine resonances taking place in the PnC. 17

Figure 8 – Wavelengths over which scattering of an elastic wave is expected to take place in a PnC in the \( \Gamma X \) direction .......................................................................................................................... 19

Figure 9 – The reflection coefficient vs. frequency using the PAM for a W-SiO\(_2\) PnC with \( r/a = 0.32 \) and \( a = 45 \) µm showing the resonance width for the fundamental resonance expected in the \( \Gamma X \) direction ........................................................................................................................................ 22

Figure 10 – Bandgap width in the \( \Gamma X \) direction using the planes approximation method ........................................................................................................................................... 23

Figure 11 – \( \Gamma X \) and \( \Gamma M \) Bragg resonance widths as well as their overlap. Light green represents only \( \Gamma X \) resonance width while black represents only \( \Gamma M \) resonance width. Dark green represents the overlap between the two resonance widths, i.e. the phononic bandgap ................................................................. 24

Figure 12 – A comparison between bandgap width vs. \( r/a \) using FDTD[32], PWE and PAM ........................................................................................................................................... 25

Figure 13 – A portion of a PnC, which extends to nine layers of W, and the corresponding chosen RLC tank model ......................................................................................... 27

Figure 14 – The RLC circuit model response for a PnC with W rods in SiO\(_2\) host medium with \( r/a \) ratio of 0.12 – two resonances are shown at 83.75 and 211 MHz, respectively, indicating the resonance frequency within the W rod as well as that within the SiO\(_2\) medium between two adjacent W rods, assuming a one-dimensional model. .......... 32

Figure 15 – Resonance frequencies in the W-SiO\(_2\) PnC model for various \( r/a \) ratios – as the \( r/a \) ratio increases, the higher frequency resonance moves to a lower frequency. This is expected since the resonance length within the W rods increases with the higher \( r/a \) ratio, which indicates that the wavelength, \( \lambda \), is longer which is why the resonance
frequency moves to a lower value. The lower frequency resonance, however, moves to a higher frequency as the r/a ratio increases. This is expected since the resonance length within the SiO$_2$ medium decreases as the r/a ratio increases, which indicates that the wavelength, $\lambda$, is shorter which is why the resonance frequency becomes higher with higher r/a ratios.  

Figure 16 – A demonstration of a phononic crystal showing the radius of the inclusions r and the lattice pitch a, as well as the directions referred to in the derivation of the plane wave expansion method  

Figure 17 – A comparison between the elastic band structure for the bulk 2D PnC made of an array of W of cylindrical cross section, arranged in a simple cubic lattice, embedded in a SiO$_2$ background with an r/a ratio of 0.32 using the CPWE and NPWE formulations mentioned above - The inset represents the first Brillouin zone (TXM) of the square array. The components of the wave vector $\vec{k}$ at the $\Gamma$, X and M points are $\pi/a (0,0)$ $\pi/a (1,0)$ and $\pi/a (1,1)$, respectively. A dimensionless frequency, $oa/C_t$ is reported on the vertical axis, where $C_t$ is the transverse elastic velocity in SiO$_2$. Note the faster convergence of the NPWE when compared to the conventional method for (a) 81 RLVs as well as (b) 441 RLVs.  

Figure 18 – The band structure of the same W-SiO$_2$ PnC using 1369 RLVs with the CPWE compared to the NPWE using only 81 RLVs - It is clear that even with 1369 RLVs, the CPWE fails to fully converge, asserting the need for using even more RLVs to reach full convergence. The computation time ratio between the two results, namely the NPWE using only 81 RLVs vs. CPWE using 1369 RLVs, is around 1:1000, which is extremely significant.  

Figure 19 – A comparison between the band structure obtained using 81 RLVs and 441 RLVs using the (a) NPWE and (b) CPWE for the same W-SiO$_2$ structure as in Figure 17.  

Figure 20 – Normalized Band gap width comparison (vs. r/a ratio) using FDTD (green diamonds) [32] and the NPWE (blue circles) with only 81 RLVs showing the agreement in band gap widths when both methods are utilized  

Figure 21 – The percent error in the first five bands at the X point ($\pi/a (1,0)$) showing the results obtained from using the CPWE and NPWE methods with 9, 25, 49, 81, 441, 841 and 1369 RLVs for the W-SiO$_2$ PnC. Notice that only 49 RLVs are needed for the modes obtained with the NPWE method to have an error less than 0.5%. Also notice the pseudo-convergence the CPWE shows at a lower number of RLVs (up to 81 RLVs), which can be deceiving, after which the modes start converging.  

Figure 22 – A qualitative example of the received signal when launched in (a) bulk material and (b) a phononic crystal  

Figure 23– (a) Individual couplers’ response and (b) overall couplers’ response  

Figure 24– (a) The Al-AlN-Al drive and sense set-up used to interrogate a phononic crystal showing the bottom electrode, the AlN film and the top electrode constituting the IDT fingers and (b) a top view of the Al fingers of the IDT showing the longitudinal wavelength, $\lambda_l$, and in-plane transverse wavelength, $\lambda_{in-plane}$  

Figure 25 – Experimental results for a single-frequency IDT showing the narrow-bandwidth nature of such couplers  

Figure 26 – The stack of Al-AlN-Al-Host in which the displacement wave propagates, used to calculate an average elastic wave speed in the composite
Figure 27 – An example of chirped coupler design for wider bandwidth IDTs, where $\lambda_3 < \lambda_2 < \lambda_1$ such that the higher frequency fingers are closer to the phononic crystal........ 53
Figure 28 – Experimental results for a chirped IDT showing the wider-bandwidth nature of such couplers if compared to Figure 25 ................................................................. 54
Figure 29– (a) Slanted coupler design and (b) experimental results for such design........ 55
Figure 30 – Fabrication Process for Solid-Solid phononic crystals comprised of W cylindrical inclusions in a SiO$_2$ host matrix, interrogated by AlN couplers................. 57
Figure 31 – (a) Angled and (b) planar SEM images of a W rod with release hole of 7.5 $\mu$m in its center. The circular profiles in the W ring are clear in the image, and are due to the two-step processs (steps b and c above) in the W deposition .............................. 58
Figure 32 – An example of the non-uniformity of the chemical mechanical polishing fabrication step, seen in the inset around the W rods, likely due to the large difference in flow stress mismatch between the W inclusions and the SiO$_2$ host medium ............... 60
Figure 33 – An SEM of a W-SiO$_2$ phononic crystal with $a = 45$ $\mu$m and $r/a = 0.32$ ...... 64
Figure 34 – PWE results for elastic propagation through a W-SiO$_2$ PnC with various release hole size, shown on each figure. Filled circles represent longitudinal branches and the crosses represent in-plane transverse modes. The shaded region in (a) is the full bandgap with no release holes, and as the release hole size gets progressively bigger; a longitudinal mode appears in the bandgap splitting it into two band gaps while progressively moving to a lower frequency. (b) $r_{air} = 2.5$ $\mu$m, (c) $r_{air} = 3.75$ $\mu$m, (d) $r_{air} = 5$ $\mu$m, (e) $r_{air} = 6.25$ $\mu$m, (f) $r_{air} = 7.5$ $\mu$m......................................................... 65
Figure 35 – FDTD (dashed line) [32] and experimental (line) transmission results through a W-SiO$_2$ PnC with a release hole radius of 3.75 $\mu$m compared with a band structure with longitudinal modes (filled circles). The in-plane transverse modes were ignored. The arrows show the corresponding y-axis ............................................................. 67
Figure 36 – FDTD (dashed line) [32] and experimental (line) transmission results through a W-SiO$_2$ PnC with a release hole radius of 7.5 $\mu$m compared with a band structure with longitudinal modes (filled circles). The in-plane transverse modes were ignored. The arrows show the corresponding y-axis .............................................. 68
Figure 37 – A comparison between transmission through a W-SiO$_2$ PnC with various release hole sizes, where $r_{air}$ is the radius of the airhole ......................................................... 69
Figure 38 – The fabrication process for the W-Si PnC ........................................................................ 73
Figure 39 – An SEM image showing the AlN layer, the Si membrane, Aluminum IDTs and the W inclusions in the PnC crystal ........................................................................ 74
Figure 40 – An SEM image showing the AlN layer, the Si membrane, Aluminum IDTs and the W inclusions in the matrix ........................................................................ 75
Figure 41 – (a) Normalized results for transmission through a PnC comparing FDTD [32] and experimental results, (b) the un-normalized experimental crystal and matrix responses.................................................. 76
List of Tables

Table 1 – Elastic speed, mass density and elastic impedance for materials commonly-used in the micro fabrication industry.............................................................................................................. 13
Table 2. The values of $\lambda$, $\omega$, $L$ and $C$ for the RLC resonator simulating the W rods’ response ........................................................................................................................................ 30
Table 3. The values of $\lambda$, $\omega$, $L$ and $C$ for the RLC resonator simulating the SiO$_2$ coupling response ................................................................................................................................... 31
Table 4 – Mass density $\rho$, longitudinal sound velocity $C_l$, elastic impedance $Z$, Young’s modulus $E$ and Poisson’s ratio $\nu$ for W, SiO$_2$ & Si...................................................................................................................... 40
Chapter 1 – Introduction

1.1 Definition

Phononic crystals (PnCs) are periodic composite structures comprised of two linear-elastic materials that differ in their elastic impedances [1]. The increasing interest in PnCs stems from the existence of complete phononic bandgaps (PnBGs), which are ranges of frequencies over which elastic waves are forbidden to propagate in any direction or polarization inside the crystal. Thus the crystal acts as a mirror to frequencies within the bandgap, and therefore many applications can utilize the rejection of propagating waves over this range of frequency.

PnCs are usually referred to as the mechanical analogues of photonic crystals [2] since in both cases the two-dimensional periodic array of scattering centers is embedded in a homogeneous host material (matrix) and the coherent scattering of phonons and photons, respectively, results in the creation of frequency gaps where wave propagation is forbidden. In the course of phononic crystals research, macro-scale PnCs were the first to be constructed and tested, limiting the operating frequency of the devices to the sub-MHz range, with the matrix material either being epoxy or water [3, 4]. After a number of theoretical [5-11] and experimental [12-14] studies were performed proving the existence of PnBGs in PnCs, devices on the micron-level were fabricated utilizing techniques from the well established microelectronics fabrication industry [15]. Fabricating such small devices has many advantages. First, the operating frequency is tremendously, at least 3 orders of magnitude, higher in the case of micron-level devices because of their smaller feature sizes, as will be discussed later. Furthermore, such miniature PnCs have applications in microelectronics and micro systems, especially in physically isolating
devices from the vibrations of other devices on the same substrate, or from the vibration of the substrate itself. Like other Micro-Electro-Mechanical Systems’ (MEMS) technologies, micro-machined PnCs utilize the tools of the microelectronics fabrication industry, leading to accuracy, precision, flexibility, speed and relative-ease of realizing new research ideas as well as a method to fabricate multiple devices in parallel. For these same reasons, micro-machined PnCs have higher yield when compared to hand-assembled macro-scale PnCs. An example of a PnC is shown in Figure 1, where six layers of inclusions are shown between the drive and sense areas of the device. The larger the number of layers between the sense and drive pads, the more scattering takes place and therefore the stronger this elastic-wave mirror acts to propagating waves. At least 9 layers were used in all simulations and fabricated devices in this manuscript unless otherwise stated.

It is worth noting that the naming convention of phononic crystals is not fundamentally accurate, but is widely accepted in the research community. Although ‘acoustic’ generally refers to frequencies between 20 Hz and 20 kHz, ‘phononic’ refers to extremely high frequencies (100’s of GHz to THz) and the terms ‘mechanical’ and ‘elastic’ are usually used irrelevant of frequency. The ‘phononic crystals’ name adopted in this field of study is used independent of the frequency range over which the bandgap exists. It is surmised that the similarities between the names photonic crystals and phononic crystals are what encouraged the general use of phononic for the entire range of frequencies rather than a more broadly applicable terminology. ‘Acoustic crystals’ is another name used by many researchers because of PnCs’ possible applications in
acoustic signal processing. All of the above names will be used interchangeably throughout this manuscript.

![Diagram of a phononic crystal](image)

*Figure 1 – An illustration of a phononic crystal showing the radius of the inclusions, \( r \) (green), in a host material (blue) and the lattice pitch, \( a \)*

### 1.2 Figures of Merit

We first define commonly-used terms in this field. The ‘width’ of the bandgap refers to the range of frequency over which transmission is suppressed. The ‘location’ of the bandgap refers to the center frequency of the bandgap. Finally, the ‘depth’ refers to the amount of rejection, in dB, of waves traveling through the crystal at frequencies within the bandgap, as compared to those traveling at frequencies outside of the bandgap.

The most important figure of merit for a PnC is the bandgap width. Precisely determining the width of a bandgap is crucial to the operation of a device. The wider the bandgap means that more operation bandwidth is available. However, a bandgap of 500
MHz, for example, is much more significant at 1 GHz than it is at 100 GHz; therefore the gap to mid-gap ratio is another figure of merit introduced to normalize the bandgap width with respect to the operating frequency range. This figure of merit is only necessary when comparing bandgaps at different frequencies. Finally, the last figure of merit for PnCs to be discussed here is the bandgap depth. A bandgap can be defined as the range of frequency over which the incident signal is attenuated more than 3 dB, which is the half power mark used in many communications applications. It can also be defined as 10 dB, 20 dB or any other rejection level of choice, since there has not been a standard set in the research community as of yet. The deeper the bandgap the more rejection that takes place for signals traveling with frequencies within the bandgap, which results in higher signal-to-noise ratios for devices operating within the bandgap. In this manuscript, 20 dB is used to demarcate the bandgap width.

### 1.3 Applications

To motivate PnCs as devices with a bright future, this section is included to highlight some of the possible applications in which PnCs can be utilized. Elastic bandgaps are especially important in communications where the suppression of noise and having a high signal-to-noise (SNR) ratio are essential to the operation of any filter. With rejection over a large range of frequency exhibited by a PnC for up to 30 dB [16], the bandgap frequency range can be manipulated to allow only desired signals to pass in a controlled filtering procedure. Such a feature can be explored further to perform multiplexing and creating devices leading to acoustic-logic based devices.

A PnC with specifically sized features can also act as a heat insulator or enhance thermal conductivity of the matrix material. By proper choices of material properties and
geometry the phononic crystals could act as perfect phonon-reflectors. Reflecting phonons over a desired range of frequency alters the density of states and therefore allows for controlling the amount of released heat associated with waves propagating at the desired frequency range [17].

Furthermore, PnC-based time delay devices can utilize the five orders of magnitude difference between the light and sound velocities to realize devices up to 100,000 times smaller than optics-based devices of similar functionality. For example, while it would require 300 m of fiber to realize an optical delay line with 1 µs total delay, it would only require 5.8 mm to realize a similar delay acoustically. The only extra step needed in PnCs (when compared to photonic crystals, its optical analogue) is the wave conversion from the electric to the mechanical domain as well as from the mechanical to the electric domain. Piezoelectric materials have been utilized with PnCs to perform this conversion. The field of piezoelectric materials is a relatively mature technology for which reason PnC-based devices are practical and can be very affordable.

Phononic crystals have also been used in liquid sensing [18]. In this case the peak shifts in transmission of waves with the liquid in a cavity, compared to the case with no liquid present in the cavity, describe some properties of the liquid in the cavity leading to identifying the liquid. This, however, has only been demonstrated in the macro scale at lower frequencies, which may be sufficient for many materials.

Other PnC-based devices such as waveguides [19-22], filters [23-26], structures for acoustic collimation [27], focusing [28], negative refraction [29, 30] and resonators [31] have also been demonstrated. With all of the above applications and many more,
phononic crystals have a very strong potential to be implemented in various commercial applications.

### 1.4 Parameter and Material Choice

There are a few parameters one can control to alter the characteristics of PnBGs. Specifically, material properties of the inclusion and the host media, the lattice pitch \( a \), the radius-to-lattice-pitch ratio \( r/a \), and the type of inclusions’ periodicity (i.e. lattice type) are all parameters that contribute to the width, location and depth of the bandgap created.

Varying the filling fraction \( ff \) (i.e. varying the \( r/a \) ratio, since in a simple cubic arrangement \( ff = \frac{\pi(r/a)^2}{a} \)), of the inclusions will alter the bandgap width. Generally speaking, there is an optimum filling fraction for which the bandgap width is maximized. Figure 2 shows the gap to mid-gap ratio vs. the \( r/a \) ratio for a device comprised of Tungsten (W) cylindrical inclusions periodically placed in a simple cubic arrangement in a host medium of Silica (SiO\(_2\)), taken as an example. It is clear that there is a maximum bandgap width which occurs at \( r/a = 0.32 \) for this specific device; therefore controlling the \( r/a \) ratio, which means changing the \( ff \) will have a profound effect on the width of the bandgap.
The lattice pitch, $a$, is generally linked to the frequency range over which the bandgap exists. To demonstrate this we consider the PnC shown in Figure 1, where the inclusions are placed in a simple cubic cell arrangement in the host medium. A repeating cell, called a unit cell, is examined below, and because of the periodicity of the structure we can extend the analysis on a unit cell to the entire structure. The unit cell shown in Figure 3 is of size $a^2$. The average elastic wave speed in the unit cell can be approximated by using a simple ‘rule of mixtures’ formulation as follows:

$$C_{\text{avg}} = \left( \frac{\pi r^2}{a^2} \right) C_i + \left[ 1 - \left( \frac{\pi r^2}{a^2} \right) \right] C_{\text{host}},$$

(1)

where $C_i$, $C_{\text{host}}$ and $C_{\text{avg}}$ are the propagation speeds in the inclusion, host and unit cell, respectively.
respectively. The average speed is used to find an estimate of the center frequency of the bandgap where if a first harmonic (shown in Figure 3 as well) is assumed, the center frequency of the range of frequencies to be rejected by the crystal can be calculated as follows:

\[ f_{\text{center}} = \frac{C_{\text{avg}}}{\lambda} = \frac{C_{\text{avg}}}{2a}, \]  

(2)

where \( f_{\text{center}} \) is the center frequency of the bandgap and \( \lambda \) is the wavelength of the propagating elastic wave. Therefore, the location of the PnBG is inversely proportional to the lattice pitch; as such it is a key parameter in designing PnCs.

![Phononic Crystal Diagram](image)

*Figure 3 – Repeating cell (unit cell) in a phononic crystal*

From Eqn. (2) it is clear that a smaller and smaller lattice pitch, \( a \), is needed to design PnCs with bandgaps at higher frequencies. At such small sizes (when, say, \( a < 1 \mu m \)), liquid-solid (liquid inclusions in a solid host medium) PnCs are not practical because of packaging limitations as well as stiction issues during release (the entire PnC fabrication process is discussed in Section 4.2. Hence there are two remaining practical options at higher frequencies, air-solid and solid-solid PnCs.
Air-solid PnCs have the advantage of having at least three steps less (inclusion deposition and CMP as well as release hole etching) than solid-solid PnCs. Fewer fabrication steps make air-solid PnCs cheaper and may allow for more precise fabrication of devices. Furthermore, eliminating release holes in the center of the inclusions (applicable only to air-solid PnCs, and solid-solid PnCs operating in the GHz range) is also very advantageous as it helps avoid many problems during the fabrication of solid-solid PnCs, as discussed in Section 4.2. The release hole issue, however, becomes irrelevant at higher frequencies for solid-solid PnCs (around 500 MHz or higher, depending on chosen materials) where devices can be released entirely through the release pits on both sides of the device and no release holes are needed.

As shown in Figure 2, varying the \( r/a \) ratio will change the width of the bandgap leading to an optimum \( r/a \) for the widest bandgap. For air-solid PnCs, because the velocity mismatch between air and any solid is very high \( (C_{\text{host}} >> C_{\text{inclusion}}) \), a very high filling fraction is needed to obtain the optimum (widest) bandgap, as predicted by Figure 4. This translates to a very small minimum feature size, i.e. the spacing between the inclusions is \(< 0.1a\), during lithography and therefore the air-solid PnC requires greater fabrication precision at a given frequency. On the other hand, solid-solid PnCs have larger minimum feature size, i.e. the spacing between adjacent inclusions is \(< 0.36a\) because of the lower elastic velocity mismatch between the carefully-chosen solid material constituents used in the PnC when compared to the velocity mismatch between air and any solid. This translates into more reliable devices as well as wider bandgaps as can be seen when comparing results reported in [34] to those reported in [16] where the gap-to-mid-gap ratios for an air-solid and a solid-solid PnC were 23% and 44%,
respectively. Therefore, it is clear that solid-solid PnCs have a wider bandgap and a larger minimum feature size because the solid inclusion has a lower elastic velocity mismatch than air does with a solid host medium, which makes solid-solid PnCs advantageous despite the extra fabrication steps and the associated cost. As shown in Figure 4, the lower the velocity mismatch, the lower the filling fraction needed for an optimum bandgap and therefore the larger the minimum feature size; i.e. the easier and more repeatable the fabrication process is. Because the optimum bandgap is obtained with a solid-solid PnC with a relatively small filling fraction ($r/a = 0.32$ compared to $r/a = 0.44$ for air-solid), we choose to address solid-solid PnCs throughout this manuscript. Air-solid PnCs will not be discussed further in this manuscript except for contrast. The following is a discussion of how Figure 4 was created.

![Figure 4](image)

*Figure 4 – Velocity mismatch versus the inclusions radius to lattice pitch, r/a, ratio required for optimum bandgap*
To investigate the reason for solid-solid PnCs having a larger minimum feature size we first introduce the physical origins of PnBGs, which will be discussed in detail in Chapter 2. Phononic bandgaps arise when the Bragg resonances overlap leading to a wide resonance and a decline in transmission for those resonating frequencies. The two Bragg resonance directions are shown in Figure 5 along with the Mie resonance. With the Mie resonance adding to the width of either Bragg resonance, the overall unidirectional bandgap width is expected to be wider when all three resonances partially overlap. Figure 4 was obtained by setting the fundamental Mie resonance equal to the two Bragg resonance frequencies for the square lattice arrangement obtained using

\[ f_{\text{Mie}} = \frac{C_i}{4r}, \quad (3) \]

\[ f_{\text{Bragg}X} = \frac{C_{\text{Bragg}X}}{2a}, \text{ and} \quad (4) \]

\[ f_{\text{Bragg}M} = \frac{C_{\text{Bragg}M}}{2\sqrt{2}a}. \quad (5) \]

In Eqns. (3) through (5), \( C_{\text{Bragg}X} = C_{\text{Bragg}M} = C_{\text{avg}} \) and are calculated as an average shown in Eqn. (1) above, \( f_{\text{Mie}} \) is the Mie resonance frequency based on each inclusions’ size, \( f_{\text{Bragg}X} \) is the resonance frequency based on two adjacent inclusions in the \( \Gamma X \)-direction in the first Brillouin zone, and \( f_{\text{Bragg}M} \) is the resonance frequency based on two adjacent inclusions in the \( \Gamma M \)-direction in the first Brillouin zone. Setting Eqns. (3) & (4) equal and rearranging, we get:

\[ \frac{r}{a} = \frac{C_i}{2C_{\text{avg}}} \quad (6) \]
for the first case in which $f_{\text{Mie}}$ is set equal to $f_{\text{Bragg}}$. Similarly, setting Eqns. (3) & (5) equal and rearranging, we get:

$$\frac{r}{a} = \frac{C_i}{\sqrt{2C_{\text{avg}}}}$$

(7)

for the second case in which $f_{\text{Mie}}$ is set equal to $f_{\text{Bragg}}$. Figure 4 is a plot demonstrating the difference between Eqns. (6) and (7). This plot demonstrates the superiority of solid-solid PnCs compared to air-solid PnCs, as discussed earlier in this section.

![Figure 5](image)

**Figure 5** — Schematic diagram of a 2D square lattice phononic crystal showing the distinct $\Gamma X$ and $\Gamma M$ directions of elastic wave propagation inside the crystal, the lattice pitch, $a$, the lattice filling fraction, $r/a$, the wavelength of the incident elastic wave $\lambda$, and the Bragg and Mie resonance conditions necessary for realizing a spectral band gap [35].

The main factor, however, that controls the width of the bandgap is the mismatch of the elastic impedances ($Z$) of the inclusion and matrix materials. $Z$ is defined as

$$Z = \sqrt{E\rho},$$

(8)
where \( E \) is Young’s modulus (in Pa) and \( \rho \) is the mass density (in kg/m\(^3\)) and \( V^2 = E/\rho \). It was believed initially that the mass density mismatch is the main factor controlling the PnBG width [5], which was later corrected [1, 6]. The inclusions act as mirrors to the propagating waves, and therefore the higher the elastic impedance mismatch between the inclusions and the host medium the stronger the elastic wave will be scattered at the interfaces therefore the deeper and wider the bandgap is. Table 1 shows the phononic-crystals-relevant material properties for some of the commonly-used materials in the micro / nanofabrication laboratories.

### Table 1 – Elastic speed, mass density and elastic impedance for materials commonly-used in the micro fabrication industry

<table>
<thead>
<tr>
<th>Material</th>
<th>Young’s Modulus (GPa)</th>
<th>Elastic Speed ( C = \sqrt{E/\rho} ) (m/s)</th>
<th>Mass Density (kg/m(^3))</th>
<th>Elastic Impedance (kg/(m(^2)s))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poly-Si</td>
<td>155</td>
<td>8,520</td>
<td>2,330</td>
<td>19.8 x 10(^6)</td>
</tr>
<tr>
<td>Silica</td>
<td>75</td>
<td>5,840</td>
<td>2,100</td>
<td>12.8 x 10(^6)</td>
</tr>
<tr>
<td>Tungsten</td>
<td>410</td>
<td>4,611</td>
<td>19,250</td>
<td>89 x 10(^6)</td>
</tr>
</tbody>
</table>

Finally, because the Bragg and Mie resonances are different for different lattice structures, the order in which the inclusions are arranged in the host medium (i.e. the inclusion’s lattice type) is also another parameter that alters the PnBG width and location. The bandgap width for a PnC with inclusions arranged in a simple cubic array versus one with inclusions arranged in a hexagonal or honeycomb array will be different; this is shown in Figure 6. In this manuscript, we will discuss only the simple cubic arrangement.
The resonances in the square lattice are similar to those in the hexagonal lattice in the \( \Gamma X \) direction, whereas in the \( \Gamma M \) direction the resonance in the hexagonal lattice is longer. This indicates that the frequency at which the resonance in the \( \Gamma M \) direction takes place is lower in the hexagonal lattice than that in the simple cubic lattice, which in turn means that less overlap takes place between the resonances in the \( \Gamma X \) direction and the \( \Gamma M \) direction. We will introduce the concept of overlapping resonance frequency in different lattice directions in Section (2.4).
Chapter 2 – Physical Origins of Phononic Bandgaps

2.1 Introduction

Various methods have been utilized to model elastic propagation in phononic crystals including the plane-wave-expansion \([36]\) and finite difference time domain \([33]\) methods, both of which will be used in this manuscript. However, both methods provide no insight in the physical origins of phononic bandgaps. Furthermore, both methods rigorously solve equations of motion for elastic waves in a complex structure, which inevitably consumes resources. This section explains how PnBGs are realized and provides a simple method to pre-determine whether the choices of materials, filling fraction, lattice pitch ‘\(a\)’ and inclusions’ arrangement in the host medium will provide the desired PnBG.

To understand how phononic bandgaps are formed we employ a new method dubbed the Planes Approximation Method (PAM). This method estimates, using the underlying physics principles, the PnBG that would result with a specific material set for any physically allowed filling fraction. The PAM renders a two-dimensional problem into a one-dimensional problem as a means by which the time to complete a simulation run is tremendously reduced. Analyzing scattering within the crystal using the PAM (as opposed to studying and adding the scattering of every cylindrical inclusion) helps avoid the more complex problem of cylindrical scattering throughout the crystal, which is a sum of terms of periodic functions \([36]\), and gives insight to explain why PnBGs exist and how to manipulate them. In the following sections, the formulation of the method is introduced followed by a discussion of the obtained results.
2.2 Formulation

The PAM assumes a two-dimensional PnC to be a number of alternating layers placed in the path of a longitudinal elastic wave instead of the cylindrical inclusions in the host matrix, as shown in Figure 7. For a PnC of square lattice type, with lattice constant ‘a’ and made of cylindrical Tungsten (W) inclusions in a silicon dioxide (SiO₂) matrix (host medium), we assume that the PnC is split into planes P₁, P₂, P₃…Pₙ, where n is the total number of planes in the structure. Each plane can be treated as a “hybrid” plane made of a new homogenized material, the properties of which can be obtained using the effective material properties of the plane’s material constituents via a weighted averaging formulation. The material properties of each plane are obtained proportionally using the properties of the material constituents of the plane as well as the filling fraction each material within the plane occupies, as seen by Eqns. 10 and 11. For plane P₁, the effective impedance, mass density and elastic velocity are $Z₁$, $ρ₁$ and $C₁$; these same properties of plane 2 are $Z₂$, $ρ₂$ and $C₂$, respectively. For the specific case shown in Figure 8, the material properties of P₃ are the same as those of P₁, due to the periodicity.

To calculate the effective elastic speed within plane P₁, the filling fraction of the inclusions within P₁ ($ff_1$) is obtained using a repeating cell (the white-background square shown in Figure 7a) such that,

$$ff_1 = \frac{πr^2}{2ra},$$

(9)

where $r$ is the radius of the cylindrical inclusion and $a$ is the lattice constant of the PnC. The filling fraction is a measure of the amount of inclusions material present in the repeating cell and therefore the entire structure. Then, the effective elastic impedance within plane P₁, $Z_{eff1}$, is given by
Figure 7 – Tungsten inclusions in SiO$_2$ host matrix. The planes approximation method uses a number of planes, Plane $P_1$, with effective impedance ($Z_1$) and effective velocity ($C_1$) based on the filling fraction of the material constituents in plane $P_1$, and Plane 2, with effective impedance ($Z_2$) and effective velocity ($C_2$) in Plane $P_2$ for the (a) $\Gamma X$ and (b) $\Gamma M$ directions in a square lattice to determine resonances taking place in the PnC.
\[ Z_{\text{eff}1} = f f_1 Z_W + (1-f f_1) Z_{\text{SiO}_2}, \]  

and the effective elastic speed of plane P₁, \( C_{\text{eff}1} \), is given by

\[ C_{\text{eff}1} = f f_1 C_W + (1-f f_1) C_{\text{SiO}_2}, \]

where \( Z_W, C_W, Z_{\text{SiO}_2} \) and \( C_{\text{SiO}_2} \) are the elastic impedance and elastic speed of W and SiO₂, respectively. Utilizing the symmetry of a square lattice, the first Brillouin zone includes only two directions, \( \Gamma X \) and \( \Gamma M \) [38], as shown earlier in Figure 5. \( \Gamma X \) and \( \Gamma M \) directions will contribute scattering in a similar manner since both directions look identical to a normal incident wave, and therefore will not be calculated separately to avoid redundancy; only scattering and reflection along the \( \Gamma X \) and \( \Gamma M \) directions are needed to yield a complete solution for scattering within the PnC slab.

We now study the reflection (and transmission) off of each interface between adjacent planes. Using the conditions shown in Figure 5, the resonant frequency for a plane is calculated from

\[ f_{\text{res}} = \frac{C_{\text{eff}}}{\lambda}, \]  

where \( C_{\text{eff}} \) is the effective elastic speed in the plane and \( \lambda \) is the wavelength of the incident elastic wave.

Bragg resonances, which inevitably occur due to the creation of standing waves between adjacent cylinders, must overlap to create a wide bandgap. At this point we have a way by which to calculate the resonant center frequency for each homogenized plane. Indeed, the resonant frequency in each distinct direction in the phononic crystal is not a single-mode resonance. Rather, the resonance possesses a bandwidth of scattering that extends from frequencies corresponding to wavelength \( \lambda_{\text{min}} = 2(a - 2r) \) to frequencies corresponding to wavelength \( \lambda_{\text{max}} = 2(a + 2r) \). This is the wavelength range over which
disturbance and scattering will occur at any given period of an incident elastic wave, as shown in Figure 8. To obtain such a bandwidth we employ a recursive method borrowed from electromagnetic theory and transformed to apply to the elastic wave case. This method allows for finding an approximation to the resonance width per frequency and therefore the overall reflection at each single frequency leading to identifying the frequencies over which transmission is tremendously reduced, i.e. the bandgap. In the next section we discuss the recursive reflection equation borrowed from electromagnetic theory and how to transform it to apply to our elastic wave reflection problem.

Figure 8 – Wavelengths over which scattering of an elastic wave is expected to take place in a PnC in the ΓX direction

2.3 Recursive Reflection Equation

In electromagnetic theory [39] if a similar structure as in Figure 7a exists, the total reflection for a wave propagating at a specific frequency is obtained by finding the single reflection off of each surface, $r_i$, where $i$ is the interface index, which is then used in the recursive relation
$$\Gamma_i = \frac{r_i + \Gamma_{i+1}e^{-2jk_i l_i}}{1 + r_i \Gamma_{i+1}e^{-2jk_i l_i}},$$  \hspace{1cm} (12)$$

Where \( \Gamma_i \) is the total reflection off of the entire surface at a given frequency, \( k_i = 2\pi\lambda_i \), is the wave number, \( \lambda \) is the corresponding wavelength within the plane and \( l_i \) is the width of the plane. The entire derivation of Eqn. 12 can be found in [39]. Replacing \( k_i l_i \) with \( 2\pi L_i / \lambda \), where \( L_i \) is the length of the elastic resonance in the \( i^{th} \) plane (shown in Figure 7) and replacing the electromagnetic wave impedance, \( \eta \), with the inverse of the elastic impedance, \( 1/Z \), we transform Eqn. (12), used for electromagnetic wave reflection, into an equation that can be used for elastic wave reflection in a periodic one-dimensional medium. Then, the overall reflection coefficient using the PAM, \( \Gamma_i \), can be determined by using the recursive relation

$$\Gamma_i = \frac{R_i + \Gamma_{i+1}e^{-4\pi l_i \lambda}}{1 + R_i \Gamma_{i+1}e^{-4\pi l_i \lambda}},$$  \hspace{1cm} (13)$$

where \( i = n, n-1, \ldots, 2, 1 \) is the number of interfaces between planes, \( n+1 \) is the number of planes chosen for the calculation, \( L_i \) is the width of the \( i^{th} \) plane, \( j = \sqrt{-1} \), \( \lambda \) is the wavelength of the incident wave and is calculated as \( \lambda = C_{\text{medium}}/f \) for each frequency step in the frequency range of interest, and \( R_i \) is the reflection coefficient between the \((i-1)^{st}\) interface and the \(i^{th}\) interface, and is calculated by

$$R_i = \frac{Z_i - Z_{i+1}}{Z_i + Z_{i+1}}.$$  \hspace{1cm} (14)$$

The recursive relation above is initialized by

$$\Gamma_n = R_n.$$  \hspace{1cm} (15)$$
This recursive relation determines the width of the resonance by calculating the total reflection coefficient off of the multilayered structure per frequency.

2.4 Results

Figure 9 shows the results for the overall reflection coefficient vs. frequency over the frequency range of interest for a W-SiO₂ PnC with a lattice constant of 45 μm and an inclusion radius of 14.4 μm arrayed in a simple cubic lattice \((r/a = 0.32)\). The fundamental resonance was taken since the bandgap center frequency is expected to be at \(f = C_{avg}/2a\), which corresponds to a frequency of 60 MHz in our device. The criterion for a bandgap was taken to be 20 dB reduction in transmission for any given frequency. Choosing a 20 dB reference to determine the frequencies constituting the edges of the gap for all relevant \(r/a\) ratios, 0.1 – 0.49, gives the bandgap width for every \(r/a\) ratio for the specific direction \((IX\) is the direction that has been discussed so far.)
Figure 9 – The reflection coefficient vs. frequency using the PAM for a W-SiO$_2$ PnC with $r/a = 0.32$ and $a = 45$ µm showing the resonance width for the fundamental resonance expected in the $\Gamma X$ direction.

The bandgap width obtained using the PAM is shown in Figure 10 for the W-SiO$_2$ PnC in the $\Gamma X$ direction. It is clear from the figure that the resonance width in a plane in the $\Gamma X$ direction using the PAM changes smoothly versus $r/a$ ratio. However, this bandgap is really a pseudo-bandgap since it only takes into account one of the two independent directions in a square lattice or in a simple cubic arrangement. The calculation for the other direction, the $\Gamma M$ direction, is similar to that of the $\Gamma X$ directions with slight changes. For the $\Gamma M$ direction, a set of planes as shown in Figure 7b are considered. The calculation above is repeated for the $\Gamma M$ direction with the main difference that the width of $P_2$ is now $(a\sqrt{2})$.

Figure 10 – Bandgap width in the $\Gamma X$ direction using the planes approximation method
Figure 11 shows the resonance widths in both directions as functions of the $r/a$ ratio. The bandgap in the $\Gamma X$-direction is at a higher frequency than the bandgap in the $\Gamma M$-direction. This is to be expected since the planes are wider in the $\Gamma M$-direction than they are in the $\Gamma X$-direction. This means that in each direction within the crystal the Bragg resonances prevent certain frequencies from propagating through and instead form a standing wave within the planes. A direct result of the difference in frequency is that the two resonances will never directly overlap, but with some design considerations, a partial overlap (shown in dark green in Figure 11) is possible. A phononic bandgap will be created only in the region in which the two Bragg resonances overlap. In the regions in which there is no overlap, propagating waves outside of the overlap spectrum will only be suppressed in one direction and not the other, therefore propagating through the crystal and do not become a part of the bandgap.

Frequencies outside of the overlap region will propagate through the other direction, in which that specific frequency does not create a bandgap. This becomes clear when considering a mode propagating in this device at a frequency of 70 MHz. While that frequency is inhibited to exist in the $\Gamma X$ direction, it can freely propagate in the $\Gamma M$ direction and therefore will not lead to a complete phononic bandgap. Rather, only frequencies in the overlap region will constitute the phononic bandgap.

The one-dimensional solution to the two-dimensional problem is not expected to give exact results. However, many qualitative pieces of data can be obtained. Bandgap width obtained using the plane wave expansion (PWE) method (discussed in Chapter 3) and finite difference time domain (FDTD) [32] are compared to those obtained using the PAM, i.e. the overlap region between the Bragg resonances, in Figure 12. While the
Figure 11 – $\Gamma X$ and $\Gamma M$ Bragg resonance widths as well as their overlap. Light green represents only $\Gamma X$ resonance width while black represents only $\Gamma M$ resonance width. Dark green represents the overlap between the two resonance widths, i.e. the phononic bandgap.

The phononic bandgap width is not entirely as accurate as those given by PWE and FDTD [32], PAM serves two main purposes. From the figure, it is seen that PAM shows good qualitative agreement with the other two methods, albeit requiring very little computational resources and time. First, it shows a great agreement in the general form of the curve. This is extremely helpful for a designer in determining the best $r/a$ ratio to use for a wide PnBG to appear with very little time consumed. In fact, the amount of time for the results to be obtained by the PAM vs. FDTD [32] is on the order of 1: 2800. Second, the PAM captures the physical origins of phononic bandgaps while generating a bandgap as
well, which is a feature that cannot be obtained using any of the two-dimensional methods such as PWE or FDTD.

![Graph](image_url)

*Figure 12 – A comparison between bandgap width vs. r/a using FDTD[32], PWE and PAM*

A worthy observation to be noted is that the resonance, or the bandgap, in the \( \Gamma X \) direction is wider than that in the \( \Gamma M \) direction. One possible explanation for such a difference is that in the \( \Gamma X \) direction, the planes have a higher elastic impedance mismatch than that in the \( \Gamma M \) direction. This is clear when comparing plane P2 in both cases. In the \( \Gamma X \) case, P2 has material properties of SiO2 only, whereas P2 in the \( \Gamma M \) direction has hybrid material properties depending on both W and SiO2. This creates a higher elastic impedance mismatch in the \( \Gamma X \) direction, which in turn results in a wider bandgap that that in the \( \Gamma M \) direction. This can be contrasted with the hexagonal lattice where the width of the bandgap in the \( \Gamma M \) direction is wider for the hexagonal lattice that that of the square lattice because of the longer resonance width, and therefore the lower
filling fraction in $P_2$ in the hexagonal case. The lower filling fraction in plane $P_2$ in the $\Gamma M$ direction of the hexagonal lattice compared to that of the square lattice means that the elastic impedance between $P_1$ and $P_2$ in the $\Gamma M$ direction in the hexagonal lattice is lower; therefore the resonance width is also lower than that of the $\Gamma M$ direction of the square lattice. Therefore, the overlap between the $\Gamma X$ and $\Gamma M$ resonances in the hexagonal lattice is less than that in the square lattice, which explains why the hexagonal lattice has a slightly narrower bandgap than that of the square lattice, as shown in Figure 6.

2.5 Modeling the Mie Resonance

After establishing that the Bragg resonances are the main reason for a phononic bandgap to be created using the PAM, it is desired to learn the contribution of the Mie resonance, if any, to the creation of the phononic bandgap. For this reason, a one-dimensional RLC circuit model that simulates the Mie resonance within a phononic crystal was designed. Figure 13 shows a portion of a PnP and the corresponding circuit model to-be used. In this model, the W rods are simulated by a parallel RLC tank, RLC$_1$, with a resonant frequency corresponding to the resonant frequency inside the W rods, with resonance length of $2r$, while the SiO$_2$ host medium, with resonance length $(a-2r)$ was also simulated by a parallel RLC tank, RLC$_2$, with a resonant frequency corresponding to that in the SiO$_2$. This one-dimensional RLC model was taken in the $\Gamma X$ direction.
To get an accurate model of the Mie resonance that takes place inside the inclusions, three design criteria were introduced, as follows:

1. The quality factor of the RLC tanks should be equal, i.e. $Q_{RLC_1} = Q_{RLC_2}$, since $Q$ is directly related to $\Gamma$, the reflection coefficient at the cylinders’ interface, via the equation:

$$Q = 2\pi \frac{E_{\text{stored}}}{E_{\text{lost}}/\text{cycle}},$$

where $E_{\text{stored}}$ is the power reflected back into the W rod and $E_{\text{lost}}$ is the power transmitted through the W rod’s interface into the SiO$_2$ medium. $|\Gamma|$ is equal from either side of the interface between the two materials because the magnitude of $\Gamma$ depends only on the material properties around the interface and therefore is the same on either side of the interface. Therefore:

$$E_{\text{stored}} = \Gamma^2 \text{ and } E_{\text{lost}} = (1 - \Gamma)^2.$$
Considering there are two reflections that take place inside the W rod per cycle, we get

\[ E_{\text{stored}} = (\Gamma^2)^2 \] and \[ E_{\text{lost}} = ((1 - \Gamma)^2)^2. \] \hfill (18)

Therefore, quality factors \((Q)\) for both tanks have to be the same since \(|\Gamma|\) is the same on all interfaces between the W rods and the SiO\(_2\) medium. By substituting Eqn. (18) in Eqn. (16) we have

\[ Q = 2\pi \frac{\Gamma^4}{(1 - \Gamma^2)^2}. \] \hfill (19)

and the \(Q\) of a parallel RLC tank is also equal to:

\[ Q = \frac{R}{\omega_o L}. \] \hfill (20)

where \(R\), \(L\), and \(\omega_o\) are the resistance, inductance, and resonance frequency of the RLC tank, respectively.

2. The resonant frequency inside the W rod is

\[ \omega_{\text{res}} = 2\pi \frac{C}{\lambda}, \] \hfill (21)

where \(\frac{\lambda}{2} = 2r\), i.e. \(\lambda = 4r\) and \(C\) is the elastic wave velocity for W, and the resonant frequency of an RLC tank is defined as

\[ \omega_o = \frac{1}{\sqrt{LC_i}}. \] \hfill (22)

\(C_i\) is the capacitance of the RLC tank. The resonant frequency, and therefore the RLC circuit components, will change value as the \(r/a\) ratio changes according to a number of equations, which are defined presently. Because the parameters of the circuit model change with \(r/a\), a circuit model per \(r/a\) value is required.
3. The ratio of the impedances in the RLC tanks have to be equal to the ratio of the elastic impedance between W and SiO₂, and we have

\[
\frac{Z_1}{Z_2} = \frac{Z_W}{Z_{ox}} = \frac{89}{12.8}, \tag{23}
\]

while the equation for the impedance of a parallel RLC tank is:

\[
Z = \frac{\sqrt{L}}{\sqrt{C}}, \tag{24}
\]

We can now use the above equations to obtain the design values for \( R, L, C \), and \( \omega_0 \), as follows:

Using Eqn. (24), we get

\[
L = Z^2 C, \tag{25}
\]

and using Eqns. (22) and (25), we get:

\[
C_i = \frac{1}{\omega Z}. \tag{26}
\]

To get the resistance and the resonance frequency, which are the only parameters needed to complete the design of RLC, we first find the reflection coefficient, \( \Gamma \) using

\[
\Gamma = \frac{Z_1 - Z_2}{Z_1 + Z_2} \tag{27}
\]

and the quality factor, \( Q \) using Eqn. (19) to be 10.202. Then, the resistance and resonance frequency of the RLC tank are obtained using Eqns. (20) and (21), respectively, such that

\[
R = Q\omega L, \tag{28}
\]

and

\[
\omega = 2\pi \frac{C}{\lambda}. \tag{29}
\]
where $\lambda_1 = 2L_i$ is obtained by the resonance length dictated by the specific $r/a$ ratio and $C$ in Eqn (29) is the elastic wave speed. The equations used are the same for both RLC tanks except that the length of $\lambda$ is calculated differently based on the $r/a$ ratio. For the RLC tank representing the W rods, $\lambda/2 = 2r$ or $\lambda = 4r$, whereas in the case of the RLC tank simulating the resonance in the SiO$_2$ medium $\lambda/2 = a-2r$, or $\lambda = 2(a-2r)$. Eqns. (25, 26, 28) and (29) define the design parameters for the RLC tanks used to simulate the Mie resonance in the W and in the SiO$_2$. It is worth noting that in Eqn. (28), the product $\omega L$ is

<table>
<thead>
<tr>
<th>$r/a$</th>
<th>$\lambda$ (µm)</th>
<th>$f_{\text{res W}}$ (MHz)</th>
<th>$\omega_{\text{W}}$ (MHz)</th>
<th>$L_{1, \text{W}}$ [H]</th>
<th>$C_{1, \text{W}}$ [F]</th>
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<td>335.32</td>
<td>2.65E-01</td>
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</tr>
</tbody>
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always a constant, yielding a constant value for the resistance, \( R \), for each RLC tank. The values for these RLC tanks were obtained from Eqn. (28) for the case of W-SiO\(_2\) PnC model to be \( R_W = 908 \) M\( \Omega \) and \( R_{SiO_2} = 131 \) M\( \Omega \), independent of the \( r/a \) ratio.

Table 2 and Table 3 demonstrate how the equations above were used to model the Mie resonance in a phononic crystal using an RLC model, along with the values obtained when the equations above are used. Using the design criteria above, we obtain the Mie resonance for several \( r/a \) cases sufficient to show the trend of the location of the Mie resonance.

**Table 3. The values of \( \lambda, \omega, L \) and \( C \) for the RLC resonator simulating the SiO\(_2\) coupling response**

<table>
<thead>
<tr>
<th>( r/a )</th>
<th>( \lambda ) (( \mu m ))</th>
<th>( f_{res, SiO_2} ) (MHz)</th>
<th>( \omega_{SiO_2} ) (MHz)</th>
<th>( L_{2, SiO_2} ) [H]</th>
<th>( C_{2, SiO_2} ) [F]</th>
</tr>
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<tbody>
<tr>
<td>Range</td>
<td>= 2(a-2r)</td>
<td>= ( C_{SiO_2}/\lambda )</td>
<td>= 2( \pi f_{res, SiO_2} )</td>
<td>= ( Z_{SiO_2} / \omega )</td>
<td>= 1/(( \omega Z_{SiO_2} ))</td>
</tr>
<tr>
<td>0.12</td>
<td>68.4</td>
<td>85.38</td>
<td>536.46</td>
<td>2.39E-02</td>
<td>1.46E-16</td>
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<tr>
<td>0.14</td>
<td>64.8</td>
<td>90.12</td>
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<tr>
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<td>599.57</td>
<td>2.13E-02</td>
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<tr>
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<td>1622.22</td>
<td>10192.72</td>
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resonance. Figure 14 shows the RLC circuit model response for a PnC with W rods in SiO₂ host medium with \( r/a \) ratio of 0.12. Two resonances appear in Figure 14, one at 84.17 MHz and the other at 212 MHz. When the model is repeated for higher \( r/a \) ratios, the higher frequency resonance moves to a lower frequency as the \( r/a \) ratio increases. This is expected since the resonance length within the W rods increases with the higher \( r/a \) ratio, which indicates that the wavelength, \( \lambda \), is longer which is why the resonance frequency is lower. The lower frequency resonance, however, moves to a higher frequency as the \( r/a \) ratio increases. This is also expected since the resonance length within the SiO₂ medium decreases as the \( r/a \) ratio increases, which indicates that the wavelength, \( \lambda \), is shorter which is why the resonance frequency becomes higher with higher \( r/a \) ratios. Figure 15 shows the transition of the higher and lower frequency resonances as the \( r/a \) ratio changes. Three important points arise from Figure 15. The first is that the resonance frequency in cases for \( r/a < 0.34 \) is higher than the location of
the phononic bandgap as predicted by FDTD and PWE (as will be shown later in Chapter 4, Figure 35), which means that the Mie resonance for this material set for $r/a$ ratios < 0.34 does not contribute to the creation of a phononic bandgap. However, as the Mie resonance goes lower in frequency (with higher $r/a$ ratios), it is clear that it can contribute to the bandgap operating at a frequency close to the edge of the bandgap. The second issue is that for $r/a = 0.2$ and $r/a = 0.24$, the two resonance frequencies are very close. The effect of such proximity of both resonance frequencies is that, for such an $r/a$ ratio, the Mie resonance is wider. The third issue deduced from Figure 15 is that for $r/a = 0.22$ for this material set, when the two resonances are exactly identical, the Mie resonance depth is enhanced.

Therefore, the Mie resonance can either contribute to a phononic bandgap by adding width or depth, not both, to the current phononic bandgap created by the Bragg resonances. Although this does not apply in this material set in cases where $r/a < 0.34$ since the Mie resonance appears at a higher frequency that the location of the phononic bandgap as predicted by FDTD, it does applies to higher $r/a$ ratios in this material set and it can apply for other material sets where the Mie resonance is closer in frequency to the location of the phononic bandgap. One final note here is that an output resistance of 908 MΩ, which is the same as the resistance used for the RLC tank simulating the W rods, was used for the simulation. If another resistance value was used at the output port, the $Q$ of the resonant frequency would be different from the values reported here, which limits this method to producing qualitative data and not quantitatively accurate width and depth of the Mie resonance.
Figure 15 – Resonance frequencies in the W-SiO₂ PnC model for various r/a ratios – as the r/a ratio increases, the higher frequency resonance moves to a lower frequency. This is expected since the resonance length within the W rods increases with the higher r/a ratio, which indicates that the wavelength, \( \lambda \), is longer which is why the resonance frequency moves to a lower value. The lower frequency resonance, however, moves to a higher frequency as the r/a ratio increases. This is expected since the resonance length within the SiO₂ medium decreases as the r/a ratio increases, which indicates that the wavelength, \( \lambda \), is shorter which is why the resonance frequency becomes higher with higher r/a ratios.
Chapter 3 – The Plane-Wave-Expansion Method for Modeling Phononic Crystals

3.1 Overview

Many modeling techniques have been utilized to predict the elastic transmission in PnCs. Finite difference time domain (FDTD) uses a grid in both space and time to track the wave propagation across the PnC, while recording the displacement at each spatial point [37]. The Finite Element Method (FEM) employs spatial discretization and variational methods to express the original problem into a linear algebraic equation, which is subsequently solved. The plane-wave expansion (PWE) method utilizes Bloch’s theorem, based on the periodicity of the inclusions, to obtain Fourier coefficients for the elastic displacement field and the material properties in reciprocal space (k-space). An eigenvalue problem is formed from the Fourier-transformed propagation equations and possible solutions, traditionally summarized by a list of propagating frequencies vs. momenta (k-vectors) that is called a band structure, is then obtained.

Either a transmission plot (as shown in Chapter 4) or a band structure (as shown in Figure 17 later in this chapter) is generated by these methods. A band structure is uniquely important in finding the correct range of frequencies with which to interrogate the PnC to couple into, and out of, defect modes due to devices such as waveguides and cavities. A “mode” is nothing but a configuration of the displacement field; in this case it is the direction of the displacement vector field. In addition, the group velocity and density of states can be calculated using a band structure since the slope of each mode is representative of the group velocity, through which the density of states can be obtained. Furthermore, the PWE method can model defects if combined with the super-cell technique, in which a periodic unit cell, necessary to use the PWE and to fulfill Bloch’s
theorem’s periodicity requirement, is expanded to a larger unit cell that includes the defect such that repeating the unit cell yields the structure of interest, and that the entire unit cell material properties are taken into account during the derivation of the calculation [36].

The PWE can dissect the band structure into longitudinal, in-plane transverse and out-of-plane transverse, also called flexural, branches. This is a necessary operation for obtaining the thermal conductivity of phononic crystals, since phononic crystals have been shown to alter the thermal properties of the material [17]. In this manuscript, we only discuss the details of the PWE. FDTD [32] is used without deriving how the method is formulated. The reader is encouraged to refer to Reference [12] for further information about FDTD. In the next section we show the PWE formulation for a two-dimensional phononic crystal consisting of W inclusions in SiO$_2$ host matrix and show that the PWE method converges very slowly when the material constituents of the PnC have high elastic impedance contrast. We finally introduce a method that will enhance the convergence of the PWE in obtaining the band structure for such high-contrast solid-solid (HCSS) phononic crystals.

### 3.2 Formulation for 2D Plane Wave Expansion Method

The PWE method is described in the literature [40-41]. To summarize it, for a two-dimensional PnC we start with the equation of motion for the displacement vector $\vec{u}(\vec{r},t)$ in an inhomogeneous linear elastic medium with no body force, which can be written as

$$\rho(\vec{r})\ddot{\vec{u}}(\vec{r},t) = \frac{\partial}{\partial x_j} \left( C_{ijkl}(\vec{r}) \frac{\partial u(\vec{r},t)}{\partial x_l} \right).$$

(30)
where \( \vec{r} = (x_1, x_2, z) = (\vec{x}, z) \) is the position vector, \( \rho(\vec{r}) \) and \( C_{ijkl}(\vec{r}) \) are the position-dependent mass density and elastic stiffness tensor, respectively.

Utilizing the Fourier transformation of the spatially-periodic inclusions, the material properties can be expanded, with respect to the two-dimensional RLVs, \( \vec{G} = (G_x, G_y) \), into the Fourier series:

\[
\rho(\vec{x}) = \sum_G e^{i\vec{G} \cdot \vec{x}} [\rho_G], \quad \text{and} \\
C_{ijkl}(\vec{x}) = \sum_G e^{i\vec{G} \cdot \vec{x}} [C_{ijkl}^G],
\]

where \( \rho_G \) and \( C_{ijkl}^G \) are the corresponding Fourier coefficients, and are defined as

\[
\rho_G = A_{uc}^{-1} \int \rho(\vec{x}) e^{i\vec{G} \cdot \vec{x}} d^2 \vec{x}, \quad \text{and} \\
C_{ijkl}^G = A_{uc}^{-1} \int C_{ijkl}(\vec{x}) e^{i\vec{G} \cdot \vec{x}} d^2 \vec{x},
\]

where \( A_{uc} \) is the area of the primitive unit cell of a two-dimensional PnC, as described by [42]. Expanding the displacement vector utilizing Bloch’s theorem [38] in a Fourier series, we get

\[
u_j(\vec{r}, t) = \sum_G e^{i(\vec{k} + \vec{G}) \cdot \vec{x} - i \omega t} \left( e^{ik_z z} \vec{A}_G^j \right),
\]

where \( \vec{k} = (k_x, k_y) \) is the Bloch wave vector, \( \omega \) is the angular frequency, \( k_z \) is the wave number along the z-direction, \( \vec{A}_G^j \) is the amplitude of the displacement vector. As \( k_z \) approaches zero, Eqn. (30) degenerates into the displacement vector for bulk elastic waves. Substituting Eqns. (31, 32 & 35) in (30), collecting like-terms and setting \( k_z \) to zero a generalized eigenvalue problem is formed:

\[
C \cdot \mathbf{U} = \mathbf{0},
\]
where

$$C = \begin{bmatrix} M1 & L1 & U1 \\ L2 & M2 & U2 \\ W1 & W2 & M3 \end{bmatrix}, \quad \text{and} \quad U = \begin{bmatrix} A^1_G \\ A^2_G \\ A^3_G \end{bmatrix}.$$  \hspace{1cm} (37)

Matrix elements, $M1, L1 \ldots$ etc., are each of size $n \times n$ forming a $C$ matrix of size $3n \times 3n$, where $n$ is the total number of RLVs used in the Fourier expansion. The components of matrix $C$ depend only on $\tilde{k}, \tilde{G}, \omega$ and the material properties $\rho_G$ and $C_{ijkl}^G$. The $(\omega,k)$ pairs satisfying Eqn. (36) define the dispersion relations of bulk elastic waves propagating in two-dimensional PnC.

For materials with orthorhombic symmetry or higher, the components $U1, U2, W1$ and $W2$ in matrix $C$ are zero and Eqn. (36) can be decoupled into two different polarizations as follows:

$$\begin{bmatrix} M1 & L1 \\ L2 & M2 \end{bmatrix} \begin{bmatrix} A^1_G \\ A^2_G \end{bmatrix} = 0$$ \hspace{1cm} (39)

for mixed polarization modes (longitudinal and in-plane transverse), and

$$M3 A^3_G = 0$$ \hspace{1cm} (40)

for modes with polarization displacement along the axial direction of the cylinders, the $z$-direction shown in Figure 16, which is identical to Figure 1, repeated for the reader’s convenience. In all PWE calculations in this manuscript, we will consider only the mixed
polarizations calculated by Eqn. (39). A detailed derivation of the PWE method as well as the contents of matrices M1, L1, etc can be found in Appendix A.

Figure 16 – A demonstration of a phononic crystal showing the radius of the inclusions $r$ and the lattice pitch $a$, as well as the directions referred to in the derivation of the plane wave expansion method

3.3 Convergence Comparison for High-Contrast Solid-Solid Phononic Crystals

The formulation above has been known to have convergence difficulties, especially when considering HCSS materials [6, 14, 36, 43-50]. To enhance the convergence, it has been shown that using an alternative formulation is necessary. Specifically, one should use the inverse rule when obtaining the Fourier coefficients of $C_{ijkl}(\vec{x})$ instead of the conventionally used Laurent’s rule, according to the procedure of
Fourier factorization of a product of two piecewise smooth, bounded, periodic functions.

This leads to substituting $C_{ijkl}$ with $\left[\frac{1}{C_{ijkl}}\right]^{-1}$ in eq. (18) above. The inverse rule was observed to yield a faster and more stable algorithm especially in the case of HCSS-PnCs, in agreement with the suggestion and observations in [45].

The dispersion relations obtained using the new formulation of the PWE (NPWE) are presented and compared to results obtained by using the conventional formulation (CPWE) here. In this section we study the number of RLVs (equivalently the number of plane-waves) needed for the convergence of the band structure modes for HCSS PnCs and show that faster convergence is achieved using the inverse rule. We choose to study a PnC comprised of cylindrical W inclusions arrayed in a square lattice arrangement in SiO$_2$ as well as Si background materials. These two solid sets, namely W-SiO$_2$ and W-Si, have two of the largest elastic impedance ($Z$) mismatch among solids commonly used in the microelectronics fabrication industry, as shown in Table 4.

<table>
<thead>
<tr>
<th></th>
<th>$\rho$ (kg/m$^3$)</th>
<th>$C_l$ (m/s)</th>
<th>$Z$ (kg/(m$^2$s))</th>
<th>$E$ (GPa)</th>
<th>$\nu$ (unitless)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tungsten (W)</td>
<td>19300</td>
<td>4611</td>
<td>$89 \times 10^6$</td>
<td>410</td>
<td>.28</td>
</tr>
<tr>
<td>Silica (SiO$_2$)</td>
<td>2200</td>
<td>5840</td>
<td>$12.8 \times 10^6$</td>
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<td>.17</td>
</tr>
<tr>
<td>Silicon (Si)</td>
<td>2331</td>
<td>8520</td>
<td>$19.8 \times 10^6$</td>
<td>155</td>
<td>.22</td>
</tr>
<tr>
<td>Aluminum (Al)</td>
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<td>5091</td>
<td>$13.7 \times 10^6$</td>
<td>700</td>
<td>.33</td>
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<tr>
<td>Aluminum nitride (AlN)</td>
<td>3260</td>
<td>9592</td>
<td>$31.3 \times 10^6$</td>
<td>300</td>
<td>$0.17 - 0.24$ [$51$]</td>
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</table>

Using Eqn. (39) above, we calculate the dispersion relations of bulk elastic waves in a PnC comprised of W cylindrical inclusions periodically placed in a simple cubic
arrangement in SiO$_2$ host medium with an r/a ratio of 0.32. We use the NPWE to compare with dispersion relations obtained with the CPWE.

Convergence in a series is usually achieved by taking a finite number of terms added to the series such that the solution(s) obtained with $m + 1$ terms is within a defined error margin from those obtained with $m$ terms. In our case, since accurately identifying the

**Figure 17** – A comparison between the elastic band structure for the bulk 2D PnC made of an array of W of cylindrical cross section, arranged in a simple cubic lattice, embedded in a SiO$_2$ background with an r/a ratio of 0.32 using the CPWE and NPWE formulations mentioned above - The inset represents the first Brillouin zone ($\Gamma$XM) of the square array. The components of the wave vector $\vec{k}$ at the $\Gamma$, X and M points are $\pi/a$ (0,0) $\pi/a$ (1,0) and $\pi/a$ (1,1), respectively. A dimensionless frequency, $\omega a/C_t$ is reported on the vertical axis, where $C_t$ is the transverse elastic velocity in SiO$_2$. Note the faster convergence of the NPWE when compared to the conventional method for (a) 81 RLVs as well as (b) 441 RLVs.

whereas only 81 RLVs are needed for the band structure to fully converge with the NPWE, as can be extracted from Figure 18. The ratio between the computation time needed to obtain the band structure of a HCSS PnC for the CPWE using 1369 RLVs vs. NPWE using 81 RLVs is on the order of 1: 1000, which is substantial.
A comparison between the band structure obtained using the NPWE and the CPWE methods with various RLVs is shown in Figure 19. The excellent agreement in the lower bands of the dispersion relations obtained using the NPWE with 81 and 441 RLVs confirms the full convergence of the band structure when 81 RLVs. This is a very short and acceptable computation time if compared to FDTD or FEM, as well as the CPWE method.

Bandgap limits is very important for various applications, a 0.5% error is taken as a criterion. Figure 17 shows a comparison between the band structure of bulk elastic waves for the W-SiO$_2$ PnC using 81 and 441 RLVs for both formulations. It is clear from Figure 17 that using the NPWE enhances convergence of the modes dramatically; a goal which needs much more than 441 RLVs in the CPWE method before the same convergence is achieved. The superiority of the new formulation is better appreciated when the same comparison is made with a higher number of RLVs. In Figure 18, even with 1369 RLVs full convergence of the modes has not been reached with the CPWE,
Figure 18 – The band structure of the same W-SiO₂ PnC using 1369 RLVs with the CPWE compared to the NPWE using only 81 RLVs. It is clear that even with 1369 RLVs, the CPWE fails to fully converge, asserting the need for using even more RLVs to reach full convergence. The computation time ratio between the two results, namely the NPWE using only 81 RLVs vs. CPWE using 1369 RLVs, is around 1:1000, which is extremely significant.

whereas only 81 RLVs are needed for the band structure to fully converge with the NPWE, as can be extracted from Figure 18. The ratio between the computation time needed to obtain the band structure of a HCSS PnC for the CPWE using 1369 RLVs vs. NPWE using 81 RLVs is on the order of 1: 1000, which is substantial.

A comparison between the band structure obtained using the NPWE and the CPWE methods with various RLVs is shown in Figure 19. The excellent agreement in the lower bands of the dispersion relations obtained using the NPWE with 81 and 441 RLVs confirms the full convergence of the band structure when 81 RLVs. This is a very short and acceptable computation time if compared to FDTD or FEM, as well as the CPWE method.
Figure 19 – A comparison between the band structure obtained using 81 RLVs and 441 RLVs using the (a) NPWE and (b) CPWE for the same W-SiO₂ structure as in Figure 17. The excellent agreement in the lower bands of the dispersion relations obtained using the NPWE with 81 and 441 RLVs confirms the full convergence of the band structure with only 81 RLVs. This is a very acceptable computation cost when compared to FDTD or FEM, as well as the CPWE method.

Furthermore, Figure 20 shows the agreement in the location and width of the band gap obtained using the NPWE when compared to that obtained using FDTD [32]. That is to say that the NPWE is a legitimate transformation of the CPWE, and that our simulation is accurate since FDTD results closely agree with the results obtained when the NPWE, with 81 RLVs only, is used.
The first five modes are chosen for comparison because the band gap lies between the third and the fourth bands, and the PnBG width is the most important functionality of a PnC. Therefore, predicting the band gap width and location is the most important piece of information to be supplied with a modeling technique for phononic crystals. Figure 21 shows the percent error in the first five bands at the X point (\(\pi/a\ (1,0)\)) in the first Brillouin zone showing the results obtained from using the CPWE and NPWE methods with 9, 25, 49, 81, 441, 841 and 1369 RLVs for the W-SiO2 PnC. It is clear from Figure 21 that even with 1369 RLVs, modes obtained by the CPWE are not fully converged.
while only 49 RLVs are needed for the modes obtained by the NPWE method to give solutions within 0.5% error from those results obtained with 841 & 1369 RLVs using the NPWE. Although the CPWE offers around 4% error using 81 RLVs, 4% error of each of the bands bounding the PnBG would cause a significant error in the gap to mid-gap ratio, which are usually on the order of only 25% at higher frequencies [34]. The NPWE provides much faster convergence and gives results within 0.5% error in a fraction (around 0.00014) of the time needed by the CPWE to offer results within 1% error. Only
with 1369 RLVs does the CPWE have a percent error around 1%. Noteworthy is the pseudo-convergence the CPWE shows at a lower number of RLVs (up to 81 RLVs), which can be deceiving, after which the modes start converging toward the values achieved by the NPWE with only 25 RLVs.

The above section showed the strong influence of the inappropriate use of the Laurent’s rule to express the elastic tensor Fourier coefficients [45], and suggests great convergence can be achieved with the new formulation. It also suggests that the lack of convergence of the plane wave expansion method should not be attributed to the slow convergence of the Fourier series for the elastic parameters in the interfaces of different materials comprising a PnC.

It is worth noting that one could use a brute force numerical technique to solve the eigenvalue problem in Eqn. (36) by sampling over both $\omega$ and $k$ and finding pairs satisfying Eqn. (36) [36]. However, although similar results are achieved by both methods, solving the eigenvalue problem is much faster than using a numerical technique to obtain the band structure, even when shared memory multi-processing (such as OpenMP) is utilized because the eigenvalue problem approach allows for sampling over one parameter only, $k$. The discussion above regarding the CPWE vs. NPWE applies to the numerical approach as well, since identical eigenfrequencies are obtained when both the numerical technique and the eigenvalue approaches are undertaken.
4.1 Electro-elastic Transduction

Piezoelectricity is the ability of a material to produce an electric field in response to an applied mechanical stress [1]. A material exhibiting such behavior exhibits the reverse behavior where a mechanical stress is produced in response to an applied electric field or potential difference. The concept of piezoelectricity is used in many commercial applications used daily. A simple example is the use of piezoelectric materials for ignition. A cigarette lighter, for example, uses a piezoelectric material which responds to the pressure applied by the user (when one applies pressure to light a cigarette) with a large-enough electric field creating a spark. The spark causes the ignition of a flammable fluid. Push-start grills also use the same concept. Furthermore, piezoelectricity has also been used in various technological applications such as sensors. In a sensor, the piezoelectric material detects any mechanical pressure and produces electrical charge which can easily be read by a user or recorded on a computer. A piezo-electric sensor also detects a mechanical signal converting it into an electric signal.

For phononic crystals, one of the biggest challenges is to propagate elastic waves through the crystal at the frequency of interest. The reverse problem applies to detecting the transmitted signal on the other side of the phononic crystal to compare with the launched signal. Comparing both the launched and received signal proves whether the phononic crystal actually suppressed frequencies within the phononic bandgap or not. Since it is easy to create electric signals at most frequencies of interest, piezoelectric
materials become a perfect fit for such a task (up to 5 -10 GHz because of material and fabrication limitations). Piezoelectric materials convert electrical energy into elastic energy and convert elastic energy into electrical energy, which makes them an excellent candidate to be used to interrogate a phononic crystal. Examples of piezoelectric materials used for such a task are aluminum nitride (AlN), lead zirconate titanate or PZT (PbZr$_x$Ti$_{1-x}$O$_3$, 0<x<1) and zinc oxide (ZnO.)

The bandwidth of signals launched through a phononic crystal has been a challenge, since thin film piezoelectric transducers generally have a narrow-band response, quantified by their coupling coefficient $k_r^2$. A wide-band launched signal is required (as shown in Figure 22a) such that if the phononic crystal rejects a band of frequencies, it can be observed at the other end of the phononic crystal (as shown in Figure 22b).

![Figure 22](image_url)

*Figure 22 – A qualitative example of the received signal when launched in (a) bulk material and (b) a phononic crystal*

Figure 22a and Figure 22b show an example of the received signal when launched in bulk material and in a phononic crystal, respectively. A bandgap can only be observed if the couplers used to interrogate the phononic crystal launch a signal with a wide enough bandwidth to cover the entire frequency range over which the bandgap exists.
However, in most cases the desired bandwidth cannot be achieved using only one coupler. For example, a bandwidth of at least 1 GHz was needed to interrogate the device discussed in Section 4.5. Such bandwidth is not practically achieved using one Inter-Digitated Transducer (IDT). Therefore, to create a profile similar to that in Figure 22a, a number of IDTs are designed at slightly different frequencies, as shown in Figure 23a. The overall response collected from all of the couplers combined gives a profile similar to Figure 22a, as shown in Figure 23b. When this collective response is launched through a phononic crystal with the appropriate design, a bandgap, qualitatively similar to that shown in Figure 22b, is observed. This method leads to somewhat noisy bandgaps, although the ‘noise’ is created because of the partial overlapping between adjacent couplers used to interrogate the phononic crystals [15, 32, 51]. The ‘noise’ in the bandgap can be eliminated or reduced by designing couplers which partially overlap to decrease the ripple shown in the overall response in Figure 23b.

![Graph](image)

**Figure 23** – (a) Individual couplers’ response and (b) overall couplers’ response

There are many ways to design AlN transducers. In the phononic crystal designs discussed in Sections 4.2 – 4.5, slanted couplers and chirped inter-digitated transducers (cIDTs) were used. In this section we discuss the design of such transducers and show some experimental results of fabricated transducers. We begin with inter-digitated
transducers used for devices discussed in Section 4.5 after which we discuss the design of slanted couplers discussed in Sections 4.2 – 4.4.

a. Inter-digitated Transducers

Inter-digitated transducers have been used in many applications. Figure 24 shows the usual setting for a resonator used to interrogate a phononic crystal at frequency $f$ (or equivalently wavelength, $\lambda$).

![Diagram](image)

**Figure 24** – (a) The Al-AlN-Al drive and sense set-up used to interrogate a phononic crystal showing the bottom electrode, the AlN film and the top electrode constituting the IDT fingers and (b) a top view of the Al fingers of the IDT showing the longitudinal wavelength, $\lambda_l$ and in-plane transverse wavelength, $\lambda_{\text{in-plane}}$.

An AlN film is deposited on top of an Al film acting as the bottom electrode, or ‘ground.’ Then Al fingers are deposited on top of the AlN film forming the IDTs. A signal is launched between the top and bottom electrodes (the inter-digitated fingers and the bottom Al film) creating an electric field with flux lines through the AlN film. The electric field creates a displacement in the AlN film which occurs at a specific frequency, largely based on the dimensions of the top Al fingers as discussed below. The displacement in the AlN film is transformed through the thin bottom electrode to the host material through which a displacement field gradient is desired. This displacement field
propagates as an elastic wave through the host material below the bottom electrode (in which the phononic crystal resides) and can be sensed at the other end of the phononic crystal by a similar set-up of Al-AlN-Al layers, as shown in Figure 24a. The displacement transfer between the AlN and the host medium is slightly affected by the presence of a thin film of Al; the bottom electrode. However, losses are minimal through such a layer since the thickness of this layer is much smaller compared to the wavelength.

The elastic wave launched through the host material below the bottom electrode (in which the phononic crystal resides) is mostly in the form of longitudinal waves and flexural modes, though in-plane transverse modes can also be launched and received by

![Graph](image)

*Figure 25 – Experimental results for a single-frequency IDT showing the narrow-bandwidth nature of such couplers*
the couplers. However, the in-plane transverse modes will be launched and detected at a much lower frequency due to the length of the IDTs in the fundamental transverse direction, as shown in Figure 24b.

![Diagram](image)

*Figure 26 – The stack of Al-AlN-Al-Host in which the displacement wave propagates, used to calculate an average elastic wave speed in the composite*

Figure 25 shows an example of an experimental IDT launched and received through a bulk material of Si with the dimensions of the device discussed in Section 4.5. To determine the design dimensions (the width, specifically) of such Al fingers needed to launch an elastic wave at a center frequency, $f$, $\lambda = c/f$ should be used, where $c$ is the elastic wave speed, and $\lambda$ is the wavelength. The width of each Al finger is then obtained since the width of each Al finger should be $\lambda/4$. The displacement from the AlN, through the Al and to the Si host medium layer encounters different media forcing the wavelength to change throughout the path to the Al-AlN-Al-Si stack on the other side of the phononic crystal. Therefore, to get a good estimate for the wavelength, $\lambda$, an average elastic speed, $c_{avg}$ should be used to find the wavelength corresponding to the desired frequency, $f = c/\lambda$. Therefore, each film’s thickness, $t$, as shown in Figure 26, is used to find the average elastic speed of the wave through the stack as follows:
where \( t_x \) is the thickness of the \( x \) film, and \( c_x \) is the elastic speed in the \( x \) film, the values of which are mentioned in Table 4 above. Using Eqn. 41 to find the wavelength, \( \lambda = c_{avg} / f \), at the desired frequency, \( f \), the top electrode IDT fingers are designed. Since a number of transducers covering a very wide bandwidth are being produced, variations in the calculated \( c_{avg} \) from the true average speed are quite irrelevant to the overall characterization. The design of such single frequency couplers relies on having top-electrode Al fingers with the same width as well as the same spacing between two adjacent Al fingers. While designing such IDTs is easy, the bandwidth achieved with each coupler is not nearly sufficient to interrogate a phononic crystal, leading to the need for a large number of couplers as is obvious from Figure 25. An alternative to designing single frequency IDTs is to use a chirped coupler design, where \( \lambda_1 \) in Figure 24b slightly changes such that the fingers and spacing between fingers are not constant across each coupler, as shown in Figure 27. This allows for a relatively broader bandwidth if

\[
c_{avg} = \left( c_{Al} t_{Al} + c_{AIN} t_{AIN} + c_{Al} t_{Al} + c_{host} t_{host} \right) / \left( t_{Al} + t_{AIN} + t_{Al} + t_{host} \right),
\]

\( \lambda = c_{avg} / f \), at the desired frequency, \( f \), the top electrode IDT fingers are designed. Since a number of transducers covering a very wide bandwidth are being produced, variations in the calculated \( c_{avg} \) from the true average speed are quite irrelevant to the overall characterization. The design of such single frequency couplers relies on having top-electrode Al fingers with the same width as well as the same spacing between two adjacent Al fingers. While designing such IDTs is easy, the bandwidth achieved with each coupler is not nearly sufficient to interrogate a phononic crystal, leading to the need for a large number of couplers as is obvious from Figure 25. An alternative to designing single frequency IDTs is to use a chirped coupler design, where \( \lambda_1 \) in Figure 24b slightly changes such that the fingers and spacing between fingers are not constant across each coupler, as shown in Figure 27. This allows for a relatively broader bandwidth if

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\[
\lambda \approx \left( \right) / \left( \right),
\]
compared to single-frequency IDTs such that fewer couplers are needed to cover the frequency range of interest. Experimental results for a single chirped coupler are shown in Figure 28. Comparing Figure 28 and Figure 25, the width of the passband with the chirped IDT design is around 50 MHz, which is greater than that of the single-frequency IDT, being 10 MHz at the -10 dB point. For this reason, chirped IDTs were used in the design of the W-Si phononic crystal operating at 1.4 GHz, which is discussed in Section 4.5.

Figure 28 – Experimental results for a chirped IDT showing the wider-bandwidth nature of such couplers if compared to Figure 25
Figure 29 – (a) Slanted coupler design and (b) experimental results for such design

b. Slanted Transducers

An alternative to chirped IDTs is slanted couplers, the design of which is shown in Figure 29a. The idea of a slanted coupler is having one continuous Al trace, on top of the AlN film, with dimensions that vary along the fundamental longitudinal direction. Since the wavelength launched by the coupler is related to the width of the coupler, $W$, by $W = \lambda/4$, and because this width changes along the fundamental longitudinal direction, the frequency at which the coupler launches elastic displacements also changes adding to the bandwidth of the coupler. The bandwidth of such device extends from frequency $f_n$ to $f_1$ where $f_n = \frac{c_{avg}}{\lambda_n}$ and $f_1 = \frac{c_{avg}}{\lambda_1}$. Experimental results of the fabricated device, shown in Figure 29b, show wideband transduction with a region with a lack of transduction at
around 65 MHz. It is worth noting that chirped couplers are too large to be designed at low frequencies.

In the above section we presented an overview of the design of the electro-elastic transducers we used in creating our devices. In this chapter, we present two devices successfully fabricated and show their results. Specifically, in Sections 4.2 – 4.4 we discuss the fabrication process, design, characterization and results of phononic crystals comprised of W inclusions in a SiO₂ host medium designed to operate around 47 MHz range. In such regime, release holes are essential for releasing the phononic crystal devices. However, release holes introduce modes in the bandgap leading to its closure as will be discussed in Section 4.3. Therefore, careful design of the implementation of solid-solid phononic crystals is necessary for devices operating at such frequencies. In Section 4.5 we discuss the fabrication process, design, characterization and results of phononic crystals comprised of W inclusions in a Si host medium designed to operate around 1.4 GHz range. In such regime, no release holes are needed because of the relative small size of such devices.

4.2 Fabrication Process for W-SiO₂ Phononic Crystals [52]

Similar to most MEMS devices, the fabrication process for a PnC consists of a combination of material deposition and material etching steps followed by a device release step. The process flow for creating a PnC comprised of W inclusions in SiO₂ and designed to operate at around 47 MHz is shown in Figure 30. The micro-machined PnC process begins with:

(a) An oxide deposition of 0.6 µm followed by the deposition of a 2 µm undoped poly-Si release layer. The poly-Si is then removed around each device, limiting the area to which
the release gas, SF$_6$, has access to prevent suspension from the substrate in non-device areas of the wafer and to avoid etch loading, which is described in the next section. The poly-Si patterning is followed by a deposition of a conformal oxide layer. By polishing this oxide layer to the level of the deposited poly-Si, mechanical support for the suspended membrane is secured and higher efficiency of SF$_6$ etching is achieved, as less poly-Si is available. Next a 0.4 µm Al bottom interconnect layer is sputter-deposited and patterned. This Al also serves to protect the bottom of the W inclusions during release from the SF$_6$. The PnC is formed through the deposition of 4 µm of SiO$_2$ which is subsequently polished to remove the topography created by the Al.

Figure 30 – Fabrication Process for Solid-Solid phononic crystals comprised of W cylindrical inclusions in a SiO$_2$ host matrix, interrogated by AlN couplers

(b) Trenches in the oxide are etched followed by conformal deposition of a 1.2 µm thick layer of W which forms contacts to the bottom electrode of the AlN couplers and parts of the high density W inclusions. The W layer is polished until it remains only where the trenches were etched in the SiO$_2$ producing W rings.
(c) The formation of the W cylindrical scattering centers is completed by filling the rings using an additional oxide etch, W deposition and polish. The W inclusions have to be deposited in two steps to avoid stress associated with thicker W film deposition. The two step process can be seen in Figure 31 where the circular profile between the various W deposition layers is apparent. Next a Ti/TiN/Al bottom electrode is deposited followed by the sputter deposition of 0.75 µm of AlN. The AlN film is highly c-axis oriented with an x-ray diffraction rocking curve full width half maximum of 1.5°, which results in strong electro-acoustic coupling. The AlN is patterned and a 0.4 µm Al top electrode is deposited. This Al layer protects the top of the W inclusions during release from the SF₆. 

(d) Finally, release holes are etched through the SiO2 in the center of the W inclusions, 

![Figure 31](image)

*Figure 31 – (a) Angled and (b) planar SEM images of a W rod with release hole of 7.5 µm in its center. The circular profiles in the W ring are clear in the image, and are due to the two-step processs (steps b and c above) in the W deposition*

down to the poly-Si layer. The device is then released using SF₆, using release pits (large areas exposing the SF₆ to the release Si layer) that are adjacent to the device (not shown
in Figure 30 because the release pits are located adjacent to the PnC structure in the direction perpendicular to this page.)

**4.3 Fabrication Challenges in Solid-Solid Phononic Crystals [52]**

We choose solid-solid PnCs to design and characterize because, as discussed earlier, the $r/a$ ratio for optimum bandgap is 0.32 (for the W-SiO$_2$ system), which allows for the minimum feature size to be $0.36a$ (distance between two adjacent rods in a square lattice), which is easily fabricated. This becomes obvious when compared to the $r/a$ ratio for optimum bandgap in an air-solid PnC, which is around 0.44, which allows for the minimum feature size to be only $0.12a$, which is much harder to fabricate especially at higher frequencies when the size of $a$ is significantly smaller.

A step that is needed in fabricating some MEMS devices is polishing a surface after depositing a metal in a trench. The deposition step fills up trenches with the desired material, but leaves residual deposited material on the adjacent matrix material. This is detrimental for two reasons. First, if the inclusion has a rough surface, leakage and reflection at those interfaces will minimize resonators’ quality factor, $Q$, which is a measure of frequency selectivity, of the signal through the device. Furthermore, if other films are to be deposited on top of such a surface, the new film will not be uniform and therefore may cause other scattering mechanisms and a lower quality AlN film. The chemical mechanical polishing process is a well-known process that creates a uniform surface and removes any excess material from the surface. However, with two materials with large flow stress mismatch, namely W (~700 MPa) and SiO$_2$ (~70 MPa) in our case,
the chemical mechanical polishing process becomes less uniform and introduces the problems mentioned above. Thus, if a material system with an acceptable mismatch of

![Figure 32](image)

*Figure 32 – An example of the non-uniformity of the chemical mechanical polishing fabrication step, seen in the inset around the W rods, likely due to the large difference in flow stress mismatch between the W inclusions and the SiO2 host medium*

elastic impedances could be found while at the same time maintaining a nearly equivalent flow stress for both materials then this may solve the chemical mechanical polishing (CMP) problem. However, this optimization is beyond the scope of this work. An example of the non-uniformity in the CMP process is shown in Figure 32. The device shown in Figure 32 will be discussed in Section 4.4 below.
For a W-SiO₂ PnC, the fabrication process for a PnC is usually to deposit a Si sacrificial layer, deposit a SiO₂ device layer, etch holes in the SiO₂, backfill the holes with W, polish the surface for uniformity, deposit the AlN piezoelectric film which will launch (and detect) the elastic wave through the crystal, and then release the device through etching parts of the device layer away from the PnC to expose the sacrificial Si layer to an etchant that will react with it. The volatile outcome of this reaction exits the chamber and the PnC is now suspended (after the entire sacrificial layer under the PnC has chemically reacted and exited the chamber) except for supports on either sides of the PnC. One of the problems arising during releasing MEMS devices is etch loading. Although more complicated, one reason for etch loading to occur is when the etchant is exposed to two potential etching areas. If the area to be etched is smaller in exposed surface area to the etchant than the second area to which the etchant is exposed, the etchant takes the path of ‘least resistance’ and proceeds to etch the larger area. In our case etch loading could take place if the substrate Si is used as the sacrificial layer because the etchant will see the ‘larger’ substrate and will continue to etch vertically down instead of undercutting to release the device. To avoid etch loading, an oxide layer is deposited on the Si wafer followed by a deposition of the sacrificial thin Si layer to force the etchant to undercut the device, since the etchant is highly selective thus choosing to etch the Si instead of the SiO₂. This is the reason for adding the two layers of SiO₂ and Si in step (a) in the fabrication process.

For solid-solid PnCs operating in the sub-200 MHz range, devices’ dimensions are approximately 500 µm x 500 µm. This relatively large device size makes their release exorbitantly long, on the order of days, without the addition of release holes. In
fact, having to expose the device to the etchant for long periods of time will cause some etching of other materials on the device, albeit slower, which could cause compromising the functionality of the device. Therefore, release holes have to be included in the PnC membrane for the etchant to access the sacrificial layer to release the device. However, release holes have a profound impact on the phononic bandgap. Release holes introduce further scattering and states within the bandgap leading to compromising the bandgap. Therefore, careful design is necessary to ensure that the bandgap is minimally compromised according to the practicality of the fabrication process. Placing the release holes in the center of the solid inclusions is preferable because if they are placed outside the solid inclusions further scattering is expected to take place leading to distorting the bandgap edges. When the release holes are placed in the center of the W rods, the W inclusions partially mask the release hole from the propagating wave to minimize the bandgap distortion. In the next section we discuss the effects of release holes on elastic wave propagation through a phononic crystal.

4.4 Effect of Release Holes on Micromachined Phononic Crystals [52]

Release holes in solid-solid phononic crystals serve to allow the etchant to reach the sacrificial layer and therefore suspend the PnC membrane. However, as mentioned earlier, placing release holes in the center of the solid inclusions in a solid-solid PnC can interfere with a propagating longitudinal wave, which partially penetrates through the inclusion and is scattered again at the inclusion-air interface, causing a disruption to the observed bandgap as compared with a PnC having no release holes, the comparison of which is shown below.
In this section we experimentally and theoretically study the effects of introducing release holes on the propagation of elastic waves through PnCs made of cylindrical Tungsten (W) inclusions arrayed in a simple cubic arrangement in a SiO\textsubscript{2} host medium. Specifically, we investigate the maximum release hole size one can introduce to release the PnC membrane without disturbing the bandgap as well as maintaining a reasonable release time during the fabrication process. In the device described below, the distance in the plane of periodicity between the centers of horizontally- or vertically-adjacent W rods (the lattice pitch \(a\)) is 45 \(\mu\text{m}\) and the outer radius (\(r_W\)) of the W hoops are 14.4 \(\mu\text{m}\) resulting in an \(r/a\) ratio of 0.32, which was shown to produce the optimum bandgap in this choice of materials [1]. Figure 33 shows a scanning electron microscope (SEM) image of a PnC with release holes in the center of the W inclusions. An interesting observation is the slight curve in the PnC membrane, which happens because the gradient of residual stress in the SiO\textsubscript{2} membrane. Aluminum (Al) couplers are deposited on an aluminum nitride (AlN) film to launch and receive a longitudinal elastic wave through the PnC. Due to the inherent narrow-band behavior of these transducers, we use 12 different couplers for each crystal to cover the frequency range of interest [34].

The plane-wave-expansion (PWE) and finite difference time domain (FDTD) [32] methods were utilized to model elastic wave propagation in our device. Throughout this section, branches in the band structure have been separated into longitudinal and in-plane transverse modes. The flexural (out-of-plane transverse) are not detected by the two-dimensional PWE calculation. While comparing the results obtained using the PWE method to experimental results as well as FDTD results [32], the in-plane transverse branches were ignored. Ignoring such modes is consistent with the fact that experimental
results obtained using a network analyzer show only longitudinal modes, as does the FDTD model [32]. While scattering can force a launched mode with displacement in the longitudinal direction to transform into an in-plane transverse mode, the receivers in both the experimental and FDTD data [32] only detect longitudinal modes and flexural modes. For this reason, only longitudinal branches of the band structure obtained using the two-dimensional PWE for propagation in the $\Gamma X$ direction of the first Brillouin zone were used to compare with experimental and FDTD results [32]. For very thin structures where the thickness of the PnC, $t$, is less than $0.1\lambda$, flexural modes are not well transduced [54]. Figure 34 shows the PWE results of elastic transmission through a crystal with release hole radii of 0, 2.5, 3.75, 5, 6.25 and 7.5 $\mu$m for $r_{air}/r_{W}$ ratio of 0, 0.17, 0.26, 0.35, 0.43 and 0.52, respectively, where 625 plane waves were used in the PWE calculations. The bandgap appears in the case with no release holes (Figure 34a) between 37 and 78 MHz. Introducing a release hole of radius of 2.5 $\mu$m, as shown in Figure 34b,
leads to introducing a mode in the bandgap, leading to a slightly smaller bandgap, namely between 37 and 70 MHz, than that of PnCs with no release holes. With a 3.75 \( \mu \text{m} \) release hole, the bandgap is split into two bandgaps; one between 65 and 80 MHz and the other between 37 and 60 MHz by a mode appearing between 60 and 65 MHz, as shown in Figure 34e. Figure 34d, Figure 34e and Figure 34f further show the longitudinal branch progressively appearing at lower frequencies within the bandgap as the release hole size is increased. The longitudinal branch causing the closure of the bandgap is flat, especially on the edges of the first Brillouin zone, which means that its group velocity is extremely small (since a good approximation of the group velocity is \( d\omega/dk \), being the largest term in the Taylor expansion used to calculate the group velocity). The density of

![Figure 34](image-url)

**Figure 34** – PWE results for elastic propagation through a W-SiO\(_2\) PnC with various release hole size, shown on each figure. Filled circles represent longitudinal branches and the crosses represent in-plane transverse modes. The shaded region in (a) is the full bandgap with no release holes, and as the release hole size gets progressively bigger; a longitudinal mode appears in the bandgap splitting it into two bandgaps while progressively moving to a lower frequency. (b) \( r_{\text{air}} = 2.5 \ \mu\text{m} \), (c) \( r_{\text{air}} = 3.75 \ \mu\text{m} \), (d) \( r_{\text{air}} = 5 \ \mu\text{m} \), (e) \( r_{\text{air}} = 6.25 \ \mu\text{m} \), (f) \( r_{\text{air}} = 7.5 \ \mu\text{m} \).
phononic states is inversely proportional to the group velocity, and therefore is very large, allowing the mode to interfere with the bandgap.

The W-SiO$_2$ PnC with the aforementioned dimensions is designed with 12 different slanted Al couplers to actuate the AlN film at small frequency intervals instead of a single slanted coupler used previously. The goal of using 12 couplers per device is to cover the range of frequency of interest, since each one of these couplers transduces at a narrow bandwidth. It is clear from Figure 34 that eliminating the release holes yields the widest bandgap, and therefore is the most favorable situation. However, practically speaking, such devices are challenging to undercut using only release pits on either side of the to-be suspended PnC membrane because the structures are very large (around 500 $\mu m \times 500 \mu m$). Thus such devices must have release holes and a smaller bandgap than is optimally possible is an unavoidable compromise.

Phononic crystals with 2.5 $\mu m$, 3.75 $\mu m$ and 7.5 $\mu m$ release hole radii were fabricated to compare with the theoretical results. However the release hole of radius 2.5 $\mu m$ was not large enough to easily release the PnC membrane. A few of the difficulties in releasing such devices were reported in [55].

Figure 35 shows a comparison between FDTD [32], PWE and the experimental results for PnCs with release hole radii of 3.75 $\mu m$. The plots of the branches in the band structure are rotated 90 degree for easier comparison. Very good agreement is achieved between the longitudinal bandgap of the band structure and the bandgap shown experimentally. FDTD [32] shows the bandgap extending over a slightly-larger frequency range as compared to the experimental and the PWE band structure data. While this ~5% discrepancy is reasonably small, it can be attributed to the weak
scattering of the longitudinal modes into flexural modes of the membrane. Such modes are detected by the Network analyzer and not detected by the FDTD simulation [32] or the two-dimensional PWE calculation. The difference in the depth of the bandgap between FDTD [32] and the experimental results can be attributed to material losses which are not accounted for in the FDTD simulation [32]. The bandgap is continuous with no modes disrupting or compromising it in both the experimental and theoretical results shown.

![Graph showing transmission results](image)

*Figure 35 – FDTD (dashed line) [32] and experimental (line) transmission results through a W-SiO₂ PnC with a release hole radius of 3.75 μm compared with a band structure with longitudinal modes (filled circles). The in-plane transverse modes were ignored. The arrows show the corresponding y-axis.*
Figure 36 – FDTD (dashed line) [32] and experimental (line) transmission results through a W-SiO2 PnC with a release hole radius of 7.5 μm compared with a band structure with longitudinal modes (filled circles). The in-plane transverse modes were ignored. The arrows show the corresponding y-axis.

Figure 36 further shows the excellent agreement in predicting the location of the bandgap between the band structure and experimental results for devices with release holes of radius 7.5 μm. Comparing Figure 35 and Figure 36, representing devices with release hole radius of 3.75 and 7.5 μm, respectively, a mode is observed between 40 and 50 MHz for the device with the 7.5 μm release holes that does not exist in the case when a 3.75 μm air hole radius is introduced in the center of the W rods. The release hole
mode appears in the bandgap when the size of the release hole becomes comparable to the wavelength of the elastic wave and thus is large enough to be resolved by the propagating wave. Second-order scattering takes place at the W-air interface once the air hole is large enough to scatter the propagating modes. This creates defect modes within the rejected frequency domain.

Figure 37 – A comparison between transmission through a W-SiO2 PnC with various release hole sizes, where $r_{\text{air}}$ is the radius of the airhole.

Figure 37 shows a theoretical comparison among devices with various release hole sizes in the center of the W rods using FDTD [32]. A release hole mode (also known as air-hole mode) appears in the middle of the band gap compromising the width of the bandgap when a large enough air hole is introduced in the center of the W rods. This induced mode shifts to a lower frequency as the air hole size becomes greater, which
is consistent with the results obtained with PWE. The case with no release hole was calculated theoretically, but is impractical to fabricate experimentally with the current technology because of release difficulty previously discussed. Indeed, introducing release holes in the center of the W rods has a profound effect on the bandgap when they are large enough; therefore, these holes must be carefully designed to prevent adverse effects on the transmission through the phononic crystals.

4.5 Phononic Crystal Devices Operating in the GHz Frequency Range [52]

In this section we show the existence of a phononic bandgap (PnBG) in a solid-solid PnC made of W cylindrical inclusions embedded in a Si membrane operating at a center frequency of 1.4 GHz. In this frequency range, many applications in communications can utilize the bandgap appearing in such phononic crystals.

Utilizing Si as the host medium for phononic crystals offers several advantages. First, Si exhibits lower material loss than SiO₂. Secondly, the elastic speed in Si is higher than that in SiO₂, which results in higher frequency devices for the same lattice constant, $a$. The lower elastic speed mismatch between W and Si (compared to the mismatch between W and SiO₂) allows for the maximum bandgap to appear at a lower $r/a$ ratio (0.26) compared to that of W-SiO₂ (0.32). This means that the minimum feature size (the smallest distance between adjacent W rods) is larger for W-Si phononic crystals than that for W-SiO₂, which allows for higher frequency scaling with less lithography requirements than those of W-SiO₂ or Air-Si PnCs [1,16,34]. Thirdly, in fact, for PnCs implemented in low loss materials suitable for forming devices, the W-Si PnCs reported here exhibit the highest frequencies and widest bandgaps.
The structure is fabricated by depositing a periodic array of W cylinders in a Si film and then releasing the underlying material to suspend the PnC membrane, similar to the device discussed in the Sections 4.2 – 4.4. The main difference between the two devices, other than the host medium being SiO₂ vs. Si, is that the higher operating frequency of the device discussed in this section is advantageous in many ways. First, releasing the W-Si devices operating at higher frequency can be done without etching release holes in the center of the W inclusions. This eliminates interference leading to modes within the bandgap. Secondly, many more devices can be implemented on a single wafer because of the smaller size of such devices. The smaller size of the W-Si GHz devices, discussed in this section, is apparent by taking a look at Eqn. (2) in Chapter 1, where the higher the frequency constitutes a smaller lattice pitch, \( a \), and therefore for a smaller lattice pitch, \( a \), and the same \( r/a \) ratio, \( r/a \), the device becomes much smaller. To compare, a W-SiO₂ device operating around the MHz frequency (discussed in Sections 4.2 – 4.4) has a size of roughly (500 \( \mu \)m x 500 \( \mu \)m), whereas the W-Si devices discussed in this section have a size of roughly (45 \( \mu \)m x 90 \( \mu \)m). As is clear from the overall area each devices occupies, many more devices operating at higher frequencies can be fabricated on a single wafer compared to devices operating at lower frequencies. Both devices discussed in this manuscript are fabricated using a CMOS-compatible fabrication process and are applicable to various communications applications, if an SOI wafer is used for the GHz devices. To investigate the bandgap location and width of the W-Si PnC plate, a fabrication process was developed. The process starts with a high-resistivity Si wafer on which a sacrificial oxide layer of thickness 2.5 \( \mu \)m is thermally grown, followed by the deposition of the Poly-Si device layer of thickness 1.2 \( \mu \)m (Figure 38a).
Using an SOI wafer is also possible as long as the uniformity across such wafer is acceptable. Cylindrical trenches are then etched in the Si film followed by a chemical vapor deposition of W to fill the trenches. The wafer is then polished using chemical mechanical polishing (CMP) to ensure that the W only exists in the trenches, not elsewhere on the wafer (Figure 38b). A bottom electrode is then deposited and patterned (Figure 38c), followed by the deposition and patterning of an Aluminum Nitride (AlN) film (Figure 38d). AlN is used to launch and receive elastic waves through the PnC using its piezoelectric characteristics. The deposition of the AlN film is a very precise process to achieve a larger displacement for a given input electric field. A top electrode is then deposited and patterned (Figure 38e). The top electrodes serve to electrically actuate the AlN film, which in turn launches the elastic wave through the device. In our case, we chose to design broadband couplers by using inter-digitated transducers (IDTs) with different fingers’ width and spacing, called chirped couplers. Finally, the sacrificial oxide layer under the PnC membrane is removed using vapor phase Hydrofluoric Acid (HF) (Figure 38f). All the aforementioned steps are performed at low enough temperatures such that it can be implemented as a post-CMOS process if an SOI wafer is used. A scanning electron microscope image of the fabricated phononic crystal device is shown in Figure 39b, where the lattice pitch $a$ and the radius $r$ of the W inclusions are 2.5 µm and 0.65 µm, respectively. The thickness of the Si layer, $t$, is 1.15 µm with a thickness-to-lattice-pitch ratio, $t/a$, of 0.46, since it was shown that the bandgap is minimally compromised for $t < a$, or $t > 10a$ [33].
To characterize the bandgap observed in our fabricated PnC, we monitored the transmission in the $IX$ direction through a structure with 17 layers of W rods between launching and receiving couplers. We used a network analyzer to excite the structure by applying an electric signal over the frequency range at which a bandgap is predicted by the finite difference time domain (FDTD) [32, 33]. The electric signal creates an electric field between the top and bottom electrodes causing a displacement in the AlN film, which in turn causes longitudinal and flexural displacements in the Si membrane. The displacement field propagates through the PnC on the other side of which another set of top and bottom electrodes are placed around the AlN film. The received signal is compared with the launched signal to characterize the effect of the PnC on the propagating wave.

The IDTs, although designed chirped for broadband transduction, cannot cover the entire frequency range over which the bandgap exists using just one coupler. In fact, in our case we used 24 couplers to cover the frequency range of 0.8 – 2.2 GHz, which spans the location of the bandgap as predicted by FDTD [32]. The 24 PnC structures
were identical except that each IDT was designed to operate at a unique frequency interval such that the overall frequency range of interest is covered. To isolate the effect of the PnC we also fabricate a matrix, which is the same as Figure 38f without the W rods. An SEM image of the fabricated matrix is shown in Figure 40. Normalizing the transmission through the crystal to that through a matrix isolates the effect of the PnC at the output port [35].

Figure 39 – An SEM image showing the AlN layer, the Si membrane, Aluminum IDTs and the W inclusions in the PnC crystal
Figure 40 – An SEM image showing the AlN layer, the Si membrane, Aluminum IDTs and the W inclusions in the matrix

Figure 41 shows a comparison between our FDTD model [32] and experimental data for elastic transmission through the PnC device. A bandgap appears between 1–1.8 GHz in the experimental results. The FDTD [32] precisely predicts the upper edge of the bandgap but does not agree with the lower edge of the bandgap. This could be due to the lack of transduction exhibited by our PnC devices as can be seen in Figure 41b, or could be due to FDTD [32] not predicting flexural modes. The gap to mid-gap ratio of 57% is extremely high and surpassed the previous achieved results when compared to 25% [34] and 44% [16], and is wide enough to cover a large variety of applications in communications. A mode appears in the experimental transmission plot, Figure 41a, at
Figure 41 – (a) Normalized results for transmission through a PnC comparing FDTD [32] and experimental results, (b) the un-normalized experimental crystal and matrix responses

around 1.4 GHz. This mode can be seen in Figure 41b in the matrix's response as a dip in transmission at 1.4 GHz but not in the PnC's response. This means that such behavior in the transmission plot (shown in Figure 41a) is an artificial behavior occurring only because of the lack of transduction of the AlN resonators at that specific frequency. The experimental data in Figure 41 appears noisy for the same reason. This will be eliminated in the future by designing couplers with a wider-band response.
Conclusions

Phononic crystals are suspended MEMS or Nano-Electro-Mechanical-Systems (NEMS) made of one material periodically embedded in another material, leading to a periodic gradient in elastic properties of the final composite structure. Such devices exhibit elastic bandgaps, which are very useful in many commercial applications. Filtering, guiding and mirroring of elastic waves are but a few applications in which phononic crystals can be used and have been demonstrated. In this work, the physical origins of phononic bandgaps were successfully captured using a one-dimensional model to isolate resonances contributing to the creation of phononic bandgaps. Further, phononic crystals were modeled using a two-dimensional technique called the plane wave expansion method. Solutions for the convergence problem of the plane wave expansion method, previously believed to be a result of the elastic impedance difference between the constituent materials, were proposed and demonstrated to converge orders of magnitude faster than the original formulation of the method. Finally, phononic crystal devices operating in the MHz as well as devices operating in the GHz frequency range were modeled, designed, fabricated, and tested. Good agreement between theoretical results and experimental results is observed. In the future, phononic crystal high-Q cavities should be considered as well as development of a method by which elastic coupling into such phononic crystal resonators is readily achieved.
Appendix A

For a two-dimensional phononic crystal plate with finite thickness, the second-order elastic wave equation for the displacement field with no body force can be written as

\[ \rho \ddot{u}_j = \frac{\partial}{\partial x_l} \left( C_{ijkl} \frac{\partial u_k}{\partial x_l} \right), \text{ where } i,j,k,l = 1 - 3 \tag{A} \]

where \( \ddot{u}_k = \sum_G e^{i(K+\Gamma) \cdot r - i\omega A_k} \) is the three-dimensional vector, \( C_{ijkl} \) is the elastic tensor, \( \rho \) is the mass density and \( x_l \) is the direction of the displacement \( u_k \).

Expanding Eqn. (A) for \( j = 1 \), we get

\[
\rho \ddot{u}_1 = \frac{\partial}{\partial x_1} \left( C_{1111} \frac{\partial u_1}{\partial x_1} + C_{1112} \frac{\partial u_1}{\partial x_2} + C_{1113} \frac{\partial u_1}{\partial x_3} + C_{1121} \frac{\partial u_2}{\partial x_1} + C_{1122} \frac{\partial u_2}{\partial x_2} + C_{1123} \frac{\partial u_2}{\partial x_3} 
\right. 
\]

\[
\left. + C_{1131} \frac{\partial u_3}{\partial x_1} + C_{1132} \frac{\partial u_3}{\partial x_2} + C_{1133} \frac{\partial u_3}{\partial x_3} \right) \ldots 
\]

\[
+ \frac{\partial}{\partial x_2} \left( C_{2111} \frac{\partial u_1}{\partial x_1} + C_{2112} \frac{\partial u_1}{\partial x_2} + C_{2113} \frac{\partial u_1}{\partial x_3} + C_{2121} \frac{\partial u_2}{\partial x_1} + C_{2122} \frac{\partial u_2}{\partial x_2} + C_{2123} \frac{\partial u_2}{\partial x_3} 
\right. 
\]

\[
\left. + C_{2131} \frac{\partial u_3}{\partial x_1} + C_{2132} \frac{\partial u_3}{\partial x_2} + C_{2133} \frac{\partial u_3}{\partial x_3} \right) \ldots 
\]

\[
+ \frac{\partial}{\partial x_3} \left( C_{3111} \frac{\partial u_1}{\partial x_1} + C_{3112} \frac{\partial u_1}{\partial x_2} + C_{3113} \frac{\partial u_1}{\partial x_3} + C_{3121} \frac{\partial u_2}{\partial x_1} + C_{3122} \frac{\partial u_2}{\partial x_2} + C_{3123} \frac{\partial u_2}{\partial x_3} + 
\right. 
\]

\[
\left. C_{3131} \frac{\partial u_3}{\partial x_1} + C_{3132} \frac{\partial u_3}{\partial x_2} + C_{3133} \frac{\partial u_3}{\partial x_3} \right) \tag{B} 
\]

and expanding Eqn. (A) for \( j = 2 \), we get

\[
\rho \ddot{u}_2 = \frac{\partial}{\partial x_1} \left( C_{1211} \frac{\partial u_1}{\partial x_1} + C_{1212} \frac{\partial u_1}{\partial x_2} + C_{1213} \frac{\partial u_1}{\partial x_3} + C_{1221} \frac{\partial u_2}{\partial x_1} + C_{1222} \frac{\partial u_2}{\partial x_2} + C_{1223} \frac{\partial u_2}{\partial x_3} 
\right. 
\]

\[
\left. + C_{1231} \frac{\partial u_3}{\partial x_1} + C_{1232} \frac{\partial u_3}{\partial x_2} + C_{1233} \frac{\partial u_3}{\partial x_3} \right) \ldots 
\]
\[ + \frac{\partial}{\partial x_2} \left( C_{2211} \frac{\partial u_1}{\partial x_1} + C_{2212} \frac{\partial u_1}{\partial x_2} + C_{2213} \frac{\partial u_1}{\partial x_3} + C_{2221} \frac{\partial u_2}{\partial x_1} + C_{2222} \frac{\partial u_2}{\partial x_2} + C_{2223} \frac{\partial u_2}{\partial x_3} \right) + C_{2231} \frac{\partial u_3}{\partial x_1} + C_{2232} \frac{\partial u_3}{\partial x_2} + C_{2233} \frac{\partial u_3}{\partial x_3} \right) \]

\[ + \frac{\partial}{\partial x_3} \left( C_{3211} \frac{\partial u_1}{\partial x_1} + C_{3212} \frac{\partial u_1}{\partial x_2} + C_{3213} \frac{\partial u_1}{\partial x_3} + C_{3221} \frac{\partial u_2}{\partial x_1} + C_{3222} \frac{\partial u_2}{\partial x_2} + C_{3223} \frac{\partial u_2}{\partial x_3} \right) + 
\]

\[ C_{3231} \frac{\partial u_3}{\partial x_1} + C_{3232} \frac{\partial u_3}{\partial x_2} + C_{3233} \frac{\partial u_3}{\partial x_3} \right) \]  \tag{C}

and expanding Eqn. (A) for \( j = 3 \), we get

\[ \rho \ddot{u}_3 = \frac{\partial}{\partial x_1} \left( C_{1311} \frac{\partial u_1}{\partial x_1} + C_{1312} \frac{\partial u_1}{\partial x_2} + C_{1313} \frac{\partial u_1}{\partial x_3} + C_{1321} \frac{\partial u_2}{\partial x_1} + C_{1322} \frac{\partial u_2}{\partial x_2} + C_{1323} \frac{\partial u_2}{\partial x_3} \right) + C_{1331} \frac{\partial u_3}{\partial x_1} + C_{1332} \frac{\partial u_3}{\partial x_2} + C_{1333} \frac{\partial u_3}{\partial x_3} \right) \]

\[ + \frac{\partial}{\partial x_2} \left( C_{2311} \frac{\partial u_1}{\partial x_1} + C_{2312} \frac{\partial u_1}{\partial x_2} + C_{2313} \frac{\partial u_1}{\partial x_3} + C_{2321} \frac{\partial u_2}{\partial x_1} + C_{2322} \frac{\partial u_2}{\partial x_2} + C_{2323} \frac{\partial u_2}{\partial x_3} \right) + C_{2331} \frac{\partial u_3}{\partial x_1} + C_{2332} \frac{\partial u_3}{\partial x_2} + C_{2333} \frac{\partial u_3}{\partial x_3} \right) \]

\[ + \frac{\partial}{\partial x_3} \left( C_{3311} \frac{\partial u_1}{\partial x_1} + C_{3312} \frac{\partial u_1}{\partial x_2} + C_{3313} \frac{\partial u_1}{\partial x_3} + C_{3321} \frac{\partial u_2}{\partial x_1} + C_{3322} \frac{\partial u_2}{\partial x_2} + C_{3323} \frac{\partial u_2}{\partial x_3} \right) + 
\]

\[ C_{3331} \frac{\partial u_3}{\partial x_1} + C_{3332} \frac{\partial u_3}{\partial x_2} + C_{3333} \frac{\partial u_3}{\partial x_3} \right) \]  \tag{D}

It is worth noting that the above equations assume a slab of finite thickness, in which case plate modes are taken into consideration by examining the displacement in the \( x_3 \) direction; the direction along the cylinders’ height. For an infinite thickness phononic crystal, in which only bulk modes are assumed to exist while plate modes cannot exist, \( \frac{\partial u_i}{\partial x_3} = 0 \).

The terms in Eqns. (B), (C) and (D) can be broken down into first derivative terms and second derivative terms. The first derivative terms are:
\[
\frac{\partial \bar{u}_1}{\partial x_1} = N u_1 (k_{x_1} + G_{x_1}), \quad \frac{\partial \bar{u}_2}{\partial x_1} = N u_2 (k_{x_1} + G_{x_1}), \quad \frac{\partial \bar{u}_3}{\partial x_1} = N u_3 (k_{x_1} + G_{x_1})
\]
\[
\frac{\partial \bar{u}_1}{\partial x_2} = N u_1 (k_{x_2} + G_{x_2}), \quad \frac{\partial \bar{u}_2}{\partial x_2} = N u_2 (k_{x_2} + G_{x_2}), \quad \frac{\partial \bar{u}_3}{\partial x_2} = N u_3 (k_{x_2} + G_{x_2})
\]
\[
\frac{\partial \bar{u}_1}{\partial x_3} = N u_1 (k_{x_3} + G_{x_3}), \quad \frac{\partial \bar{u}_2}{\partial x_3} = N u_2 (k_{x_3} + G_{x_3}), \quad \frac{\partial \bar{u}_3}{\partial x_3} = N u_3 (k_{x_3} + G_{x_3})
\]
\[
\frac{\partial \bar{u}_1}{\partial t} = -N \omega u_1, \quad \frac{\partial \bar{u}_2}{\partial t} = -N \omega u_2, \quad \frac{\partial \bar{u}_3}{\partial t} = -N \omega u_3,
\]
and the thirty second-derivative expressions exist in Eqns. (B), (C) and (D) while utilizing summations over two sets of reciprocal lattice vectors, \( G \) and \( G' \), as follows:

1. \[
\frac{\partial}{\partial x_1} \left( \frac{\partial \bar{u}_1}{\partial x_1} \right) = N^2 i^2 (k + G)_{x_1} (k + G')_{x_1} \bar{u}_1 = -N^2 (k + G)_{x_1} (k + G')_{x_1} \bar{u}_1
\]
2. \[
\frac{\partial}{\partial x_1} \left( \frac{\partial \bar{u}_2}{\partial x_2} \right) = -N^2 (k + G)_{x_1} (k + G')_{x_2} \bar{u}_1
\]
3. \[
\frac{\partial}{\partial x_1} \left( \frac{\partial \bar{u}_3}{\partial x_3} \right) = -N^2 (k + G)_{x_1} (k + G')_{x_3} \bar{u}_1
\]
4. \[
\frac{\partial}{\partial x_1} \left( \frac{\partial \bar{u}_2}{\partial x_1} \right) = -N^2 (k + G)_{x_1} (k + G')_{x_1} \bar{u}_2
\]
5. \[
\frac{\partial}{\partial x_1} \left( \frac{\partial \bar{u}_3}{\partial x_2} \right) = -N^2 (k + G)_{x_1} (k + G')_{x_2} \bar{u}_2
\]
6. \[
\frac{\partial}{\partial x_1} \left( \frac{\partial \bar{u}_3}{\partial x_3} \right) = -N^2 (k + G)_{x_1} (k + G')_{x_3} \bar{u}_2
\]
7. \[
\frac{\partial}{\partial x_1} \left( \frac{\partial \bar{u}_1}{\partial x_2} \right) = -N^2 (k + G)_{x_1} (k + G')_{x_2} \bar{u}_3
\]
8. \[
\frac{\partial}{\partial x_1} \left( \frac{\partial \bar{u}_2}{\partial x_3} \right) = -N^2 (k + G)_{x_1} (k + G')_{x_3} \bar{u}_3
\]
9. \[
\frac{\partial}{\partial x_1} \left( \frac{\partial \bar{u}_3}{\partial x_3} \right) = -N^2 (k + G)_{x_1} (k + G')_{x_3} \bar{u}_3
\]
10. \[
\frac{\partial}{\partial x_2} \left( \frac{\partial \bar{u}_1}{\partial x_1} \right) = -N^2 (k + G)_{x_2} (k + G')_{x_1} \bar{u}_1
\]
11. \[
\frac{\partial}{\partial x_2} \left( \frac{\partial \bar{u}_2}{\partial x_1} \right) = -N^2 (k + G)_{x_2} (k + G')_{x_1} \bar{u}_1
\]
12. \[
\frac{\partial}{\partial x_2} \left( \frac{\partial \bar{u}_3}{\partial x_1} \right) = -N^2 (k + G)_{x_2} (k + G')_{x_1} \bar{u}_1
\]

81
\[ 13. \frac{\partial}{\partial x_2} \left( \frac{\partial u_2}{\partial x_1} \right) = -N^2 (k + G) x_2 (k + G) x_1 \bar{u}_2 \]

\[ 14. \frac{\partial}{\partial x_2} \left( \frac{\partial u_2}{\partial x_2} \right) = -N^2 (k + G) x_1 (k + G) x_2 \bar{u}_2 \]

\[ 15. \frac{\partial}{\partial x_2} \left( \frac{\partial u_2}{\partial x_3} \right) = -N^2 (k + G) x_3 (k + G) x_2 \bar{u}_2 \]

\[ 16. \frac{\partial}{\partial x_2} \left( \frac{\partial u_3}{\partial x_1} \right) = -N^2 (k + G) x_2 (k + G) x_1 \bar{u}_3 \]

\[ 17. \frac{\partial}{\partial x_2} \left( \frac{\partial u_3}{\partial x_2} \right) = -N^2 (k + G) x_1 (k + G) x_2 \bar{u}_3 \]

\[ 18. \frac{\partial}{\partial x_2} \left( \frac{\partial u_3}{\partial x_3} \right) = -N^2 (k + G) x_3 (k + G) x_2 \bar{u}_3 \]

\[ 19. \frac{\partial}{\partial x_3} \left( \frac{\partial u_1}{\partial x_1} \right) = -N^2 (k + G) x_1 (k + G) x_1 \bar{u}_1 \]

\[ 20. \frac{\partial}{\partial x_3} \left( \frac{\partial u_1}{\partial x_2} \right) = -N^2 (k + G) x_2 (k + G) x_2 \bar{u}_1 \]

\[ 21. \frac{\partial}{\partial x_3} \left( \frac{\partial u_1}{\partial x_3} \right) = -N^2 (k + G) x_3 (k + G) x_3 \bar{u}_1 \]

\[ 22. \frac{\partial}{\partial x_3} \left( \frac{\partial u_2}{\partial x_1} \right) = -N^2 (k + G) x_1 (k + G) x_2 \bar{u}_2 \]

\[ 23. \frac{\partial}{\partial x_3} \left( \frac{\partial u_2}{\partial x_2} \right) = -N^2 (k + G) x_2 (k + G) x_2 \bar{u}_2 \]

\[ 24. \frac{\partial}{\partial x_3} \left( \frac{\partial u_2}{\partial x_3} \right) = -N^2 (k + G) x_3 (k + G) x_3 \bar{u}_2 \]

\[ 25. \frac{\partial}{\partial x_3} \left( \frac{\partial u_3}{\partial x_1} \right) = -N^2 (k + G) x_1 (k + G) x_1 \bar{u}_3 \]

\[ 26. \frac{\partial}{\partial x_3} \left( \frac{\partial u_3}{\partial x_2} \right) = -N^2 (k + G) x_2 (k + G) x_2 \bar{u}_3 \]

\[ 27. \frac{\partial}{\partial x_3} \left( \frac{\partial u_3}{\partial x_3} \right) = -N^2 (k + G) x_3 (k + G) x_3 \bar{u}_3 \]

\[ 28. \frac{\partial^2 u_1}{\partial t^2} = -N^2 \omega^2 \bar{u}_1 \]

\[ 29. \frac{\partial^2 u_2}{\partial t^2} = -N^2 \omega^2 \bar{u}_2 \]
The voigt notation will be used from this point onwards to represent the elastic tensor components, therefore the above ij or kl values will be replaced with a single digit number, as shown in Table A.

Table A. Voigt notation transformation

<table>
<thead>
<tr>
<th>ij or kl</th>
<th>11</th>
<th>22</th>
<th>33</th>
<th>23 or 32</th>
<th>13 or 31</th>
<th>12 or 21</th>
</tr>
</thead>
<tbody>
<tr>
<td>becomes</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
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</tbody>
</table>

The thirty second-derivative equations above are substituted in the equations of motion for j = 1, 2 and 3 above (Eqns. B, C, and D), and the term \( N^2 \) cancels out from both sides of the equation. For j = 1, after replacing Eqns. 1-30 in Eqn. (B) above we get:

\[
30. \frac{\partial^2 \mathbf{u}_1}{\partial t^2} = -N^2 \omega^2 \mathbf{u}_3
\]
\[-\rho \omega^2 \ddot{u}_1 = C_{11}(k + G)_{x_1}(k + G')_{x_1} \ddot{u}_1 + C_{16}(k + G)_{x_1}(k + G')_{x_2} \ddot{u}_1 + C_{15}(k + G)_{x_2}(k + G')_{x_2} \ddot{u}_1 + C_{12}(k + G)_{x_1}(k + G')_{x_3} \ddot{u}_1 + C_{14}(k + G)_{x_1}(k + G')_{x_4} \ddot{u}_1 + C_{15}(k + G)_{x_1}(k + G')_{x_1} \ddot{u}_2 + C_{12}(k + G)_{x_1}(k + G')_{x_2} \ddot{u}_2 + C_{14}(k + G)_{x_1}(k + G')_{x_4} \ddot{u}_2 + C_{15}(k + G)_{x_1}(k + G')_{x_1} \ddot{u}_3 + C_{14}(k + G)_{x_1}(k + G')_{x_4} \ddot{u}_3 + C_{13}(k + G)_{x_1}(k + G')_{x_3} \ddot{u}_3 + C_{61}(k + G)_{x_2}(k + G')_{x_1} \ddot{u}_1 + C_{65}(k + G)_{x_2}(k + G')_{x_3} \ddot{u}_1 + C_{66}(k + G)_{x_2}(k + G')_{x_2} \ddot{u}_1 + C_{62}(k + G)_{x_2}(k + G')_{x_2} \ddot{u}_2 + C_{66}(k + G)_{x_2}(k + G')_{x_3} \ddot{u}_2 + C_{62}(k + G)_{x_2}(k + G')_{x_2} \ddot{u}_2 + C_{64}(k + G)_{x_2}(k + G')_{x_3} \ddot{u}_2 + C_{65}(k + G)_{x_2}(k + G')_{x_3} \ddot{u}_3 + C_{63}(k + G)_{x_2}(k + G')_{x_3} \ddot{u}_3 + C_{64}(k + G)_{x_2}(k + G')_{x_2} \ddot{u}_3 + C_{63}(k + G)_{x_2}(k + G')_{x_3} \ddot{u}_3 + C_{51}(k + G)_{x_3}(k + G')_{x_1} \ddot{u}_1 + C_{54}(k + G)_{x_3}(k + G')_{x_3} \ddot{u}_3 + C_{53}(k + G)_{x_3}(k + G')_{x_3} \ddot{u}_3 + C_{51}(k + G)_{x_3}(k + G')_{x_1} \ddot{u}_1 + C_{54}(k + G)_{x_3}(k + G')_{x_3} \ddot{u}_3 + C_{53}(k + G)_{x_3}(k + G')_{x_3} \ddot{u}_3 \]

which when rearranged with respect to \( \ddot{u}_1, \ddot{u}_2 \) and \( \ddot{u}_3 \) becomes:

\[
\ddot{u}_1 \{ \rho \omega^2 + C_{11}(k + G)_{x_1}(k + G')_{x_1} + C_{16}(k + G)_{x_1}(k + G')_{x_2} + C_{15}(k + G)_{x_2}(k + G')_{x_2} + C_{12}(k + G)_{x_1}(k + G')_{x_3} + C_{14}(k + G)_{x_1}(k + G')_{x_4} + C_{15}(k + G)_{x_1}(k + G')_{x_1} + C_{12}(k + G)_{x_1}(k + G')_{x_2} + C_{14}(k + G)_{x_1}(k + G')_{x_4} + C_{15}(k + G)_{x_1}(k + G')_{x_1} + C_{12}(k + G)_{x_1}(k + G')_{x_2} + C_{14}(k + G)_{x_1}(k + G')_{x_4} + C_{15}(k + G)_{x_1}(k + G')_{x_1} \}
\]

\[
+ \ddot{u}_2 \{ C_{16}(k + G)_{x_1}(k + G')_{x_1} + C_{12}(k + G)_{x_1}(k + G')_{x_2} + C_{14}(k + G)_{x_1}(k + G')_{x_4} + C_{15}(k + G)_{x_1}(k + G')_{x_1} + C_{12}(k + G)_{x_1}(k + G')_{x_2} + C_{14}(k + G)_{x_1}(k + G')_{x_4} + C_{15}(k + G)_{x_1}(k + G')_{x_1} + C_{12}(k + G)_{x_1}(k + G')_{x_2} + C_{14}(k + G)_{x_1}(k + G')_{x_4} + C_{15}(k + G)_{x_1}(k + G')_{x_1} \}
\]

\[
+ \ddot{u}_3 \{ C_{15}(k + G)_{x_1}(k + G')_{x_1} + C_{14}(k + G)_{x_1}(k + G')_{x_2} + C_{13}(k + G)_{x_1}(k + G')_{x_1} + C_{14}(k + G)_{x_1}(k + G')_{x_2} + C_{13}(k + G)_{x_1}(k + G')_{x_1} \}
\]

84
\[ G'_{x_3} + C_{65}(k + G)_{x_2}(k + G')_{x_1} + C_{64}(k + G)_{x_2}(k + G')_{x_2} + C_{63}(k + G)_{x_2}(k + G')_{x_3} + C_{55}(k + G)_{x_3}(k + G')_{x_1} + C_{54}(k + G)_{x_3}(k + G')_{x_2} + C_{53}(k + G)_{x_3}(k + G')_{x_3} \] = 0, \quad (E)

which is in the form \( M_1 \bar{u}_1 + L_1 \bar{u}_2 + U_1 \bar{u}_3 = 0 \), where \( M_1, L_1 \) and \( U_1 \) are the coefficients of \( \bar{u}_1, \bar{u}_2 \) and \( \bar{u}_3 \), respectively, in Eqn. (E) above. For \( j = 2 \), after replacing Eqns. (1-30) in Eqn. (C) above, and rearranging with respect to \( \bar{u}_1, \bar{u}_2 \) and \( \bar{u}_3 \) we get:

\[
\begin{align*}
\bar{u}_1 \{ & C_{61}(k + G)_{x_1}(k + G')_{x_1} + C_{66}(k + G)_{x_1}(k + G')_{x_2} + C_{65}(k + G)_{x_1}(k + G')_{x_3} + \\
& C_{21}(k + G)_{x_2}(k + G')_{x_1} + C_{26}(k + G)_{x_2}(k + G')_{x_2} + C_{25}(k + G)_{x_2}(k + G')_{x_3} + \\
& C_{41}(k + G)_{x_3}(k + G')_{x_1} + C_{46}(k + G)_{x_3}(k + G')_{x_2} + C_{45}(k + G)_{x_3}(k + G')_{x_3} \} + \\
\bar{u}_2 \{ & \rho \omega^2 + C_{66}(k + G)_{x_1}(k + G')_{x_1} + C_{62}(k + G)_{x_1}(k + G')_{x_2} + C_{64}(k + G)_{x_1}(k + G')_{x_3} + \\
& C_{26}(k + G)_{x_2}(k + G')_{x_1} + C_{22}(k + G)_{x_2}(k + G')_{x_2} + C_{24}(k + G)_{x_2}(k + G')_{x_3} + \\
& C_{46}(k + G)_{x_3}(k + G')_{x_1} + C_{42}(k + G)_{x_3}(k + G')_{x_2} + C_{44}(k + G)_{x_3}(k + G')_{x_3} \} + \\
\bar{u}_3 \{ & C_{65}(k + G)_{x_1}(k + G')_{x_1} + C_{64}(k + G)_{x_1}(k + G')_{x_2} + C_{63}(k + G)_{x_1}(k + G')_{x_3} + \\
& C_{25}(k + G)_{x_2}(k + G')_{x_1} + C_{24}(k + G)_{x_2}(k + G')_{x_2} + C_{23}(k + G)_{x_2}(k + G')_{x_3} + \\
& C_{45}(k + G)_{x_3}(k + G')_{x_1} + C_{44}(k + G)_{x_3}(k + G')_{x_2} + C_{43}(k + G)_{x_3}(k + G')_{x_3} \} \} = 0.
\]

which is in the form \( L_2 \bar{u}_1 + M_2 \bar{u}_2 + U_2 \bar{u}_3 = 0 \), where \( L_2, M_2 \) and \( U_2 \) are the coefficients of \( \bar{u}_1, \bar{u}_2 \) and \( \bar{u}_3 \), respectively, in Eqn. (F) above. For \( j = 3 \), after replacing Eqns. (1-30) in Eqn. (D) above, and rearranging with respect to \( \bar{u}_1, \bar{u}_2 \) and \( \bar{u}_3 \) we get:

\[
\begin{align*}
\bar{u}_1 \{ & C_{51}(k + G)_{x_1}(k + G')_{x_1} + C_{56}(k + G)_{x_1}(k + G')_{x_2} + C_{55}(k + G)_{x_1}(k + G')_{x_3} + \\
& C_{41}(k + G)_{x_2}(k + G')_{x_1} + C_{46}(k + G)_{x_2}(k + G')_{x_2} + C_{45}(k + G)_{x_2}(k + G')_{x_3} + \\
& C_{31}(k + G)_{x_3}(k + G')_{x_1} + C_{36}(k + G)_{x_3}(k + G')_{x_2} + C_{35}(k + G)_{x_3}(k + G')_{x_3} \} + \\
\bar{u}_2 \{ & \rho \omega^2 + C_{56}(k + G)_{x_1}(k + G')_{x_1} + C_{52}(k + G)_{x_1}(k + G')_{x_2} + C_{54}(k + G)_{x_1}(k + G')_{x_3} + \\
& C_{46}(k + G)_{x_2}(k + G')_{x_1} + C_{42}(k + G)_{x_2}(k + G')_{x_2} + C_{44}(k + G)_{x_2}(k + G')_{x_3} + \\
& C_{36}(k + G)_{x_3}(k + G')_{x_1} + C_{32}(k + G)_{x_3}(k + G')_{x_2} + C_{34}(k + G)_{x_3}(k + G')_{x_3} \} + \\
\bar{u}_3 \{ & C_{55}(k + G)_{x_1}(k + G')_{x_1} + C_{54}(k + G)_{x_1}(k + G')_{x_2} + C_{53}(k + G)_{x_1}(k + G')_{x_3} + \\
& C_{45}(k + G)_{x_2}(k + G')_{x_1} + C_{44}(k + G)_{x_2}(k + G')_{x_2} + C_{43}(k + G)_{x_2}(k + G')_{x_3} + \\
& C_{35}(k + G)_{x_3}(k + G')_{x_1} + C_{34}(k + G)_{x_3}(k + G')_{x_2} + C_{33}(k + G)_{x_3}(k + G')_{x_3} \} \} = 0.
\]
\[ \bar{u}_2 \{ \rho \omega^2 + C_{56}(k + G)_{x_1}(k + G')_{x_1} + C_{52}(k + G)_{x_1}(k + G')_{x_2} + C_{54}(k + G)_{x_1}(k + G')_{x_3} + C_{46}(k + G)_{x_2}(k + G')_{x_1} + C_{42}(k + G)_{x_2}(k + G')_{x_2} + C_{44}(k + G)_{x_2}(k + G')_{x_3} + C_{36}(k + G)_{x_3}(k + G')_{x_1} + C_{32}(k + G)_{x_3}(k + G')_{x_2} + C_{34}(k + G)_{x_3}(k + G')_{x_3} \} + \bar{u}_3 \{ C_{55}(k + G)_{x_1}(k + G')_{x_1} + C_{54}(k + G)_{x_1}(k + G')_{x_2} + C_{53}(k + G)_{x_1}(k + G')_{x_3} + C_{45}(k + G)_{x_2}(k + G')_{x_1} + C_{44}(k + G)_{x_2}(k + G')_{x_2} + C_{43}(k + G)_{x_2}(k + G')_{x_3} + C_{35}(k + G)_{x_3}(k + G')_{x_1} + C_{34}(k + G)_{x_3}(k + G')_{x_2} + C_{33}(k + G)_{x_3}(k + G')_{x_3} \} = 0. \] (G)

which is in the form \( W_1 \bar{u}_1 + W_2 \bar{u}_2 + M_3 \bar{u}_3 = 0 \), where \( W_1, W_2 \) and \( M_3 \) are the coefficients of \( \bar{u}_1, \bar{u}_2 \) and \( \bar{u}_3 \), respectively, in Eqn. (G) above.

Eqns. (E), (F) and (G) can be written as a system of linear equations as follows:

\[
\begin{bmatrix}
M_1 & L_1 & U_1 \\
L_2 & M_2 & U_2 \\
W_1 & W_2 & M_3
\end{bmatrix}
\begin{bmatrix}
\bar{u}_1 \\
\bar{u}_2 \\
\bar{u}_3
\end{bmatrix} = 0. \] (H)

Since the only unknown in the 9 matrices shown in Eqn. (H) is \( \omega \), solving the linear system above gives \( \omega/k \) pairs which represent the propagating modes within a phononic crystal. An example of the band structure obtained using this formulation is shown in Chapter 3.
References


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