Generalized Phononic Networks: Of Length Scales, Symmetry Breaking and (Non) locality

“Controlling Complexity through Simplicity”

by

Cheong Yang (Henry) Koh
B.S. Materials Science and Engineering
Cornell University (2005)

Submitted to the Department of Materials Science and Engineering in Partial Fulfillment of the Requirements for the Degree of

Doctor of Philosophy in Materials Science and Engineering

at the

Massachusetts Institute of Technology

May 2011

©2011 Massachusetts Institute of Technology. All rights reserved

Signature of Author..........................................................................................................................

Cheong Yang (Henry) Koh
Department of Materials Science and Engineering

Certified by .................................................. .................................................................

Edwin L. Thomas
Morris Cohen Professor of Materials Science and Engineering
Thesis Supervisor

Accepted by ...............................................................................................................................

Chris A. Schuh
Danae and Vasilios Salapatas Associate Professor of Metallurgy
Chair, Departmental Committee on Graduate Students
Generalized Phononic Networks: Of Length Scales, Symmetry Breaking and (Non) locality

“Controlling Complexity through Simplicity”

by

Cheong Yang (Henry) Koh

Submitted to the Department of Materials Science and Engineering on May 10th, 2011, in Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy in Materials Science and Engineering

ABSTRACT

The manipulation and control of phonons is extremely important from both a fundamental scientific and applied technological standpoint, providing applications ranging from sound insulation to heat management. Phononic crystals and metamaterials are artificially structured materials (at certain length scales) that provide promise in controlling the propagation of phonons in solids. However, the vector nature of the phonon makes the development of a governing framework with which to guide the design of these phononic metamaterials complicated and no coherent framework exists for the design of phononic structures. In this thesis, we utilize a combination of global symmetry principles, adopted from group theory and the theory of representations, together with conservation principles and broken symmetry concepts to formulate our generalized design framework. This framework allows us to exactly treat the vector nature of phonons and control their propagation, unifying the design of phononic crystals, metamaterials, waveguides and numerous other structures, both infinite and finite. In particular, utilizing only this general framework which we develop, we are able to explain the choice of a particular physical topography for a desired phononic propagation behavior in a coherent fashion. In addition, we show how we may explicitly control the dispersion relations of a phononic metamaterial in order to obtain a desired final band structure. Some of our demonstrations include a new polychromatic phononic metamaterial which possesses multiple complete in-plane spectral gaps totaling over 100% in normalized gap size to a phononic metamaterial which exhibits a single complete in-plane spectral gap of 102% and a complete spectral gap of 88%, both significant advancements over the state of the art. This thesis also removes the artificial distinction between the phononic crystal and metamaterial classifications by unifying their behavior within the same generalized framework. As a result, we show that only a few governing principles are required to design the complex band dispersion relations of phononic metamaterials. The generality of our framework allows extension to other vector and scalar waves, such as photonic, plasmonic and magnonic structures and provides a promising route
forward to the development of integrated structured material platforms that allow for the rational manipulation and interactions of phonons with other waves, such as phonons and spin waves.

Thesis Supervisor: Edwin L. Thomas

Title: Morris Cohen Professor of Materials Science and Engineering
### Table of Contents

List of Figures ............................................................................................................................ 6  
Acknowledgements.................................................................................................................. 15  

Chapter 1. Introduction, Motivation and Overview ................................................................. 17  
  1.1 Introductory remarks ........................................................................................................ 17  
  1.2 Phonons in Science and Technology ............................................................................... 18  
  1.3 Phononic Crystals and Metamaterials- A Timeline ...................................................... 20  
  1.4 Phononics and its relation to acoustics, elasticity and mechanics: Length scales and broken symmetry ...................................................................................................................... 29  

Chapter 2. Elastodynamics of Artificial Structures .................................................................. 35  
  2.1 Introductory Remarks ...................................................................................................... 35  
  2.2 Fundamental Equations and Governing Principles ....................................................... 38  
  2.3 Broken Symmetry and Polarizations of the Vector Phonon ......................................... 51  
  2.4 Concluding Remarks on Elastodynamics from a Symmetry Breaking Perspective ....... 60  

  3.1 Introductory Remarks ...................................................................................................... 62  
  3.2 Generalization of Avoided Crossings & Perturbation Theory ..................................... 66  
  3.3 Non-Locality: The effect of the Lattice and its Interactions .......................................... 77  
  3.4 Local Principles: The Variational Principle from a Geometric Viewpoint ................... 85  
  3.5 Groups & Representations: Nonsymmorphicity and Wyckoff Positioning .................. 95  
  3.6 Concluding Remarks....................................................................................................... 111  

Chapter 4. Classifications of Lattices: Physical Topology of Phononic Structures ............... 112  
  4.1 Introductory Remarks ...................................................................................................... 112  
  4.2 The Dynamical Mechanical Bond .................................................................................. 115  
  4.3 Specialization for Solid-Air/Vacuum structures: An exercise in symmetry breaking and the high impedance limit. ........................................................................................................... 133  
  4.4 Linking the Physical Topography to the Applications ................................................... 140  
  4.5 Conclusions ................................................................................................................... 158  

Chapter 5. Designing Dispersion Relations in Phononic Metamaterials I: Avoided Crossings ... 161  
  5.1 Introductory Remarks ...................................................................................................... 161  
  5.2 From Crystals to “Resonant” Meta-materials .................................................................. 164
5.3 Meso-Scale Phononic Meta-Crystal: Polarization specific spectral gaps

5.4 Conclusions

Chapter 6. Designing Dispersion Relations Phononic Metamaterials II: A Polychromatic Nonsymmorphic Phononic Crystal

6.1 Introductory Remarks

6.2 Global Symmetry: Nonsymmorphicity and Sticking Bands

6.3 Local Variational Principles: The Tight Binding Lattice (TBL) Class

6.4 Conclusions

Chapter 7. Conclusions and Future Work

7.1 Summary of Work

7.2 Technological Applications of Phononic Networks

7.3 Current and Future Work: Xoxonics?

Bibliography
List of Figures

Figure 1.1 Overview of the applications of phononics across various length scales, ranging from sub Hz to the THz, and spanning various technological areas of imaging and detection. .................................................. 18

Figure 2.1 Band Dispersion Relations of (a) Monatomic one-dimensional classical chain, (b) Diatomic one-dimensional classical chain (c) Generic Continuous one dimensional Phononic Crystal. Here we computed, at a 50-50 volume fraction, one phase utilizing (E=12Gpa, ν=0.3, ρ=2330kgm⁻³), the other utilizing (E=6Gpa, ν=0.17, ρ=1330kgm⁻³). ........................................................................................................... 39

Figure 2.2 Displacement field comparing between the (a) homogeneous system and (b) the 1D phononic crystal and the corresponding (anti)symmetric pairs along the direction of periodicity. The strain field intensity, |u(r)| ranges from red (high) to blue (low), with the vector field indicating both the magnitude and the direction of the strains. The color map indicates large (red) to zero (blue) displacement.......... 56

Figure 2.3 Eigenmode plots for the pairs of bands (5,12) at the Γ point, and pairs of bands (2,4) at the X point for the 1D phononic structure computed in Figure 2.1(c). These pairs of bands are responsible for the opening of the spectral gap in the phononic crystals at the Γ and X point respectively. The color map indicates large (red) to zero (blue) displacement.................................................................................. 59

Figure 3.1 Dispersion relations of (a) the classical Lamb plate and (b) the modified antisymmetric (AntiS) plate. The unit cells are shown in the insets, with the structures extending infinitely along the axial and into the plane, and having a finite thickness h. (a) clearly shows the two sets of solutions, symmetric (solid lines) and anti-symmetric (dotted lines) about the central mirror plane with the anti-symmetric modes represented by dotted lines. The pair of red arrows indicate the positions of avoided crossing in both systems. In (a) this takes place between the 2nd and 4th modes (both even) and in (b) we picked the 6th and the 7th bands. The exact thickness of the plates will affect the positions of the bands, but the features of the dispersion relations remain invariant to the change in thickness. Computations were performed with amorphous silicon as the material (E=156Gpa, ν=0.2152, ρ=2330kgm⁻³) ....................... 69

Figure 3.2 Avoided crossing of the 2nd and 4th modes in the Lamb plate, before (k= 0.24,0) and right after(k=0.28,0) the avoided crossing as highlighted in Figure 3.1 It is clear here that the interaction, or avoided crossing is rather weak, hence there is very little mixing of the modes, although the bands do change character after undergoing the interaction, a clear signature of the avoided crossing. The color map indicates large (red) to zero (blue) displacement................................................................. 71
Figure 3.3 Eigenmodes of modes 3 to 6 of the Lamb plate, at the \( \Gamma \) point. Modes 3 and 6 are anti-symmetric whereas modes 4 and 5 are symmetric with respect to the horizontal mirror at \( h/2 \). The color map indicates large (red) to zero (blue) displacement................................................................. 72

Figure 3.4 Eigenmodes of (a) Bands (6,7) from Anti-S Lamb plate before and (b) Bands (6,7) from Anti-S Lamb plate after the avoided crossing. A single unit cell is plotted here, the plates extend infinitely along the [100] direction. The color map indicates large (red) to zero (blue) displacement..........................74

Figure 3.5 Eigen-mode plots of (a) Mode 6 (antisymmetric), (b) Mode 5(symmetric), (c) Mode 4 (symmetric), (d) Mode 3(antisymmetric) of the AntiS Lamb Structure at the \( \Gamma \) point. The color map indicates large (red) to zero (blue) displacement.................................................................................... 76

Figure 3.6 Computed band diagrams of the 2D locally resonant structures, showing the effect of non-locality with the variation of the intermediate \( \beta \)-phase, which is our connecting (non)local phase in the LRS-type structure (a) \( \beta \)-phase has the same properties as the scatter, (b) \( \beta \)-phase has the same properties as the matrix,(c) \( \beta \)-phase has the mechanical properties lower than both (\( E=0.5GPa,v=0.3,p=1300kgm^{-3} \)) the scatter and matrix,(d) \( \beta \)-phase has mechanical properties much lower than both (\( E=0.05GPa,v=0.3,p=1300kgm^{-3} \)) phases. The scatterer phase was taken as (\( E=4GPa,v=0.3,p=4000kgm^{-3} \)), the matrix phase was taken as (\( E=4GPa,v=0.17,p=1300kgm^{-3} \)).....................79

Figure 3.7 (a) Modes 3 and 6 at the X point for Fig3.6 (a), which is what one associates with classically in a phononic crystal. The structure itself resembles the binary phononic crystal. (b) Modes 2 and 5 for Fig3.6 (d), where we have the LRS structure. The color map indicates large (red) to zero (blue) displacement............................................................................................................82

Figure 3.8 Time evolution of mode 3 at \( k=[0.3, 0] \) for LRS structure (Figure 3.6(a) and (d)). (a),(b), (c) show the time evolution of mode 3 for structure (d), which corresponds to the LRS structure typically introduced in the literature. The color map indicates large (red) to zero (blue) displacement. For (a) and (d), the vector fields have been plotted in white to act as a visual guide for the low displacement intensity case, i.e. it has the same physical meaning as the black arrows in figures (b), (c), (e), (f)...........83

Figure 3.9 Computed band diagrams of (a) the RS structure (b) the RB structure. The insets show the unit cell, with the dark phase being the material and the complimentary white phase being air/vacuum. The material is chosen to be amorphous silicon (\( E=156GPa,v=0.2152,p=2330kgm^{-3} \)). Area fractions are for RS (26.7\%) and for RB (39\%). The red dashed line represents the position \( k=(0.5,0) \). This will be used extensively in the remaining section. .............................................................................................................. 86
Figure 3.10. Eigenmode plots at M point for (a) Mode 3 for RS structure (b) Mode 3 for RB structure (c) Mode 2 for RS structure (d) Mode 2 for RB structure. Note that for each structure (both RS and RB), the degenerate pairs are accidentally degenerate, being antisymmetric and symmetric with respect to the diagonal mirror plane along [1 1]. The color map indicates large (red) to zero (blue) displacement. 88

Figure 3.11 Eigenmode displacement field plots at X point for the pair of interacting bands (a) mode 7, (c) mode 3 of RS, and (b) mode 6, (d) mode 3 of RB. The color map indicates large (red) to zero (blue) displacement and all displacement fields are plotted to the same scales. 90

Figure 3.12 Momentum-space evolution along ΓX [1 0] in k-space for bands 4, 5, 6 for the RS structure at \( k = (0,0) \), \( k = (0.5,0) \) and \( k = (1,0) \). We note that in particular, mode 4 at the X point, that there is delocalization of strains into the central scatterer. The color map indicates large (red) to zero (blue) displacement. At the Γ point, the isotropy group is the point group \( C_{4v} \{ E, C_2, 2C_2, 2m, y, 2my \} \), hence mode 4 is symmetric with respect to the horizontal mirror plane, mode 5 is symmetric with respect to the vertical mirror plane and mode 6 symmetric with respect to a \( C_4 \) rotation. Along ΓX ( [1 0] direction), there is only a single horizontal mirror plane, hence the irreducible representations are symmetric with respect to the mirror (mode 4), or antisymmetric with respect to it (modes 5, 6). Finally, at X, the isotropy group is \( \{ E, m_x, C_2 \} \), hence mode 4 is symmetric with respect to the mirror while mode 6 is antisymmetric with respect to the mirror. In addition, mode 5 is symmetric with respect to the \( C_2 \) rotation operation. 91

Figure 3.13 Eigenmode Displacement Field plots tracing the evolution along ΓX [1 0] in k-space for bands 4, 5, 6 for the corresponding RB structure at \( k = (0,0) \), \( k = (0.5,0) \) and \( k = (1,0) \). Here it is clear that the displacement fields here are localized mainly on the connecting bonds, with no mixing at the X point. The color map indicates large (red) to zero (blue) displacement. 93

Figure 3.14 Computed Band Diagrams of Structures (a) T1 and (b) T3, taken with the naive IRBZ belong to a p4mm lattice. The material is chosen to be amorphous silicon \( (E=156 GPa,v=0.2152,p=2330 kg m^{-3}) \). Area fractions are for T1 (59.35%) and for T2(54.15%). 98

Figure 3.15 Computed Band Diagram of the same T3 structure about its actual bigger IRBZ, which is that of a p2mm lattice. It is clear that the spectral gap size is maintained here. The material is chosen to be amorphous silicon \( (E=156 GPa,v=0.2152,p=2330 kg m^{-3}) \). 99

Figure 3.16 Eigenmode plots for (a) (3,7) for T1 and (b) modes (3,9) for T3 at the X point. The color map indicates large (red) to zero (blue) displacement. 100
Figure 3.17 Eigenmode plots at the $\Gamma$ point, for (a) mode 6, (b) mode 5, (c) mode 4, (d) modes 3, of structures T1 and T3, on the left and right respectively. The color map indicates large (red) to zero (blue) displacement.

Figure 3.18 Time Evolution of the eigenmodes at (i), $t=0$, (ii), $t=\pi/6$, for (a) 5th band along the $\Gamma X'$ [01] direction and (b) 5th band along the $\Gamma X$ [10] direction respectively. The color map indicates large (red) to zero (blue) displacement.

Figure 3.19 Computed Band Diagrams of Structures possessing global nonsymmorphic symmetries of (a) p2gg, (b), p4mg. The material is chosen to be amorphous silicon ($E=156$GPa,$\nu=0.2152,\rho=2330$kgm$^{-3}$).

Figure 3.20 Computation of Band diagrams for two different structures with p4gm symmetry. (a) is topologically connected along the <11> directions whereas (b) is only connected on the fundamental building blocks. The material is chosen to be amorphous silicon ($E=156$GPa,$\nu=0.2152,\rho=2330$kgm$^{-3}$).

Figure 3.21 Computed Band Diagrams of (a) p4mm structure with a cylindrical Wyckoff Decoration and (b) p4mm structure with a square Wyckoff Decoration. The material is chosen to be amorphous silicon ($E=156$GPa,$\nu=0.2152,\rho=2330$kgm$^{-3}$). The band sticking features here are invariant to the specific geometrical structures, as long as the Wyckoff decorations maintain the same structures at the (0,0) and (0.5,0.5) positions.

Figure 4.1 Shows the geometric structures of a tight-binding and an extended-lattice structure respectively. A matrix is defined as a connected phase, while the scatterer phase is the disconnected phase. A darker colored phase indicates a larger impedance value, hence the geometric matrix in the tight binding structure has a lower impedance. The corresponding eigenmode plot shows the typical trajectory of the strain fields, with high strains localized between the higher impedance scatterers. In contrast, for the extended lattice, it is clear that the strain fields are propagating through the matrix mainly, with some penetration into the scatterer phases. The color map indicates large (red) to zero (blue) displacement.

Figure 4.2 Computed band structures computed with the same geometrical structure (inset), but sweeping the impedance contrast, defined as $\Delta Z=Z_{\text{matrix}}-Z_{\text{scatterers}}$. (a) tight binding lattice($E=10$GPa,$\nu=0.2,\rho=1300$kgm$^{-3}$), with $\Delta Z<0$, has relatively flat dispersion in the higher order bands (above the first band gap) (b) the homogeneous case $\Delta Z=0$($E=156$GPa,$\nu=0.2,\rho=2330$kgm$^{-3}$), is the reference to show the unperturbed dispersion relation, taking into account the Brillouin zone reduction into the IRBZ and (c) the extended lattice case, $\Delta Z>0$($E=400$GPa,$\nu=0.2,\rho=7800$kgm$^{-3}$). The dark colored phase is always set here to be silicon, and is our reference material. The color map indicates large (red) to zero (blue) displacement.
Figure 4.3 Time evolution of phonon propagation in the same band (band 5) in the tight binding lattice (a,b,c,d), the homogeneous reference(e,f,g,h) and the corresponding extended lattice(i,j,kl), all at \( k = (0.7\pi/a,0) \). The time steps are taken at (i) \( t = \pi/6 \), (ii) \( t = \pi/3 \), (ii) \( t = 2\pi/3 \), (iv)\( t = 2\pi/3 \). The corresponding band structures are shown in Fig 4.2(a), (b) and (c) respectively. The color map indicates large (red) to zero (blue) displacement.

Figure 4.4 Computed band diagrams for the same geometric structure, but with different elastic parameters for the constituents. Both structures are chosen to have zero impedance contrast between the two phases. (a) the structure consists of a matrix with higher density but lower elastic moduli, and hence lower velocities whereas (b) consists of a matrix with lower density but higher elastic moduli, and hence higher velocities. This is to juxtapose against conventional methods whereby selected subsets of density and/or elastic contrasts are utilized. In both cases, the time evolution of the eigenmodes of the 5th band are shown in (i),(ii) for (a) and (iii),(iv) for (b). It is instructive to note that in this case, that the propagation looks very similar to the homogeneous case, and the transport essentially occurs through both phases and hence is neither extended nor localized like. (a) utilized hypothetical values of \( E=78\)GPa, \( p=4660\)kgm-3 while (b) utilized hypothetical values of \( E=312\)GPa, \( p=1165\)kgm-3. For both systems, the poisson ratio was matched to that of Silicon, which was utilized for the scatterer phase.

Figure 4.5 Computed band diagrams for the same geometric structure, but with different elastic parameters. (a) is a tight binding lattice, but with different elastic parameters that contrasts that in Figure 4.2. It consists of a matrix with higher wave velocities whereas (b) is the extended lattice, consists of a matrix with higher wave velocities as well. This is to contrast with the structures computed in Figure 4.2, where the matrix was chosen to have lower velocities. Time evolution of the 5th mode at \( k=(0,7,0) \) were also plotted for the TBL structure (a) (i,ii) as well as for the EL structure(b) (iii,iv). The time steps were taken at \( t = \pi/3 \) and \( t = 2\pi/3 \) for both cases.

Figure 4.6 The eigenmodes of the two bands bounding the spectral gap at \( k=(0.4\pi/a,0) \) in Figures 4.2 (a) TBL and (c) EL. For the tight binding lattice, band 7(a) (antisymmetric about \( \alpha \)) and band 6 (symmetric about \( \alpha \)) (b) have different irreducible representations. This implies that while these bands comprise the physical bounds for the gap size that avoided crossing did not occur between these two bands and hence the scattering strength is not responsible for the gap size in this situation. This is more common in tight binding lattice classes, where the multiple high order bands (\( >9 \)) cross each other in \( (\omega,k) \) space readily. In contrast, for the extended lattice, the gap size is clearly delimited by the avoided crossing occurring between bands 6(d) and 7(c). Another important point of note is that the interaction between the bounds occurs within the BZ, and not primarily or exclusively at the edges or boundaries.

Figure 4.7 shows a family of structures with \( p4mm \) plane group symmetry. The motifs are non-primitive, occupying Wyckoff positions at (0, 0) and (0.5a, 0.5b), with \( a=b \). From left to right, we increase the size of one of the building blocks, from small(a) to degenerate(b) to larger(c). The solid dark phase is the
matrix phase, and the white regions are the air/void phase. The red circles outline the mechanical 'connections' forming the actual geometric mechanical bonds of the structures. The material is chosen to be amorphous silicon \( (E=156 \text{ GPa}, v=0.2152, p=2330 \text{ kgm}^{-3}) \).

Figure 4.8 Eigenmodes displaying the time-evolution for the 6th band, which bounds the spectral gap from below at \( k=(0.4\pi/a,0) \) for all 3 structures, labelled as (a),(b), and (c) as per original convention. The time evolution is given by 4 exemplary time steps at (i)\( n/6 \), (ii)\( n\pi/3 \), (iii)\( n\pi/2 \), (iv)\( 2n\pi/3 \) respectively.

Figure 4.9 Eigenmode plots displaying time-evolution for the "7th" band, which bounds the spectral gap above at \( k(\pi/a)=0.4 \), for all 3 structures, labelled as (a),(b), and (c) as per original convention. The time evolution is given by 4 exemplary time steps at (i)\( n\pi/6 \), (ii)\( n\pi/3 \), (iii)\( n\pi/2 \), (iv)\( 2n\pi/3 \) respectively. It is clear that the transport trajectory gradually becomes more and more localized as the four diagonally aligned mechanical arms, connecting the four bulding blocks become more and more narrow. In solid-air/vacuum systems, the phonon propagation behavior is determined by the geometric structure. In this situation, there is an additional subtlety in the appearance of the eigenmodes. In this case, the formation of the eigenmode mirrors that closely of that in "molecular orbital" theory. Here in this case, one sees clearly that the eigenmodes resemble the anti-bonding type orbital, which gets more spatially localized and hence more tight binding like, as we move from (a) to (b).

Figure 4.10 Computed band structures of two structures with the same p4mm plane group symmetry, but with a deliberate change in the connectivity/topology between the two structures. Both structures belong to the extended lattice class, which is exemplified by their quasilinear dispersion bands, some of which are obscured by the avoided crossing by designed flat bands. In this work, we started deliberately with a structure with a large complete spectral gap (a), before we rationally induced pure negative refraction bands by increasing the connectivity of the structure(b, inset). This has the net effect of "pulling" the 4th to 6th bands into the original gap position to form negative refracting bands. These negative refraction bands are distinct from conventional systems in that these negative refracting bands have low group velocities, by virtue of the way in which we induce them. The material is chosen to be amorphous silicon \( (E=156 \text{ GPa}, v=0.2152, p=2330 \text{ kgm}^{-3}) \).

Figure 4.11 Eigenmode plots showing the corresponding pairs of bands that interact to form the lowest spectral gaps. For structure (a), the bands undergoing avoided crossing are the 13th(a,(i)) and the 6th(a,(ii)) bands. For (b), the bands undergoing avoided crossing are the 8th(a,(i)) and the 3rd(a,(ii)) bands. It is a common mistake to associate the corresponding bands by their band number, rather than their actual nature, which is given by the dynamics of the eigenvector. In this case, the band numbers have changed because of the connectivity change between the two structures, which introduces a number of extra flat bands in (a) that interact with the "original" extended type bands (with quasi-linear dispersion), hence obscuring the band structure at first glance. We note that the absolute method by which to identify the correct bands which undergo the avoided crossing and hence, are responsible for
the spectral gap formation is to classify them according to their irreducible representations. In fact, it is clear from their eigen-modes that these two corresponding pairs of bands are the same corresponding pairs of bands, with only the change in the connectivity perturbing the actual eigen-values slightly. The effect of the change in the connectivity has much greater effect on the flat bands, or slow modes, which is the purpose of this geometric connectivity change.

Figure 4.12 Eigenmode plots showing the strain field evolution of the (a) 6th, (b)5th and (c)4th bands of structure (a) and (e) 6th, (f)5th and (g) 4th bands of structure (b) as we increased the connectivity in order to create negative refractive bands. The color map indicates large (red) to zero (blue) displacement.

Figure 4.13 Eigenmode plots showing the time evolution at (i) t=0, (ii) t=\(\pi/2\), (iii) t= \(\pi\), of the 4th and 6th negative refracting bands of structure (b). All of these plots were taken at \(k = (0.3,0)\). It is clear that these two modes preserve their polarization generally as transverse-like (anti-symmetric) and longitudinal-like(symmetric) along the Gx direction. This is only possible by controlling the starting symmetries of the two flat modes in structure(a) before increasing its propagation velocity by increasing the connectivity in a rational way to permit transport.

Figure 4.14 Computed band structures of the tight binding lattice structures. (a) possesses the largest known in-plane complete spectral gap of 105% (b) possesses a smaller complete in-plane spectral gap of \(~ 60\%\). The material is chosen to be amorphous silicon (\(E=156\text{GPa}, v=0.2152, \rho=2330\text{kgm}^{-3}\)).

Figure 4.15 Eigenmode plots showing the corresponding pairs of bands that have undergone avoided crossing in order to create the complete spectral gap for structure (a) at the X and M points. The color map indicates large (red) to zero (blue) displacement.

Figure 4.16 Eigenmode plots comparing the 3rd and 6th bands at the \(\Gamma\) point of structures (a) and structure (b) respectively. The color map indicates large (red) to zero (blue) displacement.

Figure 4.17 Eigenmode plots at the X point, for the same pairs highlighted in Figure 4.16. By comparing with the respective modes in Figure 4.16, we see that in (a) the tight-binding nature of the lattice type is apparent here from the decomposition of the eigenmodes into tight-binding like combinations of the building blocks. For (b), there is still significant mixing, which leads to the more spatially delocalized eigenmode profile.

Figure 5.1 (a) Experimental Schematic of a resonant metamaterial, consisting of the lead sphere, surrounded by a soft rubber, with a stiffer epoxy matrix. (b) Computed band dispersion of the structure,
which is a simple cubic lattice. Note that the reason for the dispersion bands being so flat is due to the extremely soft rubber acting as the soft spring. Taken from Ref [55] ..................................................... 165

Figure 5.2  (a) (i) Structure of the original honeycomb unit cell (Area fraction=56%). The black region represents solid material and the grey region air/vacuum. It possesses C3v point symmetry at the Γ point if we take a two-cylinder motif. (ii) Structure of the deformed honeycomb unit cell (ICS) (Area fraction=55%). The black region represents solid material and the grey region air/vacuum. It possesses C2v point symmetry at the Γ point. (b) (i) Corresponding Band Diagram for the in-plane polarization of the original honeycomb lattice (ii) Corresponding Band Diagram for the in-plane polarization of the deformed honeycomb lattice. Calculations here utilized amorphous/polycrystalline silicon for the material. Note that the deformation opens a narrow sub-wavelength complete gap as well as enlarging the corresponding crystalline gap. The material is chosen to be amorphous silicon (E=156GPa, v=0.2152, ρ=2330kgm⁻³).......................................................................................................... 168

Figure 5.3 (a) Modes 2 and 3 along ΓM for the honeycomb lattice, (b) Modes 2 and 3 along ΓM for the ICS lattice, (c) Mode 3 at the Γ point for the honeycomb lattice, (d) Mode 3 at the Γ point for the ICS lattice. .................................................................................................................................................... 170

Figure 5.4 Eigenmodes of (a) Modes 2 and 3 along ΓK for the honeycomb lattice, (b) Modes 2 and 3 along ΓK for the ICS lattice.................................................................................................................................. 173

propagation while actually promoting antisymmetric propagation by removing the physical node in the middle of the original honeycomb. Here, the particular choice of the geometric cut is important because while there exist a multitude of ways to reduce the symmetry, we have to induce the right change in order to be able to interchange the AnS and S modes! We note there that we are also essentially creating a medium that in the longer wavelength limits, has a faster “transverse-like” wave velocity, compared to the “longitudinal-like” wave velocity, counter to homogeneous materials. However, this is perfectly legitimate because these are velocities induced from the dynamics of propagation in the microstructure, in this case a solid-air or, equivalent for finite-element modeling, solid-free surface, i.e. at the interfaces we experience symmetry breaking, hence the effective medium approximation in the conventional quasi-static limit needs to be modified [73]. The combination of these considerations, together with the symmetry reduction, finally allows us to then induce a complete sub-wavelength gap, as is shown [Figure 5.2 b (i), (ii)] .................................................................................................................................................... 174

Figure 5.5 a) (i) Derivative Metamaterial Structure with p4mm plane group symmetry (Area fraction=51.5%). The point symmetry at the Γ point retains C4v. (ii) Parent Crystal Structure with p4mm plane group symmetry (Area fraction=39%). The point symmetry at the Γ point is C4v. (b) (i) Corresponding Band Diagram for the in-plane polarization of the high connectivity p4mm structure in (a, i) (ii)
Corresponding Band Diagram for the in-plane polarization of the original parent p4mm structure in (a, ii) Calculations here utilized amorphous/polycrystalline silicon\((E=156\text{GPa}, v=0.2152, \rho=2330\text{kgm}^{-3})\) for the material. The increase in connectivity increases the fundamental \(t_1\) mode velocity, allowing for the avoided crossing to create the sub-wavelength transverse gap.

Figure 5.6 (a) Displacement Field for the \(t_1\) mode, as marked in Figure 4.4(b, i) (b) Displacement Field for the \(t_2\) mode, as marked in Figure 4.4(b, i) (c) Displacement Field for the \(l_1\) mode, as marked in Figure 4.4(b, i) (d) Displacement Field for the \(l_2\) mode, as marked in Figure 4.4(b, i). Note here that even though strictly speaking, the modes are not transverse or longitudinal, we physically can design the displacement field to make it as “transverse-like” or “longitudinal-like”. Along the \(\Gamma X\) direction, this naturally is separated into the modes which are \(AS\) or \(S\) with regards to the horizontal mirror.

Figure 6.1 (i) Band Diagram of the Tight-Binding Lattice (TBL) (ii) Band Diagram of the Lower fill-fraction Lattice (SL) (insets show the corresponding geometrical structure and the BZ convention) The corresponding bands 11 and 12 are colored green and red respectively for both structures to illustrate the different mechanisms involved in controlling the band dispersion in the two lattices. Calculations here utilized amorphous/polycrystalline silicon\((E=156\text{GPa}, v=0.2152, \rho=2330\text{kgm}^{-3})\) for the material. Area fractions are: for the TBL\((36.8\%)\) and SL\((59.5\%)\).

Figure 6.2 (i) Band Diagram along \(GX\) of TBL. Displacement Fields at \(\Gamma\) for modes (d) 9, (c) 10, (b) 11, (a) 12. (ii) Band Diagram along \(GX\) of SL. Displacement Fields at \(\Gamma\) for modes (f) 9, (h) 10, (g) 11, (e) 12. The color map indicates large (red) to zero (blue).

Figure 6.3 Displacement Fields at \(X\) point for TBL for mode (a) 12, (b) 11, (c) 10, (d) 9, and at \(M\) point for TBL for mode (a’) 12, (b’) 11, (c’) 10, (d’) 9. Note that for modes (a),(a’) and (b),(b’), the displacement fields are nearly identical whereas for modes (c),(c’) and (d),(d’), they are very slightly offset [Figure 1(i) and (ii)]. The color map indicates large (red) to zero (blue) displacement. The vector field represents the total displacement vector.

Figure 7.1 a) Map of \(ZT\) vs Temperature for state of the art thermoelectric materials [87]. b) Progress Map tracing the evolution of \(ZT\) performance of various thermoelectric materials over the years [88]. c) Map of \(ZT\) vs Temperature for various state of the art commercial bulk thermoelectric materials as well as those utilized and developed by NASA for space thermoelectric power generation [6].

Figure 7.2 Eigenmode plots. (a) a single edge mode in a semi-infinite medium(the lower bound extends to infinity) of which we show a section near the surface (b) the antisymmetric coupled surface Rayleigh mode and (c) the symmetric coupled surface Rayleigh of a Lamb plate, or a finite slab. The color map indicates large (red) to zero (blue) displacement.
Acknowledgements

It is often said that the hardest section to write in the thesis is the acknowledgements, not because of the lack of words, but more for the lack of space! My time here at MIT has been thoroughly enjoyable, enriching and challenging. Research has been a source of intense joy, in moments of success, as well a source of extreme frustration in times of struggle; the process has also uncovered many things about myself and how to push my own limits. I deeply enjoyed the culture of research here, which is to attack a problem fundamentally at its roots and to create from the understanding derived from it. This to me epitomizes the joys of doing research and I have shaped my research philosophy largely from it. I owe all of my growth and development to the dynamic scientific community around me; without them this would have not been at all possible.

First and foremost, I would like to thank my advisor, Prof Edwin (Ned) Thomas for his tutelage these past years. Besides instructing me in the scientific method with the highest standards of integrity, propriety and technical excellence, he has been a source of creative inspiration and wisdom. I remember many of our long meetings in the late afternoon where we would cover an exhausting plethora of different topics and I would then return to my office, thinking about the questions he had posed. After an even longer period of thought and mulling over, I would become greatly enlightened through those insightful remarks and deep, penetrating questions. Ned’s physical intuition is astounding and unparalleled to me and his ideas and wisdom always comes from unique angles. It is only after many years of training, I’ve finally been able to gradually receive and appreciate them. He has been the best mentor I could have ever hoped for and more. Much of my intellectual growth and development has been gained through these interactions and exchanges with Ned; I hope this work repays him at least partially for his patience and the freedom which he has given me in seeking to explain complexity through the simplicity of symmetry. I would not have completed this if not for Ned.

I thank Prof Samuel Allen and Prof Gang Chen for agreeing graciously to be on my committee and for their insightful comments and critical reading of this thesis. I would also like to thank some of the earlier ELT group members that I have worked with. Dr Ji-Hyun Jang (who doesn’t sleep much) is a tireless colleague, a source of very fruitful collaboration and a great friend. Dr Chaitanya Ullal taught me interference lithography when I first arrived in Cambridge, MA and was a source of clever ideas, we communicate regularly now and it was my good fortune to have him as my first contact in Ned’s group. Thanks to Dr Taras Gorishnyy for teaching me Brillouin light scattering and becoming my conduit into phononics. Through him, I also had the opportunity to collaborate with Prof George Fytas and his research group at Mainz and FORTH. Dr Joe Walish has been a great lab mate and mentor and I have been at the receiving end of his
generous help countless times. Dr Martin Maldovan has been a valued colleague and friend and our multiple trips to the APS meetings have been filled with great conversations ranging from Brillouin zones to life in general. Dr Jae-Hwang Lee, to me is the consummate experimentalist; his technical skill is impressive and puts me to shame! He is a great colleague to mull through ideas and thoughts with and I have learnt much from him. I would also like to thank the rest of the ELT group and past alumni whom I’ve had the fortune of working with, including Dr Taeyi Choi and Dr Rafael Mickiewicz. Prof Bruce van Dover gave me a glimpse into what a PhD undertaking was really like during my Cornell undergraduate years and I am grateful; he made me realize that research was hard work but that it was challenging and fulfilling hard work! I might not have embarked on this journey if not for his influence.

To my wife, Shireen Goh, thank you for the tremendous love and support. You complete and illuminated my life.

To my parents, whom I have been away from for far too long, thank you for supporting my selfish request with this undertaking; I dedicate this thesis to you.
Chapter 1. Introduction, Motivation and Overview

1.1 Introductory remarks

*Phononics* deals with the science *and* technology of manipulating phonons at various length scales, either alone or in combination with other forms of waves, like photons, magnons, among others. Phonons, or mechanical vibrations, have been a subject of scientific inquiry since the early years of electron-density waves and the birth of solid-state theory. In fact, the study of phonons, in the guise of continuum and analytical mechanics, precedes solid state theory and is one of the first few field theories to be comprehensively developed, exemplified by the various classical works of Sommerfield [1] and others [2, 3, 4]. One of the fields that so smoothly bridged between the mechanics of the classical continuum and the discrete quantum regime, it is somewhat an anomaly that phononics has not been more deeply explored. Thankfully, in the wake of the developments of electrons and photons, phonons are now finally catching up and receiving increasing scientific attention; this is especially so with the revitalization of thermoelectrics [5, 6, 7] as a potential candidate technology for harvesting energy. Thus attention is now directed to phonons and *phonon engineering*.

Phonons and mechanics pervade the fields of science and technology especially across the meso-scale and uniquely contribute to many different applications in technology. Phononic length scales span approximately 12 orders of magnitude, covering a multitude of applications in every frequency range [*Figure 1.1*], from seismic waves in earthquakes [<Hz] to ultrasonic imaging [MHz] to the currently popular field of thermoelectrics and heat management [THz].
Figure 1.1 Overview of the applications of phononics across various length scales, ranging from sub Hz to the THz, and spanning various technological areas of imaging and detection.

1.2 Phonons in Science and Technology

Phonons, or quantized mechanical vibrations, occur at any finite temperature, in all media. Central to the richness and ubiquitous presence of phonons in a variety of interesting scientific phenomena is the simple fact that phonons embody the allowable mechanical eigenstates in a medium. Hence, phonons can actually be regarded as an omnipresent propagator of both energy and information in media. They exist as a "universal coupler" mediating various wave-
particles such as electrons, photons, magnons, plasmons and of course other phonons [8, 9, 10]. Their inherent nonlinearity makes the field of phonons and elastic wave mechanics an extremely rich field. Examples of some interesting advances include new opto-mechanical platforms utilizing the coupling of photons with phonons to emit coherent phonons at extremely low temperature, leading to developments of the “phonon laser” [11, 12]. At the larger scale, the group of Weaver et al at UIUC, has been working on utilizing entrainment of oscillators in order to induce stimulated emission of acoustic waves in fluids. [13].

Much of the interesting phenomena in phonon physics are nonlinear in nature [14, 15]. Yet, our ability to control and mold phonon flow has been lagging, even in linear systems. An important point to note is that the ubiquitous presence of phonons in all media immediately indicates the challenge of being able to probe and understand their interactions and behavior. At the fundamental level, there is a lack of a coherent framework with which to treat phonons identically across the various length scales and wavelengths, even from a theoretical perspective. Alternatively stated, in traversing the length scales from scalar, long wavelength (sub Hz and km scale) propagations, such as oceanic waves in acoustics all the way up to the short wavelength vector thermal phonons in solids (near- THz and nm scale), what are the governing invariants and defining features of these different manifestations of mechanical/acoustic vibrations across various length scales and how do we interrelate them? Might there be a significant advantage to have such a framework?

Thus, from both the fundamental and applied perspective, we wish to understand and design phonon propagation behavior, dispersion, and other properties. Part of the desire to address this question has led to the development of phononic and acoustic crystals, and more recently,
acoustic metamaterials, in search for strategies and ways to control and indeed mold the flow of phonons/mechanical waves [16, 17 and 18]. This development in phonons was partially inspired by the scientific and technological success in molding the flow of photons as manifested by the burgeoning field of photonics.

We next provide a brief summary of the state of the art in phononic crystals and acoustic metamaterials and then recapitulate the current gaps in developing a universal framework with which to control the flow of phonons.

1.3 Phononic Crystals and Metamaterials- A Timeline

What is a phononic crystal or a meta-material [19]? We defer a technical discussion until chapters 2 and 3 but in essence these materials may be regarded as artificial structures (AS), which by virtue of their geometric structure and/or combination of the inherent properties of the particular component materials utilized in creating them, lead to exotic phonon propagation behavior, some not found in nature. These characteristics include i) the formation of complete all-angle spectral gaps forbidding propagation of mechanical vibrations in some frequency range, commonly known as a complete spectral/band gap, ii) negative refraction, whereby the energy flow and the phase velocity are anti-parallel and iii) negative dynamic mass and modulus density for hyperlensing beyond the diffraction limit, just to name a few. [16, 17, 20]
1.3.1 Phononics vs Photonics

We mentioned that the recent scientific foray into phononic crystals and metamaterials was partially inspired by the developments in photonics starting in 1987. In fact, it goes much deeper, demonstrating both the dichotomy and the important need for convergence between science and technology. Phononics actually preceded photonics in its conception, in the context of mechanical composites, acoustics and non-destructive evaluation (NDE), as exemplified in ultrasonic applications [21]. While the bulk of the work then was focused on the interpretation of the detection of reflected acoustic waves from unknown internal structures (e.g. cracks), there was nevertheless some work on the mitigation and control of acoustic waves reflecting off and their propagation through certain structures [21, 22]. In fact, the first numerical work on a phononic crystal was done in early 1976 [23]. In this early work, the authors recognized the significant effect of the periodicity of the composite had on the elastic/phonon dispersion relations. However, at that time, only the first two branches of the dispersion relation were computed, due to constraints on computing resources. However, Nel et al were the first authors to elucidate the inherent effect of artificial periodicity of a structure to bring about Bragg-like scattering, leading to the formation of a partial spectral gap. This was in marked contrast to the contemporary works in elastic wave propagation that were primarily focused on extracting the effective medium properties of a composite but not so much for exploiting any effects of artificial structuring, which typically occurred at higher frequency ranges (i.e. not at quasi-static or periodic loading at low frequencies). Thus, the birth of
phononics preceded photonics by over a decade. However, as is often true in technology driven research, there was a dearth of interest or capability in exploiting any unique or novel elastic wave propagation behavior in these structures so that research in phononics essentially became dormant until the 1990s.

In the later part of the 1990s, the work in the field of phononics experienced a strong resurgence, trailing in the wake of the photonics boom. This was due in no small part to the similarities between the electromagnetic and elastic wave equations and the basic idea of how periodicity leads to the formation of spectral gaps [24]. Both fields borrow heavily from the foundations of solid state theory dealing with electron waves in a periodic ionic core lattice. It is important next to identify the most promising areas where phononics may contribute uniquely to both science and technology. In so doing, we lay out the distinctions between the behavior of phonons, photons and electrons in periodic media.

The most striking difference between pho\textit{X}ons (X=\textit{n},\textit{t}) and electrons is the fact that the former are usually vector in nature whereas electrons are scalar in nature. The vector nature of phonons and photons adds complexity and hence, considerable richness to their behavior. Photonic structures made of non-conducting materials support two polarization degrees of freedom due to the transverse nature of electromagnetic wave propagation. In comparison, phonons propagating in solids possess three polarization degrees of freedom, making the design of structures more challenging, due to the difficulty in having to optimize more parameters [18] but also allowing for potentially richer behavior. While the wave equation form for both phonon and photon propagation is not a coincidence but a result of the same
fundamental equations (discussed in chapter 2), the details of their polarizations are distinct resulting from the thermodynamics of the medium and the associated constitutive relations.

Working with phonons can be either more or less complex than working with photons. It is less complex than photons in terms of the inherent material constitutive relations that describe the wave propagation. For photons, electric and magnetic fields are intrinsically coupled through both the dynamic permittivity and permeability, whereas for phonons, the elastic fields are controlled through the impedance and the relative speeds of sound in different media (refractive index). In addition, the inherent "leakiness" of air to photons, due to the low contrast in these susceptibilities makes the creation of large complete spectral gaps, for example, more challenging. In comparison, elastic contrasts are typically significantly larger and hence, one is typically designing for phononics in the large contrast limit, i.e. between solid and air. That said, the additional polarization degree of freedom for phonons offers a separate set of challenges. Indeed, photons and phonons need to be treated differently due to differences in their nature of propagation. This will be discussed in the following chapters. The framework which we introduce throughout the next few chapters can be generalized to treat both photons and phonons but we focus on phonons for the rest of this thesis.

1.3.2 Convergence between the Science and Technology of Scalar Phonons

A tremendous amount of progress has been made in recent years in the field of phononics, aided greatly by the development of formidable tools, both computational capabilities and fabrication advances in the photonics and electronics field. A somewhat unfortunate corollary of this is that the milestones reached in phononics research tend to mirror those of photonics,
regardless of whether they are particularly technologically attractive. In some cases, these milestones have the undesirable effect of obscuring the underlying differences between the two different fields. Nevertheless, these achievements fortunately did spark further developments in phononics which became better aligned with emerging technological needs. One of these has been the theoretical and experimental development of the ultrasonic phononic crystal lens, for imaging and detection applications [20, 25], inspired by the first works demonstrating the ability to achieve negative refraction and tunneling of acoustic waves through a fluid impregnated phononic crystal [26,27]. This subfield of phononics has recently been boosted by demonstration of both resonant and broadband phononic/acoustic metamaterials that allow hyperlensing and achieving sub-diffraction imaging [17, 28, 29, 20]. Novel phononic devices may provide technological advantages in acoustics, specifically in ultrasonic imaging applications, leading to sub-diffraction limited resolution. In this case, the convergence of both experimental techniques and theoretical developments is crucial for acoustic wave manipulation and control. To date, the application of phononic structures and metamaterials in the regime of ultrasonic imaging has seen the closest marriage of theory and experiment, due to the readily assessable length scales of the requisite structures (micron scale) required as well as the easier experimental verification (sub to MHz regime) of theoretical predictions. Moreover, as the medium of choice is a fluid, which supports only a single polarization; this makes detection and imaging more amenable.

In acoustics, the phononic structure plays the role of perturbing an essentially scalar coupling/propagation fluid medium, and hence both generation and detection are more readily accomplished and information interpretation from detection less ambiguous. [21] In contrast,
the requirements for the generation and detection of phonons in solid materials is a somewhat more complicated and of a different nature due to the inherent vector and mixed nature of the propagation of mechanical fields in solids. A further complication stems from the vector nature of elastic fields leading to numerous couplings and mode conversions between various polarizations. From the experimental end, most direct measurements, analogous to that employed in ultrasonics are based on simple transmissivity and reflectivity measurements; this immediately misses information on the vector nature of the propagating phonons within the structure, among other things. [30, 31] In addition, imaging measurements on the phonon propagation often involve the inelastic coupling of an imaging field (photons) with the propagation phonons. This brings in the additional complication of selection rules in the coupling mechanism for phonon detection (e.g. Brillouin Light Scattering) and subsequent imaging (although one may be able to exploit this, contingent on being able to elucidate the underlying selection rules within these target structures). In addition, the instrumentation involved in such imaging measurements (i.e. pump-probe imaging) is inherently limited to be in the MHz scale due to the detection optics. [32, 33] As a result of this, most of the information derived from experiments concentrating on elastic waves in smaller scale (< micron) structures has been inherently spectroscopic in nature. [34, 18, 35, 36]

1.3.3 Recent Scientific Developments in Vector Phonons

Despite these limitations, spectacular advances in the work on phononics at these higher frequencies (GHz and beyond) have still been achieved. Very recent work on opto-mechanical crystals by Vahala et al [37, 38, 39, 10], resulting in utilizing the coupling of photons with
phonons to detect single or few quanta phonons, as well as the development of phonon lasers (albeit at very low efficiencies), utilizing various approaches, highlight some of the recent truly amazing accomplishments in the field of phononics which were previously not thought possible. In an interesting twist to the inelastic spectroscopic methods for phonon detection, creative work by Russell et al. [40, 41] have also exploited a particular class of phononic structures, called phononic/photonic crystal fibers, to induce high sensitivities in Raman sensing as well as controlling and exploiting stimulated optical processes, such as optical pulse propagation, in order to quench phonon-induced transmission losses in microstructured optical fibers. The central concept underlying these developments is the inelastic coupling between photons and phonons, familiar in traditional Raman and Brillouin scattering [8]. The exciting work in the GHz range required nanostructures (100nm to <1um), only recently experimentally realizable with high fidelity. The ability to create structures at these length scales was crucial to allow the use of the techniques of Raman and Brillouin scattering to probe these artificially structured materials in order to monitor and control the inelastic photon-phonon interactions. As researchers aggressively chase this access to ever smaller length scales in artificial structures, one is able to control the interactions and behavior in wave propagation behavior at smaller and smaller length scales (a few nm in wavelength and below), thus enabling control that was previously not thought possible of the propagation of various quasiparticles, such as photons or even phonons inside the materials because of the inability to design and fabricate at these tiny length scales. A prominent example of this is in the field of thermoelectrics, where 1D Bi$_2$Te$_3$-Pb$_2$Te$_3$ superlattices first showed suppressed thermal conductivity normal to the set of interfaces and enhanced ZT( ~ 2.4 at 300K!) [42]. This demonstration led to new insights on the
possible dominant processes dictating the role of phonons in heat transport and in particular the types of length scales that are involved. “Phonon engineering” is now viewed as an attractive avenue that may be undertaken to improve the ZT figure of merit of thermoelectrics in the current drive for research for alternate and renewable sources of energy [43]. Recent work has demonstrated some interesting possibilities of both enhanced [Avi09] and reduced thermal conductivity [43, 7], by utilizing the concept of phonon engineering via structuring of the material at the correct length scales. This approach has been shown to be achievable even in the bulk state [5], through the use of clever nano-structuring of the material utilizing a traditionally high temperature (1000K) bulk ball-milling process. However, we note here that the field of thermoelectrics is intrinsically much more complicated than the previously mentioned areas of phononics research due to the inherently nonlinearity involved in phonon transport in materials. In this case, the phononics contribution to this field stems primarily in shaping the dispersion relations of the material in the entire low-wavelength (sub THz) acoustic phonon branch. The problem of heat transport, while strongly nonlinear, highlights several extremely important principles to take note of: primarily that of the length scale ratios between the propagating phonon and the structure which it is residing in; commonly summarized as the wave-particle picture of the phonon. This has been recognized in numerous recent excellent review articles, both theoretical [44] and experimental [45]. The experimental advances are allowing access into the new regimes where the length scales between the wave and particle regions are of order unity.

1.3.4 Moving Forward: Heat and Beyond
As mentioned above, the advent of improved nanofabrication techniques and characterization techniques has been instrumental in uncovering novel effects in phonon propagation in the important regime of phonon-structure interaction. Several key gaps still persist in theoretical work on phonon propagation in nanoscale (natural and artificial) structures, which greatly influences the propagation behavior and interaction with other fields/quasiparticles. One of these gaps has been alluded to earlier: the vector nature of the phonon. With the exception of early pioneering works \[46\], this fact has rarely been well treated or even considered. This partly stems from a lack of a coherent framework with which to treat phonons, or more generally vector fields and their interactions with other vector fields. More specifically, many of the experimentally observed phenomena evade a quantitative theoretical explanation due to not viewing the phonons as a vector field.

Why the obsession with the vector phonon? First of all, a vector wave and a scalar wave differ greatly in their interactions with themselves or other fields because of the polarization degrees of freedom. Polarization dictates the behavior of a phonon as it scatters off an interface, whether material or geometric, and hence determines the resultant scattering cross-section \[47\] in both the single and multiple-scattering regimes. Hence, correct treatment of the phonon polarization is of crucial importance to the formation of the band dispersion relations, to inelastic scattering and finally also to phonon transport! In fact, as we shall develop over the course of this thesis, the central framework for dealing with the vector nature of the phonon enables unprecedented control over the dispersion relations and phonon propagation. In order to close this introductory discussion and place the entire field of phonons into perspective, we next examine the deep scientific foundations behind the phonon, or mechanical wave by
juxtaposing the cutting edge of research of phononics with the classical fields of acoustics and mechanics of continua.

1.4 Phononics and its relation to acoustics, elasticity and mechanics: Length scales and broken symmetry

The previous brief survey demonstrating the remarkable breadth of the recent development in phononics both highlighted and reinforced the key role of the phonon as pervasive in many diverse fields of science and technology. It seems quite surprising then that despite the wealth of technology development achieved to date in phononics, as well as the abundant information available from traditional solid state electronic theory, that we still remain largely unable to answer fundamental questions with regards to the rational design of phononic structures.

The ubiquitous phonons present in all media have different polarization degrees of freedom depending on the nature of the medium: scalar in fluids and vector in solids. Despite recent advances, the field still lacks a rational framework to design a particular phononic structure for a particular application, with some notable exceptions in the case of fluids [17, 28]. Numerous fundamental questions persist: for example, what physical topology is optimal for phononic crystal structures, say, for obtaining complete spectral gaps in two dimensions? Which structure is optimal for performing negative refraction? What kind of topology (disconnected or network) is optimal for creating phononic structures? Are the particular choices of elastic constants, densities and Poisson ratios of the materials critical to the performance of a particular phononic device? All of these questions trace back to two main unresolved issues.

1.4.1 Taming the Vector Phonon: Broken Symmetry
The first of these issues relates to the vector nature of phonon propagation in solids and this is crucial in ordered structures. The common concept of a trivial pure longitudinal or transverse polarization loses meaning [48, 49] once artificial order is induced in the structure. For example, in a simple binary superlattice, the pure transverse and longitudinal modes are actually specific normal modes that only exist as pure modes in materials with certain symmetries. Pure transverse and longitudinal waves do not occur in all systems, they just happen to be very common! Deep understanding of how to treat the vector nature is essential to the development of a rational design framework for phononic structures for all forms of applications. The key reason for this is that the dispersion relations of the phononic structures, which dictate phonon propagation, can be designed with a high degree of control if one understands how to properly treat the vector phonon. In the course of this thesis, we will show that the vector nature of the phonon can be fully exploited to optimize the various mentioned areas of applications in phononics, from creating desired phonon propagation behavior, to coupling phonons to photons or other similar vector fields. This first point will be developed to formulate the workhorse of this thesis; we preliminarily state here that the control of this vector nature becomes transparent and intuitive in the framework which relies on a proper mathematical structure using group theory and concepts of symmetry breaking. The latter becomes especially pertinent when considering interfaces where a jump in the vector/scalar nature of the phonon occurs, e.g. at a solid-air interface. In this situation, differences in the phonon eigenmodes between elasticity and acoustics can be related to the degree and the specifically broken symmetries, each of which corresponds to a degree of polarization freedom!
1.4.2 Particles and Waves from the Discrete to the Continuum: Role of Length Scales

The second issue deals directly with the relation of phonons to acoustics, elasticity and continuum mechanics. Strictly speaking, a phonon is a vibrational normal eigenmode in a medium. From the viewpoint of a discrete harmonic lattice framework, phonons are \textit{quasi-particle} modes in the lattice, obtained from diagonalizing the degree of freedoms of the harmonic lattice into well-defined eigenmodes with conserved energy and crystal momentum, i.e. \((\omega, k)\).

The crucial question is when can a discrete lattice, with its phonon eigenstates, be treated as a continuous medium? To juxtapose from the complementary viewpoint, how can we reconcile the continuum approximation of a fluid with any sort of quantized model? The answer lies in the recognition of the relevant length scales, both of the propagating phonon and that of the medium which it propagates within, [14, 15]. It will turn out that in most of our cases of interest here that we are quite firmly in the continuum regime; hence the treatment of the phonon can be done utilizing the classical field theory of mechanics.

The concept of length-scales and the pertinent symmetries are elegant and universal; in fact, together, they allow the bridging of the scales between the geometric (short wavelength) and the effective medium (long wavelength) theory of wave propagation of photons, phonons etc quite transparently and generally. To do this, one first identifies the length-scale regime in which one is working and keeps track of the correct contributions, which are determined by both the length scale (phonon wavelength over the length scale of the structure) and more subtly, the underlying symmetries present in the system.

Hence, the \textit{relation} of phononics to acoustics, elasticity and mechanics is in
i) the relevant length-scales of interest

ii) the pertinent symmetries present

The former determines what processes (tunneling, scattering, interference) control the propagation and the latter controls the exact vector nature vis a vis the normal modes. Manipulation of the two will enable quite exciting and unprecedented control over the phonon propagation behavior.

We will emphasize this fundamental fact whenever this viewpoint illuminates previously unresolved points in the existing literature and leads to new and useful insights.

1.5 Outline of the Contributions of this thesis

In this thesis, we develop a universal design framework for conceiving and fabricating phononic structures to achieve certain desired phonon propagation behavior. Examples that we demonstrate utilizing our design framework include:

i) the largest complete spectral gap known in the literature (enhancement by more than two-fold over the current champion)

ii) meso-scale polarization sensitive complete spectral gaps

iii) polarization specific negative refractive bands for negative refraction

iv) relaxation of conditions and distinction between resonant metamaterials and phononic crystals through the explicit use of the non-locality concept

v) sub-wavelength complete gaps using only a single monolithic material and air

vi) creation of double negative modulus and density bands using only a single monolithic material and air
vii) generalized phononic networks with hierarchical defects of selected symmetry

viii) generalization of spectral gap opening mechanisms and their relation to ordered structures

ix) the first nonsymmorphic phononic crystal with multiple high order complete spectral gaps (with the total normalized gap width of over 100%)

We show that the creation of all these various novel and desired phonon behaviors can be done with the same set of governing design principles. This set of design principles is “complete” in the sense that it governs both the global properties (geometry, topology, material properties, symmetries) of the structures, as well as the local “energetics” that determine the position and curvature of each dispersion band. We demonstrate control of the dispersion of multiple bands within a frequency range in a rational fashion, with the use of this set of multi-scale design principles. We will indeed demonstrate how to “tame the vector phonon”!

From a more physically motivated perspective, we address the fundamental question of how to choose the optimal physical topology of a structure so as to achieve a specific functionality in a phononic structure. This is shown to be attributed to a surprisingly simple single parameter, which is necessarily material dependent. We name this the “dynamical mechanical bond”, which is related to the parameter of the dynamical impedance contrast between the component materials of the phononic structure. We then proceed to consider the details of the physical topology of the “scatterers” in the medium, via their geometric structure and selected connectivity as well as the correct framework to view them in. We address the important distinction between these geometric parameters and the more practical motivation
of volume fraction or area fraction (fill fraction). The later are shown to have little value in rational design when taken in a simple fashion. The fill fraction nevertheless holds value in determining the effective medium (long-wavelength) limit of the speed of propagation in the medium. We show that this method of classification offers a more insightful and physically intuitive design principle for various target functionalities of phononic crystals. Various phononic structures previously proposed by other groups are easily classified within our scheme. We show how new and improved technologically relevant functionality can be derived from such a design approach.

This framework is employed to generalize and relieve the traditionally touted requirement for absolute discrete translational periodicity for the formation of spectral gaps; this is demonstrated by applying simple surface perturbations to a slab and inducing complete spectral gaps in these slabs without requiring any form of periodicity or material inhomogeneity on the propagation direction. We will use concepts of broken symmetry to induce edge states in generalized form of phononic networks, controlling the symmetry of the two boundaries in the non-interacting as well as the strong interaction limit (which depends on the finite size of the structures being considered). We also treat the design of defects and waveguides within this broken symmetry framework and develop some governing principles for designing defects of various dimensionalities within these networks. We name these as generalized broken symmetry states (BSS).
Chapter 2. Elastodynamics of Artificial Structures

2.1 Introductory Remarks

The control of phonon propagation in artificial structures (AS) hinges heavily on the ratio of the length scale of the inhomogeneity of the medium, normalized to the wavelength of the propagating phonon under consideration. In general, we also have to consider the specific displacement field pattern, i.e. the eigenmodes; this later fact stems from vector nature of the phonon, that is, the elastic fields are vector in nature. It is quite interesting how much of this fact, although quite rudimentary in nature, often gets forgotten, once we consider artificial structures, even though, for example, one has no issues with this in considering anisotropic bulk crystals. In fact, recognizing that the distinction between artificial crystals and bulk atomic crystals lies in the length scale of the inhomogeneity is extremely pertinent towards the development of the universal framework. It allows us to renormalize, and map the viewpoints between the traditional bulk atomic crystals to the artificial structures. Many of the apparent differences or anomalies demonstrated in AS stem from not being able to access length scales not previously obtainable experimentally. Indeed, it has only been with the advent of nanotechnology that we are able to characterize artificial structures (AS) where the measurement precision and access to length scales match the length scale of fabricated structures [10,34,09,37,38]. Thankfully, this finally allows for the development of a toolset where we are able to truly test designed AS.

We mentioned briefly in chapter 1 that the connection of phononics, as we introduced it, and its relation to classical acoustics, elasticity and mechanics lies in the length scales. To be more
precise we first pose the question: Where does the classical field of mechanics fit into this modern age of nanotechnology and nanostructures? Why are we so obsessed with length scales?

The classical field theory of mechanics already serves as the primary work horse for the description of phonons and their propagation behavior, in the guise of elastic waves in a continuum. There is sometimes even confusion in the literature between a truly quantized mode in the quantum mechanical sense, and a quantized mode of motion, which is truly and strictly classical [51]. It turns out that the classical-quantum transition for phonons in media is at a much smaller length scale than we were aware of [52]; At the risk of belaboring the point, we note that it is quite remarkable, as well as quite reassuring, that in the age of advanced multi-scale computational tools and techniques, one may verify that the classical limit still holds even at very small scales, (nanostructures ~10-100nm). Hence, we need to recognize the critical length scales involved and adopt the correct computational tools most suited at those length scales.

In all of these cases, the crucial point is to always recognize the issue of length. In fact, the timelessness of classical continuum mechanics has manifested itself interestingly in recent work on phonon transport at the nanoscale; examples of these include the experimental discovery of the role of flexural and interface modes on supported grapheme [53]. While the interactions themselves may sometimes breach the quantum regime (e.g. at extremely low temperatures), in many of these cases, it is collective modes at the longer length scales that are quite rigorously predicted and accounted for in the classical field theories, that one is interested in.
Hence we state here outright that we are working in the classical limit, i.e. the frequencies and wavelengths which we deal with are much lower than the actual atomic/intrinsic optical phonon limit. The latter point is the defining feature of the non-classical limit of phonons in materials, contrary to common misuse in the literature [54], where the classically confined slab modes were regarded as exhibiting quantum effects. We focus on ways of molding the flow of phonons at the length scales where we can design and then successfully fabricate, in order to directly verify with experimental measurements the theoretical predictions. Hence we are bounded below by the ~10nm regime, this being set by current state of the art reproducible top down fabrication methods. This incidentally lies in the regime where the phonons are technologically relevant, e.g. ultrasonic (MHz) and hypersonic (GHz). It is also quite interesting that even the control of phonons in such structures and materials in the linear regime eludes our complete comprehension.

In this thesis, we develop a universal framework in order to both design and control the phonon propagation behavior in AS materials. A subset of these AS materials is also conventionally known as phononic crystals (PnC) [50], or metamaterials (MM) [55], depending on the length scales of the phonons propagating through the medium. This will be systematically elaborated as we build up the framework.

Hence, we utilize the well-developed classical field theories in mechanics, within a mathematical framework that we shall use to develop this field theory which turns out to be extremely useful and suitable for designing structures to control the propagation behavior of phonons. This universal design framework for designing phononic structures will be developed in broad strokes in this and the following chapters [Chapter 2, 3,4]. In chapters 4, 5 and 6, we
employ a selection of these principles in order to demonstrate the power and utility of this universal approach to achieve specific functionalities.

2.2 Fundamental Equations and Governing Principles

While utilizing fundamental classical field theory, we wish to remark that while extremely complete in its exposition, the roots were more algebraic, rather than geometric in nature. Hence, the solutions of various mechanical problems arrived at by researchers were more microscopic and dynamic in nature, as opposed to the geometrical approach, in which the observation of invariants and conserved quantities of the entire systems would be pursued. The former approach would solve the problem at the microscopic level and hence demonstrate its evolution along a path. The latter approach while not pinpointing the actual path that the solution evolves along would elucidate all the possible paths that were amenable, as well as impossible. We seek to combine both approaches and reconcile them, enabling us to be able to shift our viewpoint when it is more illuminating to the problem solution. Part of the reason this universal framework was not previously developed is simply a question of the disjoint timelines of the two viewpoints. To illustrate these two viewpoints, we will develop the fundamental equations of elastodynamics from both approaches. In the first, we reprise the classical discrete harmonic crystal and take the continuum limit, to obtain the conventional linear
Figure 2.1 Band Dispersion Relations of (a) Monatomic one-dimensional classical chain, (b) Diatomic one-dimensional classical chain (c) Generic Continuous one dimensional Phononic Crystal. Here we computed, at a 50-50 volume fraction, one phase utilizing (E=12Gpa, v=0.3, ρ=2330kgm⁻³), the other utilizing (E=6Gpa, v=0.17, ρ=1330kgm⁻³) acoustic dispersion curves for a homogeneous solid, highlighting the conversion from the discrete regime to the classical regime. This is the microscopic approach. This is also the only place where we are able to explicitly state the limits in which we are allowed to work within the continuum framework. We elaborate on this model to show how a phononic structure is often regarded as a “larger-scale” atomic crystal through a renormalization of the length scale which we examine [Figure 2.1]. Here we illustrate the concept of length scales involved when visualizing the relevant length scales between a bulk crystal, and that of a phononic crystal. We note that one may effectively "discretizes" the phononic crystal to the length scale of the building blocks, that is our discrete length scale is given by a, the size of the unit cell. This is equivalent to considering only the first two symmetric (bands 2 and 4 in solid black), or first two anti-symmetric branches, if we only allow one degree of freedom in comparing with our one-
dimensional building block systems. We see that these two branches are effectively analogous to the diatomic classical chain, with the two components of the phononic crystal being the two "atoms" in the chain. This is exactly the cut-off length scale which we are talking about!

By taking this into account, we show that the models can be mapped onto one another. We then highlight the distinctions that exist between the atomic and artificial that are often misunderstood, which can lead to erroneous conclusions in the literature. Our treatment leads to the concept of quasi-statics, locality and non-locality, and this turns out to be one of the central themes of our design framework. The issue of non-locality is developed in chapter 3.

We next approach the problem from a complimentary viewpoint, which is more mathematical but at the same time quite physical in nature. The premise for this is the validity of being able to describe the elastic displacements as a continuous field, and this allows us to use the tools of field theory, i.e. we may treat the medium as a continuum.

We start from the perspective of the conservation equations, namely of continuity of mass and momentum flow [14], in developing the general equations of classical waves. This is in contrast to the typical way of inducing an equation of motion based solely on the stress-strain relation from the starting elastostatics equilibrium viewpoint. Since the equations of motion are microscopic in nature, i.e. the wave propagates and is subject to certain requirements of continuity in the medium but omits critical information about the system, which is actually derivable from the conservation equations. We then discuss the implications of the equivalency of these two viewpoints, noting that the latter viewpoint will still be valid, for example in the event of shock-wave propagation for example, because of the nature of the physical induction of the equations. Another reason for utilizing the conservation equations is
the connection, often utilized in theoretical physics, to broken symmetries in the systems, and hence to the allowed symmetries of the phonon modes in the system. This serves to motivate the following chapter where, starting from the viewpoint of conservation and broken symmetries we cast elastodynamics into our mathematical framework.

2.2.1 The Discrete to the Continuum: Taking Limits

We first consider a regular lattice with a single atomic building block, i.e. a mono-atomic lattice, in $N$ dimensions. In the discrete approach, we represent the many-body potential energy, with the ionic coordinates $V(q_1, q_2, ..., q_n)$.

Within the Harmonic approximation, we may represent the deformations in the potential energy to only second order in the displacements, $u_\alpha(r)$, where $\alpha$ represents the spatial component and $r$ represents the position of the ion being considered. We may hence write this potential energy function under small perturbations as:

$$V = V^0 + \frac{1}{2} \sum_{\alpha, \beta} \frac{\partial^2 V}{\partial q_{\alpha} \partial q_{\beta}} u_\alpha(\bar{r}) u_\beta(\bar{r}) + O(u^3)$$

$q$ is the generalized coordinate of the system
$r$ is equilibrium positional coordinate of ion
$u$ is displacement variable from equilibrium position $r$

The full Hamiltonian is given by

$$H = T + V$$

where $T = \sum_{r, \alpha} \frac{p_\alpha(\bar{r})^2}{2m}, p_\alpha(\bar{r}) = momentum$
Because we are working with a lattice, the discrete translation symmetry, which implies the lack of a unique origin, shows that the potential energy function should only depend on the difference between the position vectors \( \mathbf{r} \) and \( \mathbf{r}' \) and also that this translational symmetry allows us to diagonalize the Hamiltonian using the Fourier modes (the translational symmetry implies that we may use the wave-vectors as conserved number and hence Fourier modes), i.e.

we may express the displacement as:

\[
u_n(\mathbf{r}) = \sum_{\mathbf{k}, \mathbf{r} \in \text{BZ}} \frac{e^{i\mathbf{k} \cdot \mathbf{r}}}{\sqrt{N}} u_\alpha(\mathbf{k})
\]

This sum is only restricted to lie within the first Brillouin Zone (BZ); this is due to the intrinsic discrete length scale restriction of the minimum wavelength of a propagating phonon to the first BZ edge (shortest wavelength possible for discrete lattice).

The final Hamiltonian, diagonalized in terms of the Fourier modes, is given by

\[
H = V_0 + \frac{1}{2} \sum_{\mathbf{k}, \alpha, \beta} \left[ \frac{\rho_{\alpha}(\mathbf{k})^2}{m} + K_{\alpha,\beta}(\mathbf{k}) u_\alpha(\mathbf{k}) u_\beta(\mathbf{k}) \right]
\]

This is the Hamiltonian that represents a lattice occupied by a discrete ionic basis. The discrete nature of the lattice is represented by the form of the Fourier mode decomposition, with the displacement at each ionic position given by:

\[
u_n = \int_{\mathbf{k}} \frac{dk}{2\pi} e^{-i\mathbf{k} \cdot \mathbf{a}} u(k)
\]

\( \mathbf{a} \) is the equilibrium lattice spacing.
\( n \) is the nth ion in the entire lattice

Hence, in this microscopic Hamiltonian, we essentially track the oscillating positions of all the ions in the lattice, and we describe, up to second order only, the harmonic displacement of the
lattice about each equilibrium ionic position. Because of the (discrete) translation symmetry, we may perform a diagonalization and rewrite the equation in the Fourier basis, with the wave vector $\mathbf{k}$, which is constrained to lie only within the first BZ. Because translational symmetry implies that the system is invariant to translations operations of the entire lattice, the natural space for the displacement lies in the Fourier, or the reciprocal wave vector space, hence the diagonalization into $\mathbf{k}$-space. However, we note that this group of transformations is only distinguishable up to the unit lattice vector. Physically, this just tells us that the discrete nature of the lattice only allows a wave, to possess a minimum wavelength of 2 lattice translations, with the unit cell size being half a wavelength, represented by two adjacent ions being exactly out of phase in their motions. This is all of course, done with a monoatomic lattice.

The discrete nature of the lattice is thus markedly manifest near values of the wave vector at the BZ edges, where strong interactions with wavelengths on the order of the unit cell size occur.

When can one utilize the continuum approximation? Away from the BZ edge, the wave vectors and hence, the associated wavelength of the propagating phonons typically span numerous unit cells and hence, at each atomic position, the displacement caused by the wave is incremental, with individual displacements satisfying $u_a(\mathbf{r}) \ll |\mathbf{r}^\alpha_a - \mathbf{r}^{\alpha}_{a'}|$. In addition, if we consider long wavelength (small $k$ numbers), the displacements take place at length scales $\ell = \frac{a}{\varepsilon}, 0 < \varepsilon << 1$, where $a$ is the unit cell dimension. Hence the wavelength is much longer than an individual unit cell.
Finally, provided that this lattice is approximately uniform (i.e. low defect, isotope densities etc...) and considering processes that occur at longer time scales (i.e. the fast microscopic fluctuations die out quickly), we will hence be able to coarse-grain the system and apply the continuum approximation to the discrete lattice. The essence of this is that we are then able to replace the discrete displacements of the ions in the lattice with a continuous displacement field. We now develop the continuum approach inducing the equations of motion from the Hamiltonian. By taking $\frac{\partial P}{\partial t} = \frac{\partial H}{\partial q}$, this gives us, in the original discrete form:

$$m \frac{d^2 u^n_\alpha}{dt^2} = - \sum_n K_{\alpha,\beta}(n - n') u^n_{\beta},$$

where $n, n'$ represent different ionic positions.

The continuum approximation allows us essentially to treat the displacement as a continuous field, hence we may carry out a Taylor expansion of the displacement:

$$u_{\beta}(r') = u_{\beta}(r) + \sum_a (r'_{\alpha} - r_{\alpha}) \nabla_{\alpha} u_{\beta}(r) + \frac{1}{2} \sum_{a,\gamma} (r'_{\alpha} - r_{\alpha})(r'_{\gamma} - r_{\gamma}) \nabla_{\gamma} \nabla_{\alpha} u_{\beta}(r).$$

$u$ is displacement
$r$ is the coordinate in space

Due to stability requirements of the lattice near equilibrium, only the quadratic terms remain, hence we obtain finally

$$m \frac{d^2 u_\alpha}{dt^2} = \sum_{\alpha,\beta,\gamma,\eta} C_{\alpha,\beta,\gamma,\eta} \nabla_{\gamma} \nabla_{\eta} u_\beta$$

$m$ is the relevant mass, here we assumed point mass
$u$ is the displacement
$C$ is the Elasticity Tensor

which is exactly the linearized form of the elastodynamic equation of motion for a continuous medium! This shows explicitly where the continuum approximation of the original many-body
problem is valid, i.e. whenever we are able to treat the displacements of a propagating wave as a continuous field.

Physically, this implies (ala coarse-graining), that despite the intrinsic many-body nature in most systems, that the emergent collective modes of propagation dominate the behavior of the entire system. In most situations, the classical-discrete transition limit, i.e. the situations where the quantum behavior is dominant should be considered properly and is different in considering different situations. For phonons, this cross-over is somewhere in the sub-10nm regime [22]; in all cases, one needs to consider the ratio of the various length scales present in the system, the intrinsic atomic length scale, the length scale of the propagation mode/wave which we are interested in and hence the length scales of the inhomogeneity that exists in the system that the wave may and may not see.

Now, we shall work with the displacement existing as a continuous field in the medium, which we may consider also as a continuum. We note here that our condition of being able to take limits from the discrete into the continuum only lies in the validity of representing the displacement as a continuous field. Subsequently, even when we consider artificial structures (AS), which are inhomogeneous, this fact does not change, because the length scale of those inhomogenities are “macroscopic”, compared to the intrinsic unit cell size; hence the medium is still continuous for our purposes.

Now, we utilize our two viewpoints of elastic wave propagation in the continuum limit, the first which is microscopic and hence is evolutionary (with time) in nature, while the second is based on conservation principles and hence is more variational in nature. That two viewpoints are needed is crucial because it is only through the second viewpoint that we are able to induce the
concept of broken symmetries and generalize the concept of polarizations, allowing us to treat the vector nature of the phonon subsequently.

\subsection{2.2.2 Evolution vs Conservation: The Microscopic E.O.M vs The Variational Principle}

We start first with the microscopic Equation of Motion (E.O.M). This is typically derived from the equilibrium conditions, or of force balance of an \textit{infinitesimal} element, where equilibrium requires:

\begin{equation}
\nabla_i \sigma_{ij} + X_j = \rho \frac{\partial^2 u_i}{\partial t^2}
\end{equation}

\begin{itemize}
  \item \(X_j = \text{external body forces}\)
  \item \(\sigma_{ij} = \text{stress tensor component}\)
  \item \(u_i = \text{particle displacement}\)
\end{itemize}

Subsequently, depending on the exact solid, we have to include extra information on the elasticity tensor of the particular solid. In the case of an homogeneous isotropic, linearly elastic medium, this is reduced to the familiar form:

\begin{equation}
(\lambda + \mu)\nabla (\nabla \cdot \vec{u}(\vec{r})) + \mu \nabla^2 \vec{u}(\vec{r}) + \vec{X} = \rho \frac{\partial^2 \vec{u}(\vec{r})}{\partial t^2}
\end{equation}

This is the common vector displacement equation of motion, or more commonly known as the elastic wave equation. In this microscopic approach, we only consider the conditions of equilibrium on an \textit{infinitesimal} element in the body. Physically, this is equivalent to regarding a propagating elastic wave as a very small perturbation traveling through every microscopic element and the subsequent motion at each position acts to restore the slight perturbation from equilibrium. There is no external or additional knowledge about the nature, and form of
the propagating wave through the medium, which is what we are actually interested in! The subsequent Ansatz on the solution form, namely $u(r)e^{it-k(r-rt)}$, seems more of an exercise based on experience rather than one induced from the form of the phenomenon at hand. In fact, why does this Ansatz even work? We know that this takes the form of a wave equation (although given the original vector form, it might be hard to guess initially!), but why would we choose such a form of the solution? Given say a large disturbance, such as a shockwave that propagates through the body, the assumptions underlying this E.O.M undoubtedly break down and we seem to need to formulate a new, probably nonlinear equation of motion to describe now shockwave propagation. How would we do this? What does the $k$ in the Ansatz imply? The answers to these fundamental questions lie in the second approach, which stems from conservation and will form the philosophical backbone behind the development of our framework. We now demonstrate this and reconcile this with the previous microscopic approaches.

Initially consider the medium to be a homogeneous continuum (later we relax this assumption), hence we can represent the displacement as a continuous field. Since we are interested in the propagating wave, we focus on the wave. In such a system, we know that in the absence of dissipation, energy is conserved due to continuous symmetry in time. Because the system possess continuous spatial symmetry (at the length scales which we consider), linear momentum is conserved. If the system is not rotating, angular momentum is also conserved. These conservation principles allow us to define an equation of continuity of some conserved quantity, $M(t)$, in some region of space $\Omega$, with a boundary $\partial\Omega$, and boundary gradient normal $n$ can be stated as:
\[
\frac{dM(t)}{dt} = R(t) + S(t)
\]

\[
M(t) = \int_{\Omega} \rho(\vec{r}, t) dV
\]

\[
R(t) = \int_{\partial\Omega} \vec{F}(\vec{r}, t) \cdot \vec{n} dS
\]

\[
S(t) = \int_{\Omega} s(\vec{r}, t) dV
\]

\(F(\vec{r}, t)\) represents the corresponding flux of the quantity and \(s(\vec{r}, t)\) represents any source and sink in the region. This continuity equation, which tracks all the processes that conserve the quantity \(M(\vec{r}, t)\), is valid even in the presence of shock waves \([14]\), as long as the medium doesn’t tear and hence introduce new discontinuities via cracks etc.

For elastic waves (and avoiding dealing with shockwaves), we may deal with the differential form of the conservation laws and now, recalling that our system conserves energy (mass) and linear momentum yields us two such equations of continuity:

**Momentum**: \(\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot T = 0\)

**Mass**: \(\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0\)

\(T\) is the momentum stress tensor

\(\rho\) is the mass density

\(\vec{v}\) is the relevant flux velocity

Here, we input our constitutive equations, which represent the behavior of the particular material we are interested in, e.g linear elasticity, the anisotropy of the elasticity tensor etc.

In this approach, it is only the constitutive relations which we input into our conservation equations that need to change when we are dealing with different systems. The modifications into the wave equation only occur as a result of the constitutive relations. We further assume a linearly elastic, isotropic medium, which allows us to approximate the form of the stress tensor
and if we assume that the mass density varies on length scales (L) longer than that of the wavelength of the propagating wave (λ) and hence the wave does not sample any mass density inhomogeneity, we recover the elastic wave equation:

\[(\lambda + \mu)\nabla(\nabla \cdot \vec{u}(\vec{r})) + \mu \nabla^2 \vec{u}(\vec{r}) + \vec{X} = \rho \frac{\partial^2 \vec{u}(\vec{r})}{\partial t^2}\]

\(\vec{X}\) are all the relevant external body forces, if any.

once again, this time without considering small microscopic displacements from equilibrium as before. This second formulation, which we call geometric, presents a slightly different viewpoint. By treating the wave initially as a propagation of an initial disturbance throughout the medium, we can regard this through any region in space as a flow of some quantity; in our case, this is linear momentum. In general, we may treat this propagation as a continuity equation for momentum. The constitutive relation, which in this case is the linear elastic response of an isotropic, linear elastic solid, inputs the phenomenological or material response of the material to the propagating wave. This is where the main piece of the appropriate material physical response comes into play for the system. This could include nonlinearity, viscosity and other nontrivial complexities in material response. Explicitly, these features enter through the stress tensor term, \(T\), of the momentum continuity equation.

After inputting this constitutive relation into the continuity equation, we recover back the elastic wave equation, verifying that given the linear elastic response a general propagating disturbance will fulfill the following wave equation, as represented by the vector elastic wave equation.

We note here in passing that this method of derivation acknowledges fully the role of momentum conservation in deriving the resultant wave equation, whereas the microscopic
method bypasses this knowledge. But what else does this geometrical approach offer us, in terms of insights? Because the wave equation is derived from the conservation of linear momentum, the system possesses continuous spatial symmetry (again, at these length scales); this immediately tells us that once again, the normal mode decompositions should be taken in Fourier space, $u(r)e^{i(k\cdot r-\omega t)}$, where the wave vector $k$ represents the natural space in which the eigen-solutions of this wave equation lie. This can be regarded as normal mode decomposition of the solutions in terms of Fourier modes, hence we can choose solutions to be “carried” by the $e^{i(k\cdot r)}$ forms, which are the said natural coordinates. This is precisely why the normal modes take the following form of $u(r)e^{i(k\cdot r-\omega t)}$, where $k$ takes on either a discrete set or continuous spectrum of values that depends on the actual spatial symmetry.

So now, we have utilized two countering viewpoints to derive the same elastodynamic wave equation, with the second geometrical approach giving us additional insight through correct identification of the processes that lead to the formation of the wave equation. The latter approach also identifies the significance of $k$ as the normal mode index and explains the rationale behind the well-known plane wave type solutions to the wave equation. However, we need to extend these principles further in order to be able to understand how to treat the vector nature of the elastodynamics. Right now, this equation does not possess any extra information about the vector nature of the elastic waves, or the number of polarization degrees of freedom. We need to now introduce the concept of polarization, working from the concept of broken symmetries of a continuous system. This framework of viewing polarization and hence the vector nature of the phonon field will be crucial towards our universal framework, which enables us to treat vector fields as readily as scalar fields.

50
2.3 Broken Symmetry and Polarizations of the Vector Phonon

From the discrete viewpoint, the polarization of a phonon arises from the fact that it is connected to other material building blocks/atoms by virtue of the requirements of stability and the dimensionality of the space and material. From the continuum viewpoint, the polarization of a phonon arises also from the requirements of stability and dimensionality as well, albeit from considering the relevant potential “energy” and considering possible stable solutions. In this latter case, there is no assumption on the details of the internal structure of the medium except for the fact that it is a mechanically and energetically stable continuous medium. Yet the connectivity requirement is intimately connected to the stability of the medium. How then does the dimensionality of the medium lead to the induction of the allowable polarization degrees in a structure? This is exactly related to the conservation equations and to the concept of the broken symmetries and finally, the extension of length scales once inhomogenities are introduced into the system.

To get an insight into the polarization of the vector fields, we have to consider the existence of phonons from another perspective, that from broken symmetry and Goldstone modes. The polarization degrees of freedom are constrained by both the dimensionality of the space with which we are considering the problem as well as the general rigidity of the system. The former is clearly shown by simply constricting the motion to occur in $N$ dimensions and gives the maximum permitted degrees of freedom. The second condition of rigidity, however, gives the final allowed degrees of polarization freedom permitted by considering the physics of the problem. One example of this is exemplified by the difference between a fluid and a solid. A typical fluid supports a single “polarization” mode, a scalar acoustic wave formed from mass...
density fluctuations. In contrast, an elastic solid, that resists both shear, torque and compression, possesses three polarization modes, in general, in any direction. We now elaborate somewhat on polarizations, since we have identified them as one major challenge towards the control of the designing the dispersion relations of different phononic structures.

In a homogeneous three dimensional continuous medium, it has been taken for granted that we derive these solutions to be the two transverse (shear and rotational, no dilation) and the longitudinal modes (only dilatational/compressional, but not shear). Typically, this is derived from the fact that every possible vector displacement field takes the form [57]:

\[ u(\vec{r}) = \nabla \varphi + \nabla \times \psi \]

\( \varphi = \text{scalar potential} \)

\( \psi = \text{vector potential} \)

These two potentials yield the respective longitudinal and transverse modes but do not provide much intuition for understand the resultant modes! We may choose instead, to consider the Hamiltonian which is given by:

\[
H = \frac{1}{2} \int d^d x \left[ \sum_a \left( \rho \frac{\partial u_a}{\partial t} - \mu \frac{\partial u_a}{\partial x} \right) + \sum_{a,b} \left( 2\mu u_{ab} u_{ab} + \lambda u_{aa} u_{bb} \right) \right]
\]

\( \mu, \lambda \) are the lâme coefficients

It is clear from the repeated summation that the resultant Hamiltonian is rotationally invariant and hence, in Fourier space, our Hamiltonian now should only contain rotationally invariant quantities and takes the form:

\[
H = \frac{1}{2} \int \frac{d^d k}{(2\pi)^d} \left[ \rho \left( \frac{\partial \vec{u}(k)}{\partial t} \right)^2 + \frac{\mu}{2} |k|^2 |\vec{u}(k)|^2 + \frac{\mu + \lambda}{2} (k \cdot \vec{u}(k))^2 \right]
\]
By decomposing this Hamiltonian, we can group the modes into those that are transverse (k perpendicular to u) and longitudinal (k parallel to u), with the transverse modes having a degeneracy of (d-1), where d is the dimensionality. Now we consider what governs the available polarization modes in a medium! Let us do this in steps. First of all, phonons are a simple form of Goldstone modes, which derive from breaking the continuous symmetry of our medium. We note that earlier, we have been saying that the continuous symmetry is what gives rise to the phonon modes, so have we contradicted ourselves? The distinction here is precisely the question of the length scale of ‘continuous’ which we are considering!

Let us talk about Goldstone modes first. In a solid, bonds are formed, with the formation of a crystalline lattice breaking the continuous translational symmetry at all scales, replacing the system with discrete translational symmetry instead. This broken continuous symmetry leads to the Goldstone modes which are our phonons (long wavelength). One characteristic of Goldstone modes is that their wavelength goes to infinity (frequency \( \omega \) goes to zero) at zero wave vector. Each such broken symmetry will give rise to a maximum of one new mode, hence giving rise to condition 1. This is for the Goldstone modes. At the length scales where we consider the medium to be a continuum (much larger scales) however, we have continuous spatial symmetry (continuous and homogeneous) and we have not contradicted ourselves. This is why the recognition of the correct length scales is very important in general.

Now, we need to extend this concept of broken symmetry further. That the longitudinal and transverse modes are the only eigenmodes is derived from the symmetry of the system, in this case our isotropic solid. Such a crystal is still rather symmetric! Of course, actual structures are never elastically isotropic; even the highest symmetry cubic crystals have an extra rigidity
constant. Excellent treatments for the correct classification of different crystal elasticity constants are given in Nye [58] and Landau [3].

The pertinent point here is that the polarization eigenstates of an elastic wave that exists in a structure depends on its underlying symmetry. To give an example, if instead of an isotropic medium, we have a medium which possesses spherical symmetry, the polarization eigenstates naturally need to obey the spherical symmetry. One of the eigenstates will possess spherical symmetry (depends only on |r|), with the other possible eigenstates depending on their dependence on the angular coordinates (ϕ, θ) [57]; these are commonly recognized as the radial-like 'breathing', dipolar-like, and quadrupolar-like modes, with the exact polarization of a propagating phonon depending on its propagation direction taken with respect to the crystal symmetry. In other words, it represents the eigenmodes present in the crystal along the direction which it is propagating in. This is geometrically often taken as a normal projection along the relevant quadric [58] but clearly this is exactly equivalent to the projection into the relevant subspace of the basis of eigenmodes of the relevant structure/medium, which we call the irreducible representations (Irreps). We recognize that bulk crystals have lower symmetry than the isotropic system, and hence break the symmetry of the original higher symmetry system. This leads to the formation of different polarization eigenstates, with different propagation velocities along different directions, depending on the symmetry of the new system, much like how that of a spherical symmetric system differs from those in an isotropic system. Hence the polarization eigenstates are not always purely transverse or longitudinal; they are fundamentally the polarization eigenstates of the elastic waves, which depend on the particular symmetry of the system. We can be easily misled by the conventional use in bulk
crystals typically described using orthogonal coordinates! In Figure 2.2a, we show the first two eigenmodes of the homogeneous system, which possesses the familiar transverse (i) and longitudinal (ii) modes. In comparison, the corresponding modes for a one dimensional phononic crystal [Figure 2.2(b)] seem to be mixed. In reality, this results from the fact that the system is no longer isotropic and hence the symmetry is broken in the periodic direction. As a result, the real eigenmodes are those which are (anti)symmetric with respect to the mirror plane (parallel to the periodic direction). In the homogeneous limit, one may also similarly classify the transverse as the antisymmetric, and the longitudinal as the symmetric Irreps. Once the symmetry is broken, the correct eigenmodes have to belong to the Irrep of the isotropy group of the relevant wave vector, at all times. This demonstrates the Irreps, or relevant classification of the eigenmodes in the system.
Figure 2.2 Displacement field comparing between the (a) homogeneous system and (b) the 1D phononic crystal and the corresponding (anti)symmetric pairs along the direction of periodicity. The strain field intensity, $|u(r)|$ ranges from red (high) to blue (low), with the vector field indicating both the magnitude and the direction of the strains. The color map indicates large (red) to zero (blue) displacement.
Let us now restate the crucial point about what polarization is and how we should treat polarization. The polarization degrees of freedom depend on the dimensionality of the medium and the conventionally known transverse and longitudinal modes in a system are but a subset of the larger class of possible modes, known more correctly as the polarization eigenstates.

The nature and form of these polarization eigenstates depends on the underlying symmetry of the medium; this is the most general and correct classification of polarization eigenstates.

These inhomogeneities further break the original symmetry of the homogeneous system at various length scales. In both the bulk crystal and this AS case, we break symmetry from an initially higher symmetry case, yet, the dispersion relations turns out to be clearly different, with the later becoming visibly more complex. What is the origin of this behavior?

This is where once again the length scale comes into play. In the artificial structure, the symmetry is broken above some length scale once the phonon can sense the inhomogeneity!

This causes changes in the nature of the wave-vector $k$, as well as its associated allowable spectrum of values; all of this represents the breaking of the spatial symmetry.

However, in both cases, it remains true that polarization states are derived with the only difference in the length scales present in the latter, due to the artificial structuring, or the non-locality present in the medium. Stated physically, the inhomogeneity present in the AS leads to changes in the wave propagation behavior beyond certain length scales. This leads to spatial dispersion and is commonly known as the non-locality of the structure! Mathematically, non-locality in this context implies that the response of the medium to a propagating wave (its group velocity, etc) depends on the wave-vector $k$ explicitly. One easy example would be a...
diatomic crystal; its first indication of the non-locality is at the length-scale of the sub-lattice separation and manifests itself as the optical phonon branch!

This realization clarifies that the polarization of each eigenmode in the medium, whether bulk or artificially structured, stems from the proper diagonalisation into the relevant subspaces, dictated by the symmetry of the crystal. The subsequent complexity from the polarization fields is due purely to the interactions from the non-locality of the structure. The nature of these interactions may of course differ, depending once again on their length scales, ranging from scattering ($\lambda/a<1$) to interference ($\lambda/a>1$). But once again, the complexity is due to the mechanics of the interactions present, but they are governed still by the global invariants and the symmetry of the medium.

To complete the discussion, we compute the eigenmodes for the pairs of bands (5,12) at \( \Gamma \) and (2,4) and \( \chi \) in the one dimensional phononic crystal (Figure 2.3(c)). We first look at the modes at \( \Gamma \). While we develop the machinery later on, we note here quickly that the interaction is occurring between the two modes that are both symmetric with respect to the mirror plane perpendicular to the periodic direction at the \( \Gamma \) point. In contrast, at the \( \chi \) point, both interacting modes are both anti-symmetric with respect to the perpendicular mirror. These two form the longitudinal and transverse gap respectively in the one-dimensional phononic crystal.
Figure 2.3 Eigenmode plots for the pairs of bands (5,12) at the $\Gamma$ point, and pairs of bands (2,4) at the X point for the 1D phononic structure computed in Figure 2.1(c). These pairs of bands are responsible for the opening of the spectral gap in the phononic crystals at the $\Gamma$ and X point respectively. The color map indicates large (red) to zero (blue) displacement.
2.4 Concluding Remarks on Elastodynamics from a Symmetry Breaking Perspective

We utilized two viewpoints, one the more conventional microscopic method, and the second method, more geometric in nature and based on conservation and symmetry. By utilizing conservation principles and reconciling them with the more conventional microscopic method, we are able to develop more insight into the nature of elastic wave propagation and relate it with the conservation of linear momentum (in our cases of interest here). We then showed that the polarization degrees of freedom actually derive from the broken symmetries at the atomic scale, leading to the formation of gapless Goldstone modes in homogeneous media. However, in contrast to convention, polarization eigenstates are not always decomposable into the common transverse and longitudinal modes. This decomposition is only true for systems with orthogonal symmetry, e.g. cubic, orthorhombic systems. In general, the existence of polarization stems from the broken symmetry from an initial continuous system (at all length scales). The exact form of the polarization eigenstates however, respect the details of the symmetry which the structure possesses, hence it may be arbitrary complicated depending of the symmetry of the homogeneous medium. This situation does not change in considering AS, where purposeful inhomogeneity occurs at various length scales as desired. The polarization state still follows the symmetry of the AS and while the dispersion relations may be much more complicated, the governing principle for the polarization eigenstates remains the same. What the inhomogeneity changes though, is that it changes the permissible values and actual physical meaning of the wave-vector \( k \).

Now that we have claimed that despite the apparent complexity of the polarization states, exemplified in a typical band diagram of a phononic structure, that their underlying
classification and nature is isomorphic to that of a bulk crystal. This points a way forward towards being able to identify and classify the polarization eigenstates in various AS.

While we now can place the polarization eigenstates within our framework of broken symmetry and conservation laws, the question still remains now as to how to control the polarization states in these phononic structures, in order to control the dispersion relation of these structures in a rational way. We have shown that the polarizations obey the explicit symmetries which are bestowed upon the structure which it propagates. We also realize that the restrictions/constraints which the explicit symmetry places on the structure is absolute and offers a way with which we can manipulate the polarizations, and hence the dispersion relations of phononic structures. The relation here is not so clear presently and requires a discussion of the effects of non-locality in the structure. This will be discussed in depth in chapter 3. The remarks on the importance of understanding and controlling the polarization state of the phonon will become clear as we demonstrate (in subsequent chapters) unique phonon propagation behavior as well as record performance metrics in our designs. These will be achieved simply by utilizing the notion of the length-scales and polarization to develop a transparent design framework that can dramatically improve one's control over \( \omega(k) \).

3.1 Introductory Remarks

The previous chapter highlighted the elastodynamic equations governing the propagation of classical phonons in general inhomogeneous media. The vector nature of a classical phonon, propagating in an inhomogeneous medium (waveguide, resonator, crystal or meta-material) makes it rather difficult to track microscopically.

From an applied perspective, it is desirable to be able to obtain rules for designing a particular inhomogeneous medium, in order to obtain a desired propagation behavior of a phonon to be able to develop novel and useful applications for phononics.

Hence, understanding and control over the vector nature of the phonons is both scientifically interesting and desirable from an engineering perspective. The question thus becomes are we able to find general governing relations in order to control the vector fields that propagate through the AS?

We mapped the polarization states of the phonons for an artificial structure and that of a bulk crystal onto the same network (chapter 2). We showed that the difference in the two stemmed from the relevant length scales of the inhomogeneity in the medium; this has direct implications to the non-locality (dependence on the wave vector and the material wavelength) of the medium, which controls the type of interaction causing the dispersion of the propagating phonons. The interaction due to this non-locality in turn, are bounded by global invariants, via the symmetry of the artificial structure, in terms of the possibility of an interaction occurring.
Hence, the ability to develop control over this dispersion relation would extend our capabilities beyond just, e.g. creating complete spectral gaps; we will also be able to induce bands that effect negative refraction, generate double negative index bands, and even perform hyper-lensing [17, 28]. In fact, we aim to control the curvature and the placement, i.e. frequencies of each individual band, in principle allowing unparalleled control over the propagation velocities and dispersion of the possible eigenmodes within a structure. Ideally, we would not want to be limited to a pedagogical infinite bulk system, but also to be able to incorporate the boundaries, interfaces between different media as part of our entire design framework; indeed, we would like our design framework to be as general, practical and as unrestrictive as possible. This implies that we would need to have control over the presence (or absence) of eigenstates as well as the curvature and dispersion of individual bands. How can this be done?

We remarked in chapter 2 that the projection into the correct subspace of the degrees of polarization freedom allows one to extract the eigenmodes of the system. Naturally, these eigenmodes then form an irreducible basis of that invariant subspace. The crucial question here is what governs these subspace projections? Because each new mode originates from a broken symmetry of the original system, the polarization state of each mode is controlled by the global symmetry which the structure possesses! Group theory poses global invariants on the explicit spatial symmetries which a particular phonon eigenmode may possess; it has to be explicitly an irreducible representation of the isotropy group of the wave-vector. While we refer to excellent texts for a detailed and clear exposition into groups and representations [59, 64], we note here that the representation theory is isomorphic to the subspace projection of the phonon eigenmodes which we have been mentioning and have explicitly demonstrated in
chapter 2. This will be our approach, i.e. we will use the mathematical machinery to map explicitly to the physical process of designing different phononic AS for different applications.

In this chapter, we endeavor to develop a general design framework, to mold the dispersion relations of phononic structures by casting the fundamental linear elastodynamics (section 2.2.2) governing the phonon propagation within a concrete mathematical framework. This mathematical framework allows us to extract the global possibilities of the types of interactions that may occur, that may lead, for example to the formation of a spectral gap. This framework also allows us to treat the often complicated polarization fields of phonons with a surprising transparency that automatically accounts for the vector or scalar nature of the field which we are interested in. Finally, we are also able to directly control the size and extent of desired interactions present in the system; indeed we will be able to show, quite clearly what kind of features are exactly needed in a phononic structure, in order to obtain a desired phonon mode.

We claim that these are the main ingredients which we need in order to achieve an unprecedented level of control in designing the dispersion relations of phonons in these structures.

While we will develop all the pieces of the framework in detail here, we next concisely highlight the various aspects of the mathematical framework which allows us to treat the vector nature of these fields in a transparent manner that treats both infinite, finite and (non)-periodic systems with the same footing. This framework consists of the following main ingredients:

i) The general interaction process leading to the formation of the spectral gap is the avoided crossing between bands having the same symmetries
ii) The non-locality principle, which illustrates the importance of the lattice in controlling the dispersion and dynamics of phonon propagation.

iii) The local principle, which utilizes a variational perspective to tie together the microscopic physical details of the phonon propagation and controls the eigenfrequency spectra at several \( k \) positions.

iv) The global principle, which ties together all the global invariants of a structure and the related phonon dispersion.

The combinations of these four aspects of our framework are instrumental in controlling and augmenting the position and size of complete spectral gap formation in phononic structures, both infinite as well as finite. To be clear, there is no actual restriction on the extent and presence/absence of boundaries of the structure. In fact, although seemingly purely mathematical and somewhat abstract in nature, it will turn out that the irreducible representations imparted by the group on the eigenmodes actually control the interactions due to the non-locality which is present in the structure. A more accurate statement is that the irreducible representation provides the character, or signature of the eigenmodes and the possible interactions between the various bands. For now, let us keep in mind that this global principle enforces global constraints on the allowed behavior of the eigenmodes of the phononic structure. Before we delve more deeply into the global principles, we first motivate the interaction process that allows us to design a fundamental spectral gap and now examine the conditions for the occurrence of an avoided crossing.
3.2 Generalization of Avoided Crossings & Perturbation Theory

The generality of a framework requires one to also be able to microscopically control the energetic, or in this case, the exact modes and their positions in the band dispersion relations. This is quite important as while global constraints allow us to limit the possibilities that the phonon propagation may have, it does not allow us to create a particular functionality. In order to do this we need to deal with the microscopic, or the dynamics involved in designing the dispersion relation. In general, a phonon propagating through a structured medium, involves encounters with various interfaces and subsequent multiple scattering events. In classical systems, we envision that this phonon remains a coherent wave (with no dissipation) at least to first order. In the previous chapter, we mentioned briefly that the polarization and hence, the eigenmodes of the phonons in an AS or bulk medium, depends on its underlying symmetries. We also showed, in the case of a one-dimensional phononic crystal, examples of eigenmodes and how they relate to our traditional concepts of transverse and longitudinal modes in bulk materials [Figure 2.3].

Having established that the eigenmodes in an AS are determined by the underlying symmetries of the system, we now proceed to examine the fundamental conditions that actually determine the formation of a spectral gap and hence the need for control of the eigenmodes. The phenomena of avoided crossings has been well known since the days of Zener and the early years of solid state physics with the theory of electrons and solid state band theory. However, the concept of an avoided crossing is quite general and can be traced back exactly to the study of the symmetry of the eigenmodes of the system and their behavior in (ω,k) space. We noted earlier that in a one-dimensional phononic crystal [section 2.5], the symmetries of the system
resulted in the selection of two classes of eigenmodes which were (anti)symmetric with respect to the mirror plane along the direction of periodicity. We showed clearly that Bragg-type scattering at the BZ edges only occurred between pairs of modes which were (anti)symmetric, i.e. modes with the same symmetry. In fact, this Bragg-scattering mechanism, which is well known is precisely an example of an avoided crossing. Physically, this corresponds to the fact that degeneracy at the position where two eigenmodes meet, or cross was not permitted by the symmetry of the system, hence these bands interact and as a result form a spectral gap due to this interaction. An absolutely important point to note is that the underlying fundamental condition for the interaction to occur is that these two modes need to have the same behavior with respect to the symmetry of the group which the AS possesses, i.e. they need to have the same irreducible representation. From a mathematical standpoint, the concept of avoided crossings and irreducible representations stem from the theory of representations as well as from group theory [59, 60, 61]. We leave the reader to pursue these excellent classics for a clear exposition of the theory and we shall endeavor here instead to develop a physical intuition of an irreducible representation. Let us consider now a system, that has some symmetry in the two dimensional X-Y plane and is invariant along the orthogonal Z axis, i.e. the system possesses uniaxial symmetry. Hence suppose we are describing say a general displacement in this system, we write it in the usual Cartesian coordinate as:

\[
\begin{bmatrix}
  u_x \\
  u_y \\
  u_z
\end{bmatrix} = \begin{bmatrix}
  u_x \\
  u_y \\
  0
\end{bmatrix} + \begin{bmatrix}
  0 \\
  0 \\
  u_z
\end{bmatrix} = \text{Irrep}_x + \text{Irrep}_z
\]
We note that any symmetry operation of the group in the XY plane will only change \textit{Irrep}_{xy}, leaving \textit{Irrep}_z invariant and likewise. For example, suppose we apply a rotation of $\theta$ about the z axis, in the XY plane, we get the following:

$$
\hat{R}u = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix} = \hat{R} \begin{pmatrix} u_x \\ u_y \\ 0 \end{pmatrix} + \hat{R} \begin{pmatrix} 0 \\ 0 \\ u_z \end{pmatrix}
$$

It is clear here that the rotation only affects \textit{Irrep}_{xy} and our two subspaces as we have laid out here are orthogonal, and do not interact with one another. This is a trivial example of the concept of an irreducible representation, i.e. it is basically the representation of a field variable, within the invariant subspace it exists in. Hence two eigenmodes which have the same irreducible representation exist in the same subspace may interact, leading to the avoided crossings, whereas those with different irreducible representations simply cross each other in $(\omega,k)$ space; this latter phenomenon is commonly denoted as an accidental degeneracy at the point of crossing.

The whole point of identifying the symmetry of an AS lies exactly in retrieving the irreducible representations of each and every eigenmode of the band dispersion. This knowledge enables us then to predict and hence control where avoided crossings, and hence spectral gap formation may occur. The physical problem can be viewed in a concrete mathematical framework where we may treat all physically distinct perturbations to the system, such as a change in the material components, the actual geometrical structure of the material, the inclusion of boundaries, interfaces etc with the exact same underlying mathematical framework.
Figure 3.1 Dispersion relations of (a) the classical Lamb plate and (b) the modified antisymmetric (AntiS) plate.

The unit cells are shown in the insets, with the structures extending infinitely along the axial and into the plane, and having a finite thickness $h$. (a) clearly shows the two sets of solutions, symmetric (solid lines) and anti-symmetric (dotted lines) about the central mirror plane with the anti-symmetric modes represented by dotted lines. The pair of red arrows indicate the positions of avoided crossing in both systems. In (a) this takes place between the 2nd and 4th modes (both even) and in (b) we picked the 6th and the 7th bands. The exact thickness of the plates will affect the positions of the bands, but the features of the dispersion relations remain invariant to the change in thickness. Computations were performed with amorphous silicon as the material ($E=156\text{Gpa}, v=0.2152, \rho=2330\text{kgm}^{-3}$)
Armed with this new insight, we now revisit a classical problem, to convince the reader that our efforts do yield considerable new insight and as a result surprising benefits even! We introduce the problem of elastic waves existing in an infinitely long plate [Figure 3.1(a) inset], which is confined only in a single direction (z), given by a thickness $h$. Originally solved by Horace Lamb in 1917 [62], the solutions to these elastic waves are rightfully known as the Lamb waves. Here, we consider only the solutions of the in-plane elastic waves, because the shear-horizontal modes are decoupled from the longitudinal-shear vertical modes. The dispersion relation of the Lamb plate is shown in [Figure 3.1(a)]. As stated, the presence of a mirror plane along the horizontal axis leads to the possibility for solutions, or eigenmodes, which are (anti)symmetric, what was called odd and even by Lamb in his original work. We highlighted [Figure 3.1(a)] the 2$^{nd}$ and 4$^{th}$ bands (in blue) belonging to the symmetric irreducible representations $A$, especially the position of the avoided crossing at $k$= (0.26,0). In the original work, the particular evolution of these modes was not discussed nor the cause for their behavior identified. We note that these changes in band curvatures are positions of avoided crossings, as we rightly see that they only occur between eigenmodes with the same irreducible representations, as we show here [Figure 3.2]. This is clear from the fact that both modes are clearly symmetric about the mirror plane, even though we are unable to identify them as shear or longitudinal, as their behaviors are rather mixed, this is most clear in the 4$^{th}$ modes.
Figure 3.2 Avoided crossing of the 2nd and 4th modes in the Lamb plate, before \((k = (0.24,0))\) and right after \((k=(0.28,0))\) the avoided crossing as highlighted in Figure 3.1. It is clear here that the interaction, or avoided crossing, is rather weak, hence there is very little mixing of the modes, although the bands do change character after undergoing the interaction, a clear signature of the avoided crossing. The color map indicates large (red) to zero (blue) displacement.

Clearly, the exact polarization state of the eigenmodes is represented by their irreducible representations, which in turn depends on the symmetry of the system and very often, traditional concepts of longitudinal and transverse waves lose their exact meaning. We have to bear in mind, as first mentioned in chapter 2, that longitudinal and transverse modes originated
from the original Lame solutions of elastic waves in an **isotropic** homogeneous medium [4,57], hence they are eigenmodes of such a system, not of all systems! We further show here [see Figure 3.3] the first 4 guided modes present in the Lamb plate to illustrate the utility of using irreducible representations to classify the polarization state of the eigenmodes in any system. It is clear here that while the pairs of modes (3,4) can be identified as quasi-longitudinal and quasi-transverse respectively, the same cannot be said for pairs (5,6). The reason for this is that the correct classification of modes in the Lamb plate can only be made with respect to (anti)symmetry about the mirror plane, that is their irreducible representations are now reduced to these two possibilities, as contrasted with a bulk isotropic solid where the shear (vertical) and longitudinal modes that we are familiar with are the correct irreducible representations.

**Figure 3.3** Eigenmodes of modes 3 to 6 of the Lamb plate, at the $\Gamma$ point. Modes 3 and 6 are anti-symmetric whereas modes 4 and 5 are symmetric with respect to the horizontal mirror at h/2. The color map indicates large (red) to zero (blue) displacement.
By applying this concept of **irreducible representations** to such a classical problem, we find that we are able to explain the behavior of the band dispersions without tracing the k-evolution algebraically or microscopically. In fact, from an algebraic standpoint, the fact that this avoided crossing occurs may have itself been obscured! We chose to revisit this classical problem because of two factors, one that it has the simplest group, consisting of only the two element group \{E,m\}. Furthermore, it is a bounded system, i.e. has a finite dimension. These two factors help illustrate the generality of our approach of an avoided crossing, particularly in illustrating that we may treat the entire system, including both the bulk as well as the boundaries within the same system. At the same time, the low symmetry group of this particular system helps make the irreducible representations nearly trivial and tractable. We now wish to do better and aim to induce multiple complete spectral gaps within this Lamb plate, not just a single spectral gap. We have shown this earlier [Figure 3.1(b)], and clearly the band dispersion has multiple complete spectral gaps. We notice that none of the bands in this structure **ever cross**, i.e. all the bands have undergone avoided crossings! This is incidentally the first demonstration of multiple spectral gaps in a structured slab; yet the underlying principle behind this design is exceedingly simple and quite amenable to fabrication. By recognizing that the original Lamb plate possessed two orthogonal sets of solutions, we now proceed to reduce the **irreducible representations** to a single one along the \(\Gamma X\) direction, that of only the trivial identity, i.e. we remove the mirror plane in the original Lamb plate. This structuring of the two boundaries explicitly breaks the mirror symmetry, resulting in only one class of solutions remaining for the eigenmodes. This is shown clearly in Figure 3.4, where single unit cells of modes 6 and 7 are plotted. Clearly, both these modes do not possess any
mirror (anti)symmetry, both modes have the identity (trivial) irreducible representation, hence avoided crossing occurs between them.

![Figure 3.4 Eigenmodes of (a) Bands (6,7) from Anti-S Lamb plate before and (b) Bands (6,7) from Anti-S Lamb plate after the avoided crossing. A single unit cell is plotted here, the plates extend infinitely along the [100] direction. The color map indicates large (red) to zero (blue) displacement.](image)

We recognize here once again that the underlying principle behind the separation of the two sets of modes governing the dispersion in the original Lamb plate originated from the symmetry of the system. Hence, we physically enhance the interaction between bands by changing mathematically the character of the bands in the dispersion, i.e. we are utilizing an underlying global principle of reducing all the irreducible representations to be only of the trivial identity representation.

Physically, this amounts to controlling the interactions such that the only allowed eigen modes obey the boundary conditions, which are anti-symmetric about the center of the plate.

We note there that while along ΓX, the only allowed irreducible representations are the trivial identity representations, this is not true at Γ. While this is elaborated later in the chapter (section 3.5), the irreducible representations corresponding to a particular wave vector belongs
to the isotropy group of that particular wave vector, i.e. the subgroup of symmetry elements that leave the particular wave vector invariant. In contrast, the AntiS Lamb structure [Figure 3.1(b) inset] actually can be identified with the pma2 frieze/line group. At the Γ point, the isotropy group is actually bigger, consisting of \{E, C_2\}, hence there are now two possible irreducible representations, which we see as we plot [Figure 3.5] mode pairs (4,5), which are symmetric with respect to a $C_2$ rotation and (3,6), which are antisymmetric with respect to a $C_2$ rotation at Γ.

We showed here, through the classical Lamb plate problem, that by correcting identifying the fundamental origins behind the eigenmodes of the system, that we are able to design quite novel changes to the system by altering the fundamental solutions themselves. In this particular instance, simply identifying the irreducible representations of the system and then subsequently reducing the symmetry of this system, we were able to create via anticrossings multiple spectral gaps into an otherwise homogeneous plate.
Figure 3.5 Eigen-mode plots of (a) Mode 6 (antisymmetric), (b) Mode 5 (symmetric), (c) Mode 4 (symmetric), (d) Mode 3 (antisymmetric) of the AntiS Lamb Structure at the Γ point. The color map indicates large (red) to zero (blue) displacement.
3.3 Non-Locality: The effect of the Lattice and its Interactions

The eigenmodes of the AS, be it a phononic crystal or slab, must obey the discrete symmetries of the space/plane group of the crystal and only adopt the permitted irreducible representations which correspond to the isotropy group of the relevant wave vector. [63, 61, 69, 59, 64] This can be summarized as a consequence of the discrete symmetry invariance of the physical system and the adherence of the eigenmodes solutions to adopt the corresponding irreducible representations. From a less physical and more abstract perspective, the presence of a symmetry group that an AS possesses mathematically partitions, for a particular problem such as elastic wave, or electromagnetic wave propagation, the solutions into invariant and orthogonal subspaces; this is a consequence of Schur’s second Lemma [64, 61], which states that different irreducible representations are orthogonal.

Avoided crossings may be said to be meso-scale as well as nonlocal. It occurs at all length scales, i.e. the process is meso-scale as we have made no approximations in the calculation of the spatial dispersion. Our pedagogical examples have demonstrated the same phenomenon from the simplest possible finite system (section 3.2), to an infinite lattice (section 2.2); in both cases, the avoided crossing was clearly identified to occur due to the irreducible representations.

It is also nonlocal, i.e. its behavior depends on the wave vector vis a vis the relevant isotropy groups and the formation of spectral gaps in finite plates and infinite phononic crystals are treated on the same footing. Hence, it automatically incorporates the non-locality in the system, if present. It acknowledges all the forms of symmetries that will lead to interaction,
regardless of the length-scale, the specific type of symmetries, translational, point or time-reversal etc.

Physically we understand that the strength of the spatial dispersion depends strongly on the non-locality of the medium to the wave propagation; i.e. $\varepsilon(k,\omega)$, where $\varepsilon$ is the response function of interest. This spatial dispersion is in turn inherently linked to the interaction length scales between the wave, and the geometrical structures of the medium. For example, a linear dispersion relation implies that the medium is interacting with the wave independently of the length scales involved. At the other extreme, when the dispersion relation becomes independent of the wavelength, this implies that the wave is spatially localized, and has flat or zero dispersion. This is the extreme case of dispersion whereby any form of propagating extended state is not supported.

Bands in the system typically lie between these two extremes and it seems an intractable task to be able to control how much dispersion occurs in a general system that has dimension $n>1$. Analytically, one might apply perturbation theory to specific points where the interaction has occurred and hope to be able to capture the subsequent dispersion which occurs; this becomes a question of keeping the correct terms in the perturbation of the system [5].

The crucial question for one to actually ask is then, what is causing the perturbation in some general position in k-space? The answer to this lies in the symmetry of the bands because the symmetries must persist across multiple length scales (for example, an entire band) and automatically keeps track of all the interactions, automatically manifesting itself through the final calculation.
As we alluded to earlier, the occurrence of an interaction or avoided crossing depends on the irreducible representations; this already implies the non-locality of the propagation behavior in the medium.

![Figure 3.6](image)

Figure 3.6 Computed band diagrams of the 2D locally resonant structures, showing the effect of non-locality with the variation of the intermediate \( \beta \)-phase, which is our connecting (non)local phase in the LRS-type structure (a) \( \beta \)-phase has the same properties as the scatter, (b) \( \beta \)-phase has the same properties as the matrix, (c) \( \beta \)-phase has the mechanical properties lower than both (\( E= 0.5 \) GPa, \( v=0.3, \rho=1300 \) kg\( m^{-3} \)) the scatter and matrix, (d) \( \beta \)-phase has mechanical properties much lower than both (\( E= 0.05 \) GPa, \( v=0.3, \rho=1300 \) kg\( m^{-3} \)) phases. The scatterer phase was taken as (\( E= 40 \) GPa, \( v=0.3, \rho=4000 \) kg\( m^{-3} \)), the matrix phase was taken as (\( E= 4 \) GPa, \( v=0.17, \rho=1300 \) kg\( m^{-3} \))
In fact, it is actually the **degree of non-locality** that is affected by the geometry and the contrast between the material constants of the different constituents. The non-locality in the medium is extremely important because it influences the strength of the interactions between bands, and therefore naturally controls the group velocity along the bands, i.e. the curvature and dispersion of the bands. This latter fact has been often overlooked. Indeed, in the pioneering work of the locally resonant sonic (LSR) crystal [Figure 4.1] [55], the non-locality of the medium was not mentioned, primarily due to the focus by the authors on large elastic contrast between the constituents employed, which made the structure behave in the **weakly non-local** limit.

In Liu’s work, the originality arises from the “local” nature of the spectral gap opening mechanism, which was distinct from the common Bragg-type mechanism. However, in actuality, both mechanisms for gap formation are strictly avoided crossings, albeit at different k vectors and the presence of the lattice itself implied that the mechanism was not local, but only weakly non-local. We shall encounter this model again in the next chapter where we show how one may remove any unnecessary requirements for the creation of certain elastic metamaterials.

The point which we wish to emphasize here is that the mechanism of spectral gap opening is strictly nonlocal in the presence of the lattice. It is the degree of nonlocality which is affected by specific material choices. We next show, through a series of very simple models, the clear influence of the lattice on the dispersion relations by utilizing the same building block and then introducing non-locality via tuning of only one of the material phases. In all of these lattices, we retain the material choices of the solid scatterer (E= 40GPa, v=0.3, ρ=4000kgm\(^{-3}\)) and the matrix ((E= 4GPa, v=0.17, ρ=1300kgm\(^{-3}\)), and vary only the connecting β-phase.
We note that in Figure 3.6(a), where the β-phase is taken as the same material as the solid scatterer that we recover the typical dispersion of a phononic crystal, with the spectral gap opening about a normalized frequency of ~0.5. The same situation is presented in Figure 3.6(b), where the β-phase is now the matrix. However, as we tune the β-phase, making it gradually mechanically ‘softer’ (lower Elastic Modulus, mass density, keeping Poisson ratio constant), we begin to notice the evolution of the band structure, most notably for the 3rd, 4th and 5th bands. Figure 3.6(d) already resembles the obtained band structure of the LRS model, with the 3rd band being characteristically flat and the 5th band evolving with positive curvature from zero slope at the Γ point. We note here that we have continuously tuned the LRS structure, from a classical phononic crystal into a resonant LRS by tuning only one of the material phases (i.e., β). One minor point of note is that even in (d), our β-phase is still three orders of magnitude stiffer than that in the original work [55], yet it has reproduced the same qualitative band structure. Hence, the perceived “local” mechanism was actually a result of the strength of a material perturbation on the non-locality and not a distinct mechanism by itself. In fact, one may notice that the very statement of a local mechanism is wrong, since the avoided crossing has occurred at non-zero wave vector!

In our work, the spectral gap opening has shifted from the avoided crossing of band pairs (3,6) at the X point in (a), to an avoided crossing between bands 2 and 5 along ΓX, at approximately k=0.32, below the first BZ edge (~ at a normalized frequency of 0.5).
Figure 3.7 (a) Modes 3 and 6 at the X point for Fig 3.6 (a), which is what one associates with classically in a phononic crystal. The structure itself resembles the binary phononic crystal. (b) Modes 2 and 5 for Fig 3.6 (d), where we have the LRS structure. The color map indicates large (red) to zero (blue) displacement.

Furthermore, by examining the eigenmodes, we recognize that the irreducible representations of the bands are different, as the isotropy groups are also different. In Figure 3.6(a), because the avoided crossing occurs at the X point, the isotropy group there consists of \( \{E, m, C_2\} \), hence
we note that both modes 3 and 6 are anti-symmetric with respect to the $C_2$ rotation. This is clearest from examining mode 6, which is mixed in nature. At the X point, $C_2$ is part of the isotropy group of $k = [G_{10}/2, 0]$, where $G_{10}$ is the reciprocal lattice vector along $\Gamma X$, since a $C_2$ rotation brings it into $k' = [-G_{10}/2, 0]$, making it equivalent and hence invariant because of the reciprocal lattice translations, i.e. the $k$ vectors are equivalent modulo $G$. In contrast, for (d), modes 2 and 5 are both symmetric with respect to the mirror plane, and the relevant isotropy group is only $\{E,m\}$. The irreducible representations of the eigenmodes once again emphasize the nonlocal nature of the spectral gap openings.

![Figure 3.8 Time evolution of mode 3 at k=[0.3, 0] for LRS structure (Figure 3.6(a) and (d)).](image)

(a)  (b)  (c)  
(d)  (e)  (f)

Figure 3.8 Time evolution of mode 3 at $k=[0.3, 0]$ for LRS structure (Figure 3.6(a) and (d)). (a),(b), (c) show the time evolution of mode 3 for structure (d), which corresponds to the LRS structure typically introduced in the literature. The color map indicates large (red) to zero (blue) displacement. For (a) and (d), the vector fields have
been plotted in white to act as a visual guide for the low displacement intensity case, i.e. it has the same physical meaning as the black arrows in figures (b), (c), (e), (f).

Nevertheless, the change in the material composition of the β-phase necessarily influences the dispersion and the extent of the non-locality of the bands, which we have pointed out earlier. By comparing the time evolution of the corresponding mode 3 bands of Figure 3.6 (a) and (d), the extent of spatial dispersion is clear. Figures 3.8 (a), (b), (c) show the time evolution of mode 3 of Figure 3.6 (d), corresponding to the LRS case. It is clearly seen from the time evolution snapshots that the eigenmode is localized strongly within the center cylinder; this gives rise to the relatively flat dispersion of the band, indicating that there is no transport in the structure and that the displacement fields are strongly localized within the solid scatterer.

In contrast, by utilizing a slightly stiffer connecting phase [Figure 3.6(c)], the eigenmode becomes less localized and the displacement field actually propagates through the medium, as shown in Figure 3.8 (d), (e), and (f). In Figure 3.6(c), there is also an onset of non-flat dispersion in this band (mode 3), which corroborates the observed time evolution of the displacement field.

Finally, we wish also to note that, as is common in the literature, that sub-wavelength spectral gaps are classified as occurring below the first BZ regime, occurring at a normalized frequency of ~ 0.5. Hence, Figures 3.6(a), (b) and (c) are conventionally identified as phononic crystals, while Figure 3.6(d) would correspond to a sub-wavelength metamaterial. In chapter 4, we shall show that this strict distinction is actually artificial.
3.4  Local Principles: The Variational Principle from a Geometric Viewpoint

We have shown that we are able to control the extent of non-locality both through a choice of materials (section 3.3), and the symmetries governing the system (section 3.2) vis a vis avoided crossings. These principles have thus far been global in nature, i.e. they apply to all structures that fulfill a particular choice of space or plane group symmetry (section 3.3). We have utilized the materials choices to only tune the extent of the non-locality, but not i) the strength of the interactions in the spectral gap, ii) the positions of the bands, i.e. their eigenfrequencies and iii) the evolution of the bands across $k$ space.

In the design of a phononic crystal, one usually considers the scattering strength of the scattering phase, the mechanical contrasts between the different material phases and the fill fraction. However, these design factors neither recognize the actual role of avoided crossings nor the lattice (nonlocality), which we have shown to be crucial for spectral gap formation. For example, while sub-wavelength and Bragg gaps are readily identified to originate from avoided crossings in our network, this underlying similarity is not so clear from the microscopic viewpoints of resonant tunneling or Bragg scattering respectively. Furthermore, these two microscopic mechanisms are strictly tractable only in isolated or simpler systems or lower dimensionality, i.e. structures with no long range order (resonant tunneling) or simple one-dimensional lattices (Bragg scattering). There is a need as well for developing a general principle that governs the eigenfrequency distribution and hence, the ability to treat the energetics involved in scattering and in tunneling equivalently. This need is met by the local design principle which we discuss next utilizing the variational perspective.
The variational perspective provides a natural approach with regards to the symmetries of the eigenmodes and their eigenfrequencies. In fact, most equations of motion can be converted into a variational form, in a method analogous to how we converted an equation of motion into a conservation equation in chapter 2. The fundamental governing idea is that in the variational method, we formulate a relevant energy functional, \( E(\mathbf{u}(r,t),\mathbf{u}_t(r,t),\mathbf{u}_{tt}(r,t),r,t) \), before projecting out each eigenmode, \( |u_\lambda> \) and its eigen-frequency, \( \lambda \). A simple example of this is to examine a freely vibrating acoustic sphere. The eigenmodes, in ascending order of eigenfrequencies, are

Figure 3.9 Computed band diagrams of (a) the RS structure (b) the RB structure. The insets show the unit cell, with the dark phase being the material and the complimentary white phase being air/vacuum. The material is chosen to be amorphous silicon \((E=156\text{GPa},v=0.2152,p=2330\text{kgm}^{-3})\). Area fractions are for RS (26.7%) and for RB (39%). The red dashed line represents the position \( k=(0.5,0) \). This will be used extensively in the remaining section.
the fully radial breathing mode, followed by an m-fold degenerate set of dipolar modes etc [8].

From a physical perspective, one may recognize that the eigenfrequencies increase with the number of nodes in the eigenmode profiles. This is linked to the exact form of the energy functional [3, 8], which contains first order spatial derivatives in the displacements, hence the presence of increasing number of nodes increase the energies and hence the associated eigenfrequencies. While simplistic, this example of an acoustic sphere is actually quite representative of the variational method and the subsequent eigenmodes which it yields. We next illustrate this design principle and focus on developing physical intuition for the reader. We
Figure 3.10. Eigenmode plots at M point for (a) Mode 3 for RS structure (b) Mode 3 for RB structure (c) Mode 2 for RS structure (d) Mode 2 for RB structure. Note that for each structure (both RS and RB), the degenerate pairs are accidentally degenerate, being antisymmetric and symmetric with respect to the diagonal mirror plane along [1 1]. The color map indicates large (red) to zero (blue) displacement.

first discuss the issue of design of the geometric structure in order to optimize a particular avoided crossing interaction.
In Figure 3.9, we compare the band structure of the RS(a) and RB(b) structure, where we geometrically modified the structure by simply increasing the size of the scatterer. This particular structure resembles a two-dimensional grid, exemplified by the mechanical connections, with the central nodes occupied by scatterers of different sizes. Since this is a solid-air structure (the impedance contrast is >99%), the transport occurs essentially through the solid structure alone. It is clear that by changing the size of the central scattering unit that the size of the spectral gap increases significantly, by a factor of ~40%. Figure 3.10 shows the eigenmodes of band pairs (mode 2, mode 3) in the respective structures. The 2nd mode in both modes have the same kind of localization of the displacement fields within the central block, however, the size of the scatterer in RB is optimized to the unit cell size, this is clear from the fact that bands 2 and 3 in RB form the lower bound of the spectral gap, whereas, for the RS structure, additional bands 4 and 5 are present, which diminish the spectral gap greatly. This is due to non-optimal interaction, leading to the formation of propagation channels within the original spectral gap. This is made clearer from examining the eigenmodes at the X point with the two corresponding mode pairs of (3, 7) in RS and (3, 6) in RB. We can see that the avoided crossing interactions are stronger between the 3rd and 6th modes in RB [Figure 3.11], as compared with RS, as we see the stronger localization in mode 3 for RB as compared with RS. This is further corroborated by examining the k-evolution of the 4th to 6th bands along ΓX, which are the bands which are absent in RB and are responsible for diminishing the gap [Figure 3.12].
Figure 3.11 Eigenmode displacement field plots at X point for the pair of interacting bands (a) mode 7, (c) mode 3 of RS, and (b) mode 6, (d) mode 3 of RB. The color map indicates large (red) to zero (blue) displacement and all displacement fields are plotted to the same scales.
Figure 3.12 Momentum-space evolution along ΓX [10] in k-space for bands 4, 5, 6 for the RS structure at k=(0,0), k=(0.5,0) and k=(1,0). We note that in particular, mode 4 at the X point, that there is delocalization of strains.
into the central scatterer. The color map indicates large (red) to zero (blue) displacement. At the Γ point, the isotropy group is the point group $C4v \{E, C_2, 2C_4, 2m_y, 2m_x\}$, hence mode 4 is symmetric with respect to the horizontal mirror plane, mode 5 is symmetric with respect to the vertical mirror plane and mode 6 symmetric with respect to a $C_4$ rotation. Along $ΓX$ ([1 0] direction), there is only a single horizontal mirror plane, hence the irreducible representations are symmetric with respect to the mirror (mode 4), or antisymmetric with respect to it (modes 5, 6). Finally, at X, the isotropy group is $\{E, m_y, C_2\}$, hence mode 4 is symmetric with respect to the mirror while mode 6 is antisymmetric with respect to the mirror. In addition, mode 5 is symmetric with respect to the $C_2$ rotation operation.
Figure 3.13 Eigenmode Displacement Field plots tracing the evolution along ΓX [10] in k-space for bands 4, 5, 6 for the corresponding RB structure at \( k = (0,0), k = (0.5,0) \) and \( k = (1,0) \). Here it is clear that the displacement fields here are localized mainly on the connecting bonds, with no mixing at the X point. The color map indicates large (red) to zero (blue) displacement.

This shows by considering the problem from a variational perspective, we account simultaneously for all the microscopic processes that lead to the final evolution of the eigenfrequencies and all that we have to focus on is the eigenfrequency placement of each mode by considering the terms in the strain energy functional and the allowed irreducible representations in each \( k \) direction. For example, Figure 3.12 shows the evolution along ΓX for bands 4, 5, 6 for the RS structure respectively. The displacement fields at Γ are localized mainly on the connecting bonds, with modes 4 and 5 differing only by a \( C_4 \) rotation, which energetically has no penalty. Mode 6, in comparison, has strain localization along all 4 connecting arms, and forms two more nodes along the \([01]\) direction; naturally, its irreducible representation is also different from that of modes 4 and 5, which forms a degenerate pair (due to the equivalent perpendicular mirror planes along \([10]\) and \([01]\) at Γ).

The situation is more telling at X, where mode 4 [Figure 3.12] is similar to mode 3 [Figure 3.11c]; in fact it has the same irreducible representation as mode 3! This indicates that the geometry of the structure was not optimal for the avoided crossing occurring near the X point (along ΓX), which is commonly identified with “Bragg-scattering”. Comparing the 4th and 5th bands of the RS structure [Figure 3.12] and the RB structure [Figure 3.13], it becomes clear that these two bands form the same degenerate pair at the Γ point as in RS. Due to the geometrical structure,
no mixing between the 3rd and 4th bands occurs near the X point; as a result, the mode remains localized at the connecting arms without any mixing, unlike the situation in the RS structure.

This was done by solely considering the irreducible representations possible from the isotropy group (at some k) and how the eigenfrequency changes with the geometry of the structure.

Comparison of the eigenmodes of the 3rd band [Figure 3.11(c)] and 4th band [Figure 3.12] of RS at X indicate mixing between these modes, suggesting that we need to repel them more strongly in order to increase the size of the gap, since X does not allow for degenerate pairs (i.e. we cannot, for example, pair bands 3 and 4 together and lower band 4 instead). In addition, from observing the eigenmode profiles of modes 4 to 6 at Γ [Figure 3.12], we recognize that the strain localization in the connecting arms needs to be decoupled from the strain localization in the scatterer to repel these bands further apart; this is exactly equivalent to enhancing the Bragg-like scattering process! The key difference is that we are now free from working in a particular regime of scattering; instead we consider the energetics based solely on the allowed symmetries to enhance the avoided crossing between modes 3 and (4,5) at Γ in the RS.

The above discussion demonstrated how one would apply variational principles based on the symmetry of the system; it turned out that this particular geometrical optimization process is equivalent to enhancing the Bragg scattering process (in a phononic structure) to increase the size of the spectral gap. Our final principle is that of the global principle of utilizing group theory and the theory of representations [59]. While the concept of irreducible representations has been utilized in all our discussions and we did motivate the concept of irreducible representations from a simple uniaxial system, we did not address their relation to the entire
band structure and dependence on the **particular choice** of the plane/space group. The choice of the global symmetry dictates the **possibilities** and bounds possible for a band structure; this will be the final development we shall undertake in this chapter.

The variational method, together with the avoided crossing, covers most possibilities for designing most of the major features in band structure, such as the formation of a spectral gap, one of the main interests in the phononics community. By complementing these local principles with the **global** symmetry principle, which governs the evolution of the dispersion bands in momentum space, we will be able to truly mold the dispersion relations to create the desired propagation behavior, or spectral gap.

### 3.5 Groups & Representations: Nonsymmorphicity and Wyckoff Positioning

We now discuss the global design principle, which pertains to the group symmetry and its representations. Group symmetry is global because it controls the likelihood for interactions (avoided crossings) and determines the character of each eigenmode vis a vis their irreducible representations [59, 64]. Unfortunately, it has been used mainly as an analysis tool [59] and not so much as a design principle; in reality the two are equivalent, merely reversed in causality. It is no surprise then that group theory may be used as the underlying foundation as well as the language for our generalized design framework.

In this section, we focus on two uncommon facts in group theory in its applications to solid state physics: 1) the concept of factor groups in plane groups, and specifically, the dressing of Wyckoff positions to modify the band structure of phononic metamaterials, and 2) the global
properties of nonsymmorphic groups and specifically, the special property that they impart band sticking along certain directions along BZ boundaries/edges.

3.5.1 Translation Subgroups and Wyckoff Positions

It has been commonly conjectured that large optimal spectral gaps will be favored in structures possessing the smallest irreducible Brillouin Zone (IRBZ). The reasoning behind this was a direct extension of Bragg scattering from one-dimension to greater than one dimension. This usually implied high symmetry plane groups, such as hexagonal plane groups (p6mm) as candidate space groups. However, this need not be the case, and recent works have suggested that certain lower symmetry plane groups, such as a honeycomb-like lattice with a two-‘atom’ basis (p3m1) has a slightly larger spectral gap than the corresponding parent p6mm lattice [68]. This discord originates from a lack of understanding of what the symmetries of a plane group actually impart upon an artificial structure (AS). Our AS structures, chosen with a certain plane/space group may be regarded as having broken the symmetry from an initial structure which is isotropic at all length scales. Naturally, these eigenmodes, which reflect this broken symmetry, necessarily adopts the irreducible representations that result from this lower symmetry plane group [59]. This is exactly analogous to how transverse and longitudinal modes are borne out of an elastically isotropic and homogeneous medium! Mathematically, when we say that an AS possesses a certain symmetry group, it implies that all functions (susceptibilities, fields such as displacements etc), have to conform to this set of symmetry operations. To summarize, the symmetry group which the AS possesses, be it spatial, spatio-temporal, or others, controls the nature of the eigenmodes, especially their vector polarization
states vis a vis the **irreducible representations**. All forms of interactions, propagations and motions in the AS are governed by the symmetry group; the most classical examples of these include the selection rules in **Raman** and **Brillouin** inelastic scattering. Now we make the explicit connection between our earlier use of irreducible representations (section 3.2, 3.3 and 3.4) concretely from its induction from broken symmetry and an explicit space group.

As the irreducible representations govern the vector polarization states of each eigenmodes, they also determine the absence/presence of avoided crossings which are crucial in spectral gap formation. Avoided crossings are only allowed between eigenmodes with identical **irreducible representations**. We also understand that along a particular direction in k-space, the irreducible representations are determined by the isotropy group and not the entire point symmetry group. We now proceed to develop the role of point group symmetry in controlling the band structure.

We remind the reader that a plane or space group is actually an infinite (countable) group, because the translation operations are infinite. For symmorphic groups, i.e. groups that do not possess glide lines (in 2D) or glide planes or screw axes (in 3D) as primary group generators, the group of translations is actually a normal subgroup of the entire plane/space group. This implies that we only need to deal with the relevant factor group, given by:

\[ F = \frac{G}{H} \]

*G* is entire symmetry group  
*H* is the translation subgroup  
*F* is commonly known as the **Factor Group/Quotient Group**
Each element of the factor group is conjugate to an element of the point group and since \( G \) is homomorphic to \( F \), we need only to deal with only the point symmetry elements in designing the band structure. Let us consider the computed band structures of the two structures shown [Figure 3.14], which we labeled \( T_1 \) and \( T_3 \).

![Figure 3.14 Computed Band Diagrams of Structures (a) \( T_1 \) and (b)\( T_3 \), taken with the naive IRBZ belong to a p4mm lattice. The material is chosen to be amorphous silicon (\( E=156\text{GPa}, v=0.2152, \rho=2330\text{kgm}^{-3} \)). Area fractions are for \( T_1 \) (59.35%) and for \( T_2 \) (54.15%).](image)

While both structures possess the same lattice vectors, hence identical translation subgroups, \( T_1 \) possesses 4mm maximal point group symmetry while \( T_3 \) possesses 2mm symmetry at \( \Gamma \) [Figure 3.14 insets]. So while their translation subgroups are identical, their point groups are not and their factor groups are different.
It is clear from Figure 3.14 though that T3 has a larger complete spectral gap compared to T1 (~20% larger)! We further plot the band structure of T3 [Figure 3.15] around its correct, larger IRBZ, since the IRBZ for the p4mm is reduced by half (compared to the p2mm) due to an extra diagonal mirror (absent in T3) and confirm that the spectral gap is indeed maintained.

Figure 3.15 Computed Band Diagram of the same T3 structure about its actual bigger IRBZ, which is that of a p2mm lattice. It is clear that the spectral gap size is maintained here. The material is chosen to be amorphous silicon (E=156GPa, v=0.2152, p=2330kgm⁻³).

Following our approach in section 3.4, we start with the p4mm T1 structure and then induce changes to the geometric structure from the variational perspective to augment the spectral
gap. From Figure 3.14(a), we note that the spectral gap is bound below by mode 3 near the X point and we hence plot the eigenmodes [Figure 3.16(a)] of the interacting band pairs (3,7) that open.

**Figure 3.16** Eigenmode plots for (a) (3,7) for T1 and (b) modes (3,9) for T3 at the X point. The color map indicates large (red) to zero (blue) displacement.
up the spectral gap in T1. We note that the isotropy group here for $k = [k_x, 0]$ along $\Gamma X$ consists of $\{E, m_x\}$, i.e. the identity and the horizontal mirror; both modes 3 and 7 have irreducible representations symmetric with respect to this mirror plane. What is perhaps more interesting is the formation of the node in mode 3. From a variational perspective (section 3.3), inducing a topographical cut would reduce the eigenfrequency and allowing for strain localization near these new ‘free’ surfaces, which is what we do in T3. We point here as well that along $\Gamma X$, the isotropy groups of both T1 and T3 are identical; this permits us to variationally alter the eigenfrequencies of the modes. Comparing the corresponding 3rd bands for both structures validates this approach, as the 3rd band is considerably lowered in frequency for T3. To show that the maximal point symmetries are indeed different, Figure 3.17 shows the corresponding eigenmodes at the $\Gamma$ point, for modes 3 to 6; it is clear that the irreducible representations are different for T1 and T3. For example, mode 3 for Top 1 is symmetric with respect to both $C_4$ and $C_2$ rotations, whereas mode 3 for Top 3 is symmetric only with respect to $C_2$. Although both modes have nearly the same eigenfrequencies, they strictly belong to different irreducible representations. Comparing the rest of the modes (4, 5, 6) between T1 and T3, we note that the eigenmodes look similar in that they are localized about the center; but from the band diagram [Figure 3.14] we observe that modes 4, 5 and 6 in T3 are relatively flat in $k$ space since these modes are topographically cut from propagating. This is not so for T1, where we do see some negative dispersion, associated with slow but non-flat dispersion.
Figure 3.17 Eigenmode plots at the $\Gamma$ point, for (a) mode 6, (b) mode 5, (c) mode 4, (d) modes 3, of structures T1 and T3, on the left and right respectively. The color map indicates large (red) to zero (blue) displacement.
In this work, the T1 and T3 structures possessed the same lattice basis and hence the same translation subgroup and same primitive Brillouin Zone (BZ). While group elements from the 4mm point group halved the IRBZ of T1 with respect to T3 (due to the set of diagonal mirror lines), however, as we have shown, this does not guarantee that the spectral gaps will be larger. We may regard our topographical modification of T1 into T3 as a change in the Wyckoff position occupations, with our modification bringing the point group from C4v down to C2v. The crucial fact that we exploited was that the avoided crossings depended on the relevant isotropy group, enabling us to modify the geometric structure while preserving the same isotropy group! The outcome of this was a local alteration of the phonon dynamics, allowing us to lower the 3rd band and increase the size of the spectral gap in the process. No assumptions on the possible microscopic mechanism governing the interaction processes were required; rather we looked at the total representation and energetics and utilized that as the fundamental starting point for our design process. Figure 3.18 shows the corresponding 5th bands along (a) the ΓX' [01] direction and (b) the ΓX [10] direction respectively for T3. Referring the band diagram of T3 [Figure 3.15], we notice that the 5th band is relatively flat along ΓX but possesses quasilinear dispersion along ΓX'. In this case, even though the bands possesses the same irreducible representation, i.e. antisymmetric about the mirror planes along their respective k directions, our choice of the motif, or the Wyckoff position occupation, leads to the distinction in their dynamics, which is ultimately characteristic of a structure with p2mm symmetry.
Figure 3.18 Time Evolution of the eigenmodes at (i), t=0, (ii), t=π/6, for (a) 5th band along the ΓX' [01] direction and (b) 5th band along the ΓX [10] direction respectively. The color map indicates large (red) to zero (blue) displacement.
3.5.2 Non-symmorphicity and Sticking Bands

We now discuss the nonsymmorphic plane groups and what they offer that symmorphic groups do not. In two-dimensions, they are only 4 (out of 17) nonsymmorphic groups but 157 (out of 230) in three dimensions. The role of group symmetry has been regarded as the underlying foundation for a framework to implement our local design principles, to shape both the physical positions of the eigenfrequencies. The global principles impart the possibilities and positions of avoided crossings for creating spectral gaps. However, there is one final aspect of the band structure which we have not yet dealt with and that is the band evolution along the BZ edge/boundaries. As an example, we refer to the band structures of T1 [Figure 3.14(a)] along the XM edge. Because the Isotropy group along XM is actually \( \{E, C_2\} \), two irreducible representations are allowed and hence the band trajectories are rather complex and intractable. This occurrence limits the creation of a single complete spectral gap and even more so for the creation of multiple complete spectral gaps. This problem, however, is reduced by employing nonsymmetric symmetry groups as they lead to the formation of sticking bands [Mermin96, 99], that is the bands are only allowed to exist as degenerate pairs along an entire BZ edge!

Let us first define a nonsymmorphic plane group. A symmetry group that is nonsymmorphic possesses generators consists of glide elements (2D) or screw axes (3D), that is they possess symmetry elements defined by:
\[ g = \{R \mid \tau\} \]
\( g \) is the glide/screw element
\( R \) is a proper point rotation, reflection operation
\( \tau \) is a translation which is not an integer multiple of the lattice basis

Figure 3.19 Computed Band Diagrams of Structures possessing global nonsymmorphic symmetries of (a) \( p2gg \), (b), \( p4mg \). The material is chosen to be amorphous silicon (\( E=156 \) GPa, \( v=0.2152 \), \( \rho=2330 \) kg m\(^{-3}\)).

Hence, all plane groups possessing glide planes as a primary symmetry element is hence a nonsymorphic group. In 2D, these are the \( \text{pmg}, p2gg, p2mg \) and the \( p4gm \) plane groups. As an example, we computed band diagrams of two structures, one with a \( p2gg \) plane group and the other with a \( p4mg \) space group [Figure 3.19]. For the \( p2gg \) structure, bands exist only as degenerate pairs along both the XM and the X'M edges, whereas for the \( p4mg \) structure, they only exist as degenerate pairs along the XM edges. A powerful result for this is that all structures possessing either of these two plane groups will possess such “band-sticking”, regardless of the actual geometrical structure. This greatly increases in the degree of control
over the band dispersion along the BZ faces, something which was previously not thought possible nor exploited. Following the approach of Mermin & Coworkers [65,66], we develop the conditions for band sticking from Fourier Space. As a periodic structure is translational invariant (for the entire lattice), one may express the displacement (expressed in a reciprocal basis), under some arbitrary translation of the entire lattice $d$, as follows:

$$u(r) = \sum u(K) \exp(iK \cdot r)$$

**Since** $u'(r) = u(r + d)$

$$\therefore u'(K) = \exp(id \cdot K)u(K) = \exp(2\pi i \chi(K))u(K),$$

$\chi(K)$ is linear in $K$ and modulo unity

This establishes the form of the displacement coefficients (in Fourier Space) due to the translation invariance. Now, under a symmetry operation, each Fourier component obeys:

$$u(g \circ K) = \exp(2\pi i \Phi_g(K))u(K),$$

$$\Phi_g(K) = \frac{1}{2\pi}(a_g, K)$$

Fundamentally, for different eigenmodes to be non-degenerate (i.e. for them to stick), this implies that the eigenmode has to be invariant to all the symmetry operations in the relevant isotropy group. Considering two different commuting symmetry operations $g, h$ we then have the following condition for band sticking to occur, that is for the eigenmode to be *not* invariant.

$$\Phi_g(K_h) - \Phi_h(K_g) \neq 0$$

$K_h$ is the reciprocal lattice translation needed after $h$ is applied

This pair of commuting symmetry elements along the XM face is met by the p4mg with i) the $C_2$ operation (allowed along XM) and ii) the glide plane lying on XM. Because of the glide mirror,
we are guaranteed that this difference is never zero, since the glide operation guarantees that the phase function is not zero by definition! These sticking bands therefore persist along the entire XM edge!

The same holds true for the p2gg structure, which has the same set of commuting symmetry elements each along the XM and X'M edges. We demonstrate the global robustness by further computing the band structures of two very different geometrical realizations of structures with p4gm plane group symmetry [Figure 3.20]. Indeed, the global properties of the p4gm symmetry do preserve the band sticking, invariant to the specific decorations of the Wyckoff position.

Figure 3.20 Computation of Band diagrams for two different structures with p4gm symmetry. (a) is topologically connected along the <11> directions whereas (b) is only connected on the fundamental building blocks. The material is chosen to be amorphous silicon (E=156GPa,ν=0.2152,ρ=2330kgm⁻³).
Band sticking is a nontrivial property and one might make the connection that in contrast to symmorphic groups, nonsymmorphic groups do not allow the factor group decomposition of the plane group as before since the translation subgroup is no longer an invariant subgroup because of the glide translation components. The net result of the glide operations requires in the irreducible representations acquiring an additional phase factor and one has to deal with what is known commonly as the multiplier representation. Despite the abstract formulation [59], it turns out that this phase factor is intimately linked to the fact that glide translations do not render the lattice invariant modulo reciprocal lattice translations, i.e. it is a gauge transformation. Importantly, this property further links the band sticking of the eigenmodes to extinctions in the Fourier spectrum decomposition of the eigenmodes [65,66]. Essentially for both situations, this phase factor given above must be nonzero modulo $2\pi$.

Based on this abstract reasoning, we highlight yet one more application of group theory, namely utilizing a specific Wyckoff decoration of the lattice to mimic the non-symmorphicity, or more specifically the property of sticking bands. We now highlight the mathematical equivalence between the band sticking and Fourier peak extinctions in the eigenmode fourier spectrum. We recall that the displacement (expressed in a reciprocal basis), under some symmetry operation of the group, may be expressed as follows:

$$u(g \circ K) = u(K) = (\exp(2\pi i\Phi_g(K)))u(K).$$

$\Phi_g(K)$ is the phase function of interest

In order for the equality to hold for all symmetry operations $g$, either $u(K)$ or the phase function $\Phi_g(K)$ needs to vanish. Earlier we stated that for band sticking to occur, the differences in the phase functions of two commuting elements needs to be non-zero. In our
case, this automatically requires the displacement field, u(K) to vanish at those K values. In order to mimic the sticking bands we thus need to design a geometric structure that fulfills this role. This is done by considering a p4mm structure, with a two ‘building-block’ Wyckoff decoration [Figure 3.21 insets] at [0 0] and [0.5, 0.5]. The choice of this decoration is such that it fulfills the glide operation as well, although in this case, the glide planes in a p4mm lattice are not part of the group generators and hence is distinct from a true nonsymmorphic lattice. Nevertheless, we are indeed able to replicate the sticking bands along the XM edge as shown [Figure 3.21]. It is important to emphasize here that this method of ‘mimicking’ is general as we have approached the problem from only the fundamental principles guiding the band structure formation; hence all geometric structures that fulfill our guiding principles will possess these sticking bands.

![Figure 3.21 Computed Band Diagrams of (a) p4mm structure with a cylindrical Wyckoff Decoration and (b) p4mm structure with a square Wyckoff Decoration. The material is chosen to be amorphous silicon](image-url)
The band sticking features here are invariant to the specific geometrical structures, as long as the Wyckoff decorations maintain the same structures at the (0,0) and (0.5,0.5) positions. However, a cautionary note is in order; this mimicking is not robust to minor perturbations in the two Wyckoff sites. As we shall see in chapter 4 (section 4.4), topographical perturbations that preserve the p4mm symmetry yet do not fulfill our extinction conditions will immediately destroy the band sticking.

3.6 Concluding Remarks

We outlined here the mathematical framework of group theory, which established the global principles governing the possibilities of the band dispersion relation. In addition, representation theory of the groups allowed the classification of eigenmodes into their irreducible representations. By identifying all spectral gap opening processes as avoided crossings and adopting a variational like approach, we are able to rationally control and design various features of the band structure. Most notably, we are able to augment spectral gaps and generalize various design principles within the same framework, utilizing the language of symmetry and conservation. We next discuss the actual dynamics of phonon propagation in these AS, which deals with the actual propagation behavior of phonons in these AS. It will turn out that the dynamics of phonon propagation actually address the question of matching the optimal physical topology of a structure, as well as choice of materials etc, for a particular phononic application.
Chapter 4. Classifications of Lattices: Physical Topology of Phononic Structures

4.1 Introductory Remarks

We examine the unanswered question of the choice of the physical topology of a phononic structure to achieve desired phonon propagation properties. To date, there is no framework which is general, i.e. does not rely on some specific geometry of the scatterers within the artificial structure (AS), and is capable of treating different types of fields, both vector (electromagnetic, elastic, etc) and scalar (acoustic) in a coherent fashion. Current approaches suffer from their specificity to certain types of geometrical structures, either due to some particular choice of calculation methods [67,68,18, 50], or utilizing physical models which are not transitive between fields possessing different polarization degrees of freedom. In general, one might consider the contrast in elastic constants, mass density, longitudinal and transverse velocities as possible parameters for controlling the size of the spectral gaps. However, there is neither a clear trend nor rational principle guiding the theoretical works, often leading to frustrations in attempting to elucidate a coherent principle to guide selection of the optimal topology for a particular structure for phononics, photonics or any wave in general. We argue here that this is due to several reasons. First of all, not all the above mentioned parameters are independent; velocities are strictly speaking, deduced values from the set of elastic constants and only hold for "homogeneous" media or for the inhomogeneous system in the geometric (short wavelength) limit. In isotropic media (at continuum length scales), the two independent elastic constants, along with the mass density determine the longitudinal and transverse velocities and this is only strictly true in the homogeneous limit or geometric limit for
inhomogeneous systems (within each of the homogeneous component materials). In considering phonon propagation at length scales where the phonon wavelengths are on the order of the structure or the material inhomogeneity, one needs to recognize that wave velocities are highly dependent on the details of the AS.

The homogeneous phonon velocities are physically meaningful only for two situations: 1) in the long wavelength limit ($\lambda \gg a$) where the phonon samples no perturbation in the structure, or 2) in the geometrical limit ($\lambda \ll a$), where the wavelength of the phonon is so short that one may physically consider it as a particle and hence one may associate a "particle" velocity with it within each homogeneous phase. At the intermediate length scales ($\lambda \sim a$), commonly known as the scattering/diffraction regime, which is of primary interest, we need to consider not just the velocity, elastic constants or mass densities separately, but instead the generalized energy flux at any interface, together with its physical wavelength, which depends on the local refractive index. In this situation, the detailed structure becomes crucial, due to proximity in the length scales between the phonon wavelength and the structure!

Recalling that we may deduce the relevant wave equation from the original momentum continuity equation, the conservation of linear momentum is assured for all length scales. This is the motivation for insisting on utilizing the conservation as the starting point of our discussion and development of the design framework. We now show that doing so makes the final developments to the framework totally transparent. In a linearly isotropic solid, the 3 elastic constants (two Lamé coefficients with two-fold degeneracy in the shear component) lead in general to 3 Goldstone modes and hence three polarizational degrees of freedom. The
flux of phonons through a region depends on their nature, i.e. the vector and scalar nature of the fields lead to disparate behavior in their propagation and it is this distinction that holds the starting point for elucidating the underlying design principles governing the choice of the optimal physical topology for phononic and acoustic structures! It will turn out that by only considering the “dynamic impedance” at an interface between two media, we are able to develop a concept of a “dynamical mechanical bond” to classify the nature of phonon propagation in various AS comprised of different materials in a general fashion. This leads to a classification scheme for phononic structures based on the spatial extent or degree of spatial (de)localization of the phonon eigenmodes. Structures are subsequently grouped between two bounding lattice classes, depending on the mechanical bond type. We will refer to these as the extended and tight-binding lattice classes. This lattice class classification allows one to select target structure designs that achieve different phononic properties, from large spectral gaps, negative refraction bands with both isotropic and super-prism type effects. In particular, we shall demonstrate large complete spectral gaps, indeed the largest ever reported in the literature, in both classes of structures as well as controllably induce negative refraction bands which are polarization specific. To be “complete”, we examine the typical solid-solid AS lattice classes before we deal with the solid-air AS lattice class, which is advantageous due to fabrication considerations. Despite a critical difference between the two types of structures (solid-solid vs solid-air/vacuum), the classification still holds true under an appropriate transformation.

For the rest of the chapter, we develop some structures possessing various unique phononic properties. The necessary criteria for achieving various properties is discussed for various
constraints on materials choice, and the particular type of application. Finally, we choose to demonstrate this with two distinct phononic AS, belonging, approximately speaking, to the two ends of our lattice classification spectrum. We modify these structures in an entirely coherent way, utilizing only the fundamental tools and framework which we have built up over the previous few chapters to show that indeed, this method of classification and framework developed enables an entirely rational method of designing a phononic structure.

4.2 The Dynamical Mechanical Bond

We emphasized the role which the normalized wavelength ratio ($\lambda/a$) plays in understanding phonon propagation. We've mentioned geometric and material inhomogeneity, the former deals with the situation that the structure plays a role vis a vis the boundaries; the latter is the more familiar case which we shall discuss shortly. The former, we've earlier mentioned is of second order importance as it deals with the exact geometry of scatterers in optimizing a specific functionality. There are however, intrinsic characteristics inherited by the phonon transport with certain topological features of the phases. This naturally leads to the concept of the matrix and the scatterer phase. We differ here from the ad hoc usage of the network vs cermet topology for the following reasons. This analogy was borrowed from the earlier photonic crystals work where one phase is always air; hence there is no ambiguity present in defining the non-air phase as either a disconnected (cermet) or connected (network) phase. In the case of phononic crystals though, there is no standard reference material phase, where the velocity is highest (as in light/vacuum~air), hence the naming of a cermet or network phase is further convolved by assumptions about the “scattering” abilities of each material phase. Using
this new methodology of naming, the cermet and the network topology is classified according to the impedance contrast between the matrix and the disconnected phase, with the definition of the two components only dependent on the physical topography of the phases, and not their constituent material properties. This separates the actual physical network topography from the intrinsic material parameters, which is a crucial distinction because in this situation; we do not make any a priori distinction on the type of transport based on the intrinsic material parameters alone because the actual problem involves considering both the physical topography and the material impedance contrasts before the dominant mechanism of phonon transport can be deduced, vis a vis our mechanical bond. Hence this method prevents us from making any invalid assumptions on phonon transport before trying to proceed to create optimal phononic structures for certain types of propagation behavior. In fact, this methodology and approach greatly extends the framework for choosing an optimal physical topography for a particular phononic structure for desired transport properties and is not limited to just spectral gaps, but is appropriate more for properties such as negative refraction or slow modes, i.e. all aspects of phonon transport.

The fundamental framework which we developed emphasized the need to recognize the correct length scales and the role of non-locality of the eigenmodes that result from either the symmetry of the structural design and from material choices. Now we address the complementary problem, that is, how does the physical topography of the structure affect its dispersion relations? Previous works have focused attention onto the choice of topographies that favored the appearance of complete spectral gaps [69]. However, from the concepts developed of avoided crossing as the primary underlying mechanism for creating spectral gaps,
as well as the relations between the space/plane group symmetries and the probabilities of optimizing a complete gap, it suggests that one would be able to create complete spectral gaps in structures with different topographies, both cermet and network type [Figure 4.1]. While this is indeed the case, the physical topography choice for the structure possesses a tremendously more fundamental significance. It controls the dynamics of phonon propagation, i.e. the actual propagation and group velocities of the eigenmodes. This has tremendous importance in determining the optimal lattice classes for phonon propagation, such as negative refraction, slow modes etc...

**Figure 4.1** Shows the geometric structures of a tight-binding and an extended-lattice structure respectively. A matrix is defined as a connected phase, while the scatterer phase is the disconnected phase. A darker colored phase indicates a larger impedance value, hence the geometric matrix in the tight binding structure has a lower
impedance. The corresponding eigenmode plot shows the typical trajectory of the strain fields, with high strains localized between the higher impedance scatterers. In contrast, for the extended lattice, it is clear that the strain fields are propagating through the matrix mainly, with some penetration into the scatterer phases. The color map indicates large (red) to zero (blue) displacement.

In previous works, the physical topography of the structure was only considered in dealing with the possibilities of opening a complete spectral gap, i.e. only within a specific normalized frequency range, which one associates readily with either the Bragg scattering regime or the resonant tunneling regime. This viewpoint suffers from several drawbacks, including the (now clarified) point that observed gap sizes are not necessary correlated with the particular bands bounding them and indeed may have nothing very much to do with those hypothesized scattering mechanisms supposedly accounting for the presence of the gaps!

Physical topography of the structure affects the propagation behavior at all length scales. It is the length scale, i.e. the wavelength of the phonon with respect to the physical structure that determines the scattering (type), and hence propagation behavior of the phonon in the different regimes. This implies that the eigenmodes of the phonon at some wave vector \( k \), takes on different displacement profiles with different frequencies. This displacement profile, or eigenvector, depends on the choice of the physical topography vis a vis the actual material constants and the physical geometrical interfaces and boundary/interface conditions, i.e. both the material and the geometrical structure. This eigenvector physically represents the trajectory of the phonon at some \( (\omega,k) \) within each unit cell; this is clear if we consider this from a \textit{variational} viewpoint, where each eigenvector can be mapped to an irreducible
representation that physically represents the trajectory of a phonon through each unit cell, showing how the energy propagates through the structure.

The eigenvector represents the dynamics of the phonon propagation that is manifested through the slopes (linearized group velocity) and the curvature of the bands (group velocity dispersion). The variational viewpoint develops the physical concept of our dynamical mechanical bond, by considering the spatial (de)localization of the profile of the eigenmode.

From a mathematical standpoint, a variational formulation [3] induces mathematically, for every eigenvalue problem corresponding pairs of eigenvalues and eigenvectors, from an energy minimizing perspective. Physically, each eigenvector corresponds to a normal mode, i.e. the displacement field profile of a phonon mode, at some (ω,k) of the dispersion relation ω(k). In all of these cases, we define the matrix phase as the connected phase, and the scatterers as the disconnected components.[see Fig4.1] The displacement field provides information on the dynamics of phonon propagation at each (ω,k): we see the phonon propagating within the structured medium and taking on either a delocalized strain field spread throughout the matrix, or possessing a more localized strain field, for example being concentrated between scatterers along its trajectory. Of course, there can be some modes that are hybrid in between these two extreme regimes.

These two situations are reminiscent of electronic structure and chemical bonding, with the delocalized, or “metallic-like” bond, and the localized, or directional “covalent-like” bond only now we are dealing with a dynamic situation where the nature of the bonds is reflected in the “dynamic” phonon eigenmodes which represent the dynamics of phonon energy propagation in
the medium. Let us give a physical interpretation of the dynamic mechanical bond which links directly to the familiar scattering and hopping mechanisms.

Each eigenmode determines the corresponding dynamics, or type of “mechanical bond “at each \((\omega,k)\); the dynamics varies depending on the particular phonon wavelength versus the length-scale of the structure. This length scale ratio affects the scattering cross-section as the phonon propagates through the structure. While, the (an)isotropy of this scattering cross-section certainly depends on the scattering resonance profiles of the scattering components and hence their actual geometric shape, this is of secondary importance compared to the dynamic impedance, which determines the nature of the mechanical bond. For phononic structures, the nature of the bond is exhibited most clearly by the dispersion of the particular band in question. An extended ‘metallic-like’ bond exhibits a somewhat more linear dispersion, indicative of its spatially-delocalized nature (this is distinct from the non-locality discussed previously). Microscopically, this indicates that phonon energy transport is favored primarily through the matrix, with appreciable strong perturbations occurring only at specific frequencies due to the resonant scattering of the particular scatterers. This situation is what we classify as the extended lattices (EL). Subsequently, a typical characteristic of this class of lattice structure is that the dispersion of the bands is typically linear with only strong perturbations of the bands due to band-band interactions at certain positions; these are where the spectral gaps typically (but not always!) form. Next, the geometry of the scatterers comes into play. Their arrangements in the structure, and the resultant point group and little group symmetries determine the anisotropy of the spectral gaps, negative refractive bands etc. At the other extreme, we have the localized, “directional” bond; we classify these structures as tight-
**binding lattices (TBL).** The dispersion shapes of the bands in TBL structures are typically flatter, indicative that the transport of energy typically occurs along directed/localized trajectories between scatterers in direct contrast to energy transport in modes that are delocalized in the extended lattice. In TBL lattices, the strategy for designing optimal structures is somewhat different and more flexible, in the sense that the dispersion relations can be tuned more readily from *local changes* in the geometric structure. In TBL, the local point symmetries of the scatterers as well as their physical connectivity, either through the matrix or through connected architectures of the scatterers. These two considerations effectively control the dispersion of the band structure of the material, as we shall show later in the chapter.

Viewed in this classification scheme, we may now understand that structures of different physical topology exhibit different types of dynamic phonon propagation behavior; two of these examples include the EL case, where mostly extended wave propagation with resonant scatterings of the entire structure at certain spatial correlations, this is commonly associated with Bragg scattering. The second TBL case, involves mostly localized, hopping mode wave propagation among scatterers i.e., resonant tunneling mechanisms with individual resonant scattering. These regimes can be continuously spanned from one to the other by appropriate changes to the structure. For example, a periodic structure which has some spatial disorder, or as a trivial example, taking the wavelength asymptotically to infinite (all extended) for a system which is initially tight-binding. The question concerns what metric do we use as the measure for the dynamic mechanical bond? First, we note that this description depends on the *matching or not matching* the number of polarizations between the two (or more phases) present. Thus for solid-solid structures, the dynamic mechanical bond can be defined generally.
regardless of the detail of the geometric structure, as long as the matrix and scatter phase has been defined. Solid-air structures provide a different situation for two reasons: 1) the number of polarizations differs across the solid-air boundary; hence the definition of the dynamical mechanical bond is not as straightforward and 2) the elastic contrasts of solid and air is so large that one may model the solid-air interface as a free surface [57, 2, 4] for propagation in the solid. In this situation, the type of physical topology is transformed onto the physical geometrical structure. However, this classification of the lattice type, now based on the actual geometric topography, is once again valid. This method of classification has been separately verified with Painter's work on opto-mechanical slabs [70], although it was not recognized that their studied structures were only one part of our larger classification scheme. This is covered in section 4.3; we now return back to the issue at hand.

The key need now is to decide which metric to use. This choice is related to the contrast between the elastic constants and mass densities. The details of phonon propagation within an inhomogeneous medium depend on a multitude of factors, listed previously in our framework (chapters 2, 3). However, in our previous works, we did not consider the dynamics of phonon transport nor how the choice of the component, i.e. and how the material choices affect the propagation behavior. This is crucial as this offers us the ability and insight to guide phononic structural design. The metric in this case is the impedance contrast between the matrix and the scatterer phases; with the impedance is given by $Z^i = \rho v^i$, where $i$ depends on the particular polarization being considered. The concept of the impedance turns out to be quite fundamental and together with the refractive index, forms an alternate set of dynamic variables, conjugate to that of the elastic constants and mass density [71,14,72].
Hence, the choice of which pair of dynamic variables to use then depends on the particular problem we are concerned with. Recalling the equations of the conservation of linear momentum, as well as the values of the reflection and transmission coefficients at a flat interface between two media [57], we find that the fundamental quantity of interest is that of the flux of a generalized linear momentum, expressed naively as $\rho v$. The dynamical bond concept applies equally well in structures consisting of two solid phases, solid-fluid phases as well as solid-air phases, with the proviso that we have to adjust the corresponding terms in the continuity equation to account for the changes in the polarization degrees of freedom. The utility of the concept of the dynamic mechanical bond lies in its general applicability. The reason is the following: the relevant phases (matrix and scatterers), and their roles are determined by the dynamic impedance, and hence the dynamic impedance contrasts, which we define as:

$$\Delta Z = Z_{\text{matrix}} - Z_{\text{scatterer}}$$

The dynamic impedance contrast automatically determines the lattice class that the structure lies in. For solid-solid structures, we demonstrate explicitly now that by simply controlling the dynamic impedances that we may continuously tune the behavior of a given structure from an extended lattice to a tight-binding lattice. For generality, we have kept the geometric structure to be a simplistic p4mm plane group [Figure 4.2].
Figure 4.2 Computed band structures computed with the same geometrical structure (inset), but sweeping the impedance contrast, defined as $\Delta Z = Z_{\text{matrix}} - Z_{\text{scatterers}}$. (a) tight binding lattice ($E=10\text{GPa}, v_r=0.2, \rho=1300\text{kgm}^{-3}$), with $\Delta Z < 0$, has relatively flat dispersion in the higher order bands (above the first band gap) (b) the homogeneous case $\Delta Z = 0$ ($E=156\text{GPa}, v_r=0.2, \rho=2330\text{kgm}^{-3}$), is the reference to show the unperturbed dispersion relation, taking into account the Brillouin zone reduction into the IRBZ and (c) the extended lattice case, $\Delta Z > 0$ ($E=400\text{GPa}, v_r=0.2, \rho=7800\text{kgm}^{-3}$). The dark colored phase is always set here to be silicon, and is our reference material. The color map indicates large (red) to zero (blue) displacement.

By keeping the geometric structure constant, we varied the material composition, keeping the scatterer phase constant with silicon parameters in all these cases and computed three exemplary band structures corresponding to the 2 bounds of the classification scheme, with the homogeneous case as the neutral reference. A few qualitative features are immediately apparent: note in Figure 4.2(a) the flat dispersion in the bands above the region where the phonon wavelength approaches the structural length scales ($\omega a/c \sim 0.5-0.6$), in agreement with the TBL picture. In contrast, in Figure 4.2(c), the higher order bands have quasilinear dispersion. Part of this is obscured by the subsequent avoided crossings occurring between these higher order bands between $\omega a/c$ of $\sim 0.8-1.2$. As we have learned, it is instructive to
examine the symmetries of eigenmodes themselves to observe the phonon trajectories and to check for possible interactions.

Figure 4.3 Time evolution of phonon propagation in the same band (band 5) in the tight binding lattice (a,b,c,d), the homogeneous reference(e,f,g,h) and the corresponding extended lattice(i,j,k,l), all at k= (0.7π/a,0). The time
steps are taken at (i) \( t = \pi/6 \), (ii) \( t = \pi/3 \), (iii) \( t = \pi/2 \), (iv) \( t = 2\pi/3 \). The corresponding band structures are shown in Fig4.2(a), (b) and (c) respectively. The color map indicates large (red) to zero (blue) displacement.

Figure 4.3 plots the corresponding time evolution of the 5th bands for all of the three band structures. We observe that (a) to (d) shows the evolution of the phonon eigenmode at \( k(\pi/a) = 0.7 \) with time. In the TBL, the momentum transport is clearly hopping like, being localized primarily in the scatterer phase, and hopping between the scatterers through the matrix. This gives rise also to the characteristic slow group velocity of these modes. The homogenous case clearly shows no perturbation of the eigenmode, with only the profile showing its associated material wavelength(\( \lambda \sim 0.5a \)). In contrast, from the EL, the transport takes place primarily through the matrix, being only slightly perturbed by the scatterers. This is clear when comparing with the unperturbed, homogeneous case given in (e,f,g,h), where the evolution in (i,j,k,l) becomes clearly the case of extended transport with some perturbation from the scatterers. This gives rise to the quasilinear dispersion that is more characteristic of the extended lattices. We note that this behavior is generic among all the bands, provided that we are not in some resonant tunneling or scattering regime. The tight binding situation in (a,b,c,d) shows behavior remarkably different even though we are dealing with the same respective band and working in the same normalized wavelength ratio, showing a very clear transition in the propagation behavior from the extended to the tight-binding nature.

It is clear that to develop a physically accurate framework of the dynamic mechanical bond, the classification scheme employed needs to be lucid and consistent. To verify that it is only the impedances and the associated refractive index which determine the dynamics of phonon propagation, we next take various combinations of "particle (geometric limit)" velocities,
densities, parameters loosely associated with the scattering cross-sections, while maintaining the same overall impedances in each phase to show that ultimately, it is the impedances are the crucial parameters determining the classification.

![Figure 4.4 Computed band diagrams for the same geometric structure, but with different elastic parameters for the constituents. Both structures are chosen to have zero impedance contrast between the two phases. (a) the structure consists of a matrix with higher density but lower elastic moduli, and hence lower velocities whereas (b) consists of a matrix with lower density but higher elastic moduli, and hence higher velocities. This is to juxtapose against conventional methods whereby selected subsets of density and/or elastic contrasts are utilized. In both cases, the time evolution of the eigenmodes of the 5th band are shown in (i),(ii) for (a) and (iii),(iv) for (b). It is instructive to note that in this case, that the propagation looks very similar to the homogeneous case, and the transport essentially occurs through both phases and hence is neither extended nor localized like. (a) utilized hypothetical values of E=78GPa, \( \rho=4660\text{kgm}^{-3} \) while (b) utilized hypothetical values of](image-url)
E=312\,\text{GPa}, \, p=1165\,\text{kgm}^{-3}. \text{ For both systems, the poisson ratio was matched to that of Silicon, which was utilized for the scatterer phase.}

We first demonstrate this for the same geometric structure as above, but changing the material parameters of the matrix phase, choosing (a) a higher velocity phase, with higher density but lower elastic moduli and (b) a lower velocity phase, with lower density but higher elastic moduli. Note, we have purposely kept the impedance contrast for both cases to be zero. What is perhaps most striking immediately is that the dispersion is linear for most of the bands, quite similar to that of a homogeneous medium, despite the obvious differences between the elastic constants; we also chose two "opposite" cases to demonstrate the generality of the impedance. The number of bands within the structure does depend, of course on the velocity in each of the phases, but we are concerned with the dynamics of the propagation, which is crucial for our structure. By comparing the time evolution of the 5th band in each structure at \( k=(0.7\pi/a,0) \) for Figure 4.4 (a) (i,ii) and (b)(iii,iv) we note that their propagation trajectory is very similar to the homogeneous case [Fig4.3(e,f,g,h)]. This gives strong evidence that indeed the physical parameter that controls the dynamics stems from the physically motivated impedance, which is actually a generalized form of the linear momentum. To complete the picture, we will do the same for the TBL and EL lattice cases, whereby we retain the same impedance contrast as in Figure 4.3(a) and (c) but we utilize a matrix with higher velocities than the silicon scattering phase.
Figure 4.5 Computed band diagrams for the same geometric structure, but with different elastic parameters. (a) is a tight binding lattice, but with different elastic parameters that contrasts that in Figure 4.2. It consists of a matrix with higher wave velocities whereas (b) is the extended lattice, consists of a matrix with higher wave velocities as well. This is to contrast with the structures computed in Figure 4.2, where the matrix was chosen to have lower velocities. Time evolution of the 5th mode at \( k=(0,7,0) \) were also plotted for the TBL structure (a) (i,ii) as well as for the EL structure(b) (iii,iv). The time steps were taken at \( t=\pi/3 \) and \( t=2\pi/3 \) for both cases.

From (i),(ii), which illustrate modes belonging to the 5th band of Fig4.5(a), we see that the transport remains invariantly tight binding like, as demonstrated by the concentration of the high displacement regions of the fields within the scatterers with hopping between scatterers. In comparison, in (iii),(iv), belonging to Fig4.5(b), we see that the transport is similar to that of Fig4.2, which is extended like, with transport taking place primarily within the matrix, and only
weak perturbations due to the scatterers. This shows that the determinant parameter for controlling the dynamics depends on the impedance, which is related to the flux of phonons, and not independently the elastic contrasts or density contrasts alone, nor does it depend on the velocity contrasts by corollary, as demonstrated.

In summary, we have shown here that it is the dynamic impedance, essentially the linear momentum, that is the physical parameter which determines, via the impedance contrast between the constituents, the dynamics of the phonon propagation. In order to be able to rationally design a phononic structure for a particular function, it is crucial to know the dynamics of the phonon transport partly because the type of scattering and interactions that lead to the desired properties depends on the very dynamics of the interactions! To illustrate this further, we reprise again the original band structures computed in Figure 4.2(a) and (c). We observe that both of these structures have complete in-plane spectral gaps, bounded by the 6th (lower) and 7th (higher) bands. However, the mechanisms of the spectral gap opening vary greatly in each case. In the TBL case, while the 6th band undergoes an avoided crossing at the Γ point, while the 7th band, which is the upper bound on the spectral gap, does not. This is also clear from their points of inflexion, forming what they call an indirect spectral gap. An important conclusion that can be drawn from this is that the spectral gap size is then not dependent on the scattering mechanism directly, since the two bands bounding the gap sizes are not the two interacting bands! This is also quite clear from the symmetries evident in the irreducible representations of the eigenmodes of the 6th and 7th bands along ΓX. In contrast, for the EL [Fig4.2(c)], the spectral gap forms from an avoided crossing between the 6th and 7th
bands at $k=(0.5\pi/a,0)$ and $k=(0.5\pi/a,0.5\pi/a)$. This is clear from the fact that their irreducible representations are the same (see Figure 4.6(c), (d)).

Figure 4.6 The eigenmodes of the two bands bounding the spectral gap at $k=(0.4\pi/a,0)$ in Figures 4.2 (a) TBL and (c) EL. For the tight binding lattice, band 7(a) (antisymmetric about $\sigma_x$) and band 6 (symmetric about $\sigma_x$) (b) have different irreducible representations. This implies that while these bands comprise the physical bounds for the gap size that avoided crossing did not occur between these two bands and hence the scattering strength is
not responsible for the gap size in this situation. This is more common in tight binding lattice classes, where the multiple high order bands (>9) cross each other in (ω,k) space readily. In contrast, for the extended lattice, the gap size is clearly delimited by the avoided crossing occurring between bands 6(d) and 7(c). Another important point of note is that the interaction between the bounds occurs within the BZ, and not primarily or exclusively at the edges or boundaries.

In general, the actual mechanism of the linear phonon propagation through the medium depends on the wavelength of the phonon, the spatial correlation within the structure, the material components. These are all coupled into the variational formulism, which describes the trajectory of the flux of linear momentum within the domain, subject to all of the above constraints. The corresponding (λ, |λ⟩) pairs automatically set for each wavelength range (eigenvalue), the corresponding trajectory (eigenvector), based on the energy minimization. By deriving the elastic wave equation from the initial continuity equations, the problem is mapped to a variational problem. It is also this recognition that allowed us to recognize that the physical parameter or variable, which is governing the evolution of the eigenmodes, is actually the flux of linear momentum itself as modified by the impedance contrast of the structure. This is exactly why, from just considering the intrinsic material parameters that one may deduce the nature of the trajectory of phonon transport and classify the lattice types based on that. Especially key to our distinction over prior work is that we recognize the need to decouple the material contrast issue from the geometric structure issue; our assignment of the matrix and scatterer phase is geometry dependent only, not material dependent. This assignment depends on the connectivity of the geometric structure, with the connected phase always being assigned as the matrix phase. Once these assignments have been made, we then judge the dynamics of the phonon propagation, based on the materials parameters, which is reasonable,
but only in the form of the linear momentum flow, or the impedance because based on the variational perspective, the momentum flux is actually the quantity being "diagonalized" or projected out into orthogonal modes to form all the eigenmodes of the system and build up the band structure. This is our rationale for the choice of impedance as the only physical parameter related to the material choice.

4.3 Specialization for Solid-Air/Vacuum structures: An exercise in symmetry breaking and the high impedance limit.

We mentioned earlier that in the case for typical solid-air systems, that due to the extremely high impedance contrast, for the solid matrix case we may essentially ignore coupling to air (impedance contrast ~99.994% for silicon). In this situation, the solid matrix now forms the effective propagating medium which we are interested in; hence the concept of the mechanical bond needs to be recast into the geometrical structure itself. The concept of the mechanical bond is actually more intuitive from the structure itself, because the bonds are now actually physically manifested through the structuring of the system. This is illustrated clearly below (Figure 4.7) with the complement of the original p4mm structure previously dissected.
Figure 4.7 shows a family of structures with p4mm plane group symmetry. The motifs are non-primitive, occupying Wyckoff positions at (0, 0) and (0.5a, 0.5b), with a=b. From left to right, we increase the size of one of the building blocks, from small(a) to degenerate(b) to larger(c). The solid dark phase is the matrix phase, and the white regions are the air/void phase. The red circles outline the mechanical 'connections' forming the actual geometric mechanical bonds of the structures. The material is chosen to be amorphous silicon (E=156GPa, v=0.2152, p=2330kgm⁻³).

In this series of structures, we retained the plane group symmetry but we varied the building blocks, such that we slow increased the size of the building block at the (0,0) and equivalent positions. We observe the evolution of the band structure from having a more extended lattice character in(a), to the gradual flattening of bands which meet the length scales of the structures, in (b) and subsequently in the TBL (c). In all three cases, the avoided crossings result in the formation of the complete spectral gap from the 6th and 7th bands. What is perhaps more interesting of note though is that the avoided crossing takes place at different k values in (a) compared with (b) and (c), the latter pair of which take place at the Gamma point. Without the utilization of the avoided crossing framework, it could be falsely assumed that the gap formation is due to interactions between different pairs of bands. In this regime, the
mechanical bonds are manifested through the connections between the building blocks geometrically, since the high impedance contrast between the constituents indicates that mode propagation will occur essentially only through the solid matrix phase. We compare the time evolution of the 6th and 7th bands which form the spectral gap bounds and are actually involved in the spectral gap opening [Figure 4.8 and 4.9]. The time evolution is given by (i,ii,iii,iv) of all three structures for the 6th band. We note that as the mechanical connections become smaller, this implies that the transport is constrained to become more and more localized; the tight binding nature actually manifests more intuitively, as the large displacement regions of the eigenmodes progressively become more and more localized between the building blocks and resemble a bonding-type orbital as we move from (a) to (c). We observe the same trend with the 7th band of the three structures [Figure.4.9].
Figure 4.8 Eigenmodes displaying the time-evolution for the 6th band, which bounds the spectral gap from below at $k=(0.4\pi/a,0)$ for all 3 structures, labelled as (a), (b), and (c) as per original convention. The time evolution is given by 4 exemplary time steps at (i) $\pi/6$, (ii) $\pi/3$, (iii) $\pi/2$, (iv) $2\pi/3$ respectively.
We also note a more subtle effect as we geometrically alter the structure. In comparing the pairs of bands 6 and 7 for structures (a) to (c), we notice that the eigenmodes show significant increase in the spatial localization as we move from (a) to (c). In fact, those familiar with chemical bonding might note that the eigenmodes in (c) represent bonding and anti-bonding combinations of each other, if we viewed each building block as the "atom" and the mechanical connections as the bonds (as outlined in Figure 4.7 insets). That this manifests itself even at nonzero k highlights the increasing tight-binding nature of the lattice. In comparison, the eigenmode in (a) is much more delocalized spatially; this is clearest in Fig 4.9(a), where the propagation is essentially extended-like, markedly different from (b) and (c), where the momentum transport is localized around the connections in a tight-binding fashion.

From a fabrication and technological perspective, it is advantageous to be able to design and fabricate phononic structures which only require one material, i.e. solid-air systems. This is obviously due to fabrication considerations if one has to scale the structures down to smaller scales and is the reason why most of the recent demonstrations of novel behavior in phononic/acoustic crystals have been demonstrated at larger scales (mm scale or larger). To date, there is no procedure available to design targeted phonon transport, be it a simple acoustic wave or a mixed mode within the solid. Hence it was unclear whether solid-solid systems are even necessary to obtain desired phonon propagation behavior! Solving this puzzle is our rationale for seeking the governing rules for the dynamics of phonon propagation, as this complements our universal framework for the complete rational design of phononic structures. Based on the previous demonstrations, we have "abstractly" distilled our requirements for the phonon dynamics in terms of the lattice or topography class. This provides guiding principles
for applications requiring considerations on the specific dynamic propagation of key modes, e.g.
negative refraction, slow or fast modes of propagation. By showing that this classification can
be renormalized with both the most generic solid-solid lattice structure as well as the solid-
air/vacuum structures, we are able to reduce the dynamic requirements to a single material
platform system, which is extremely favorable from technological considerations as well as
scalability.
Finally, with the correct renormalization of the lattice classes into the solid-air/vacuum cases,
we are able now to design structures with desired dynamics based mainly on geometric
considerations, not the particular choice of material combinations. This leads us to then
implement our universal design framework which will enable rational design for almost all
desired forms of phonon propagation behavior. We now illustrate, using structures belonging
to both the EL and the TBL classes i) structures with polarization specific negative refraction
bands with low group velocity in a "fast" EL system, ii) an anisotropic structure which has a
higher transverse like velocity than longitudinal velocity and finally iii) a TBL structure which
possesses the largest complete spectral gap known so far (by a factor of 2-fold).
Figure 4.9 Eigenmode plots displaying time-evolution for the "7th" band, which bounds the spectral gap above at $k(p\pi/a)=0.4$, for all 3 structures, labelled as (a),(b), and (c) as per original convention. The time evolution is given by 4 exemplary time steps at (i) $\pi/6$, (ii) $\pi/3$, (iii) $\pi/2$, (iii) $2\pi/3$ respectively. It is clear that the transport trajectory gradually becomes more and more localized as the four diagonally aligned mechanical arms,
connecting the four building blocks become more and more narrow. In solid-air/vacuum systems, the phonon propagation behavior is determined by the geometric structure. In this situation, there is an additional subtlety in the appearance of the eigenmodes. In this case, the formation of the eigenmode mirrors that closely of that in "molecular orbital " theory. Here in this case, one sees clearly that the eigenmodes resemble the antibonding type orbital, which gets more spatially localized and hence more tight binding like, as we move from (a) to (b).

4.4 Linking the Physical Topography to the Applications

The reasons for the concept of a dynamic mechanical bond are manifold. One is to search for a simple classification parameter that highlights the role of the material parameter, i.e. one that is physically relevant. Previous pioneering works overly relied on the identification of different terms of a similar equation (e.g. Schrödinger equation), resulting in inferences that are sometimes incomplete [69,16,67].

The second reason for this method of classification of the lattice via the strength of the bond, while borrowing from the foundations of the concepts of elementary solid state theory, is that it is physically intuitive in allowing the researcher to choose what kind of structures, and in which combination, to design and fabricate their structure for a particular application, this is especially true in solid-air systems. Different examples of desirable applications include for example, the ability to achieve effective negative refraction, extremely large spectral gaps, as well as to provide a platform for studying nonlinear as well as defect interactions.

One would prefer relatively linear dispersion with negative refraction and thus it becomes highly advantageous to have extended state like bonds, i.e. an EL structure to ensure efficient
negative refraction behavior. At the same time, in order to produce a large spectral gap, it is less clear which class of lattice would produce an outright superior candidate for the champion structure. In the next section, we obtain structures with large spectral gaps, utilizing both categories of lattices. The complete gaps we design are much bigger than what is currently demonstrated in the literature. In this situation, the tight-binding lattice outperforms the extended lattice. However, we note there that the common physical mechanism underlying the large spectral gap is that the resonant mode of the geometric scatter lines up with the frequencies at which the Bloch symmetry (Bragg resonance) is in effect.

4.4.1 The Extended Lattice: Rational Design of Polarization Specific Negative Refraction Bands

The nature of the bond between scatterers controls the character of phonon propagation behavior ranging from a delocalized, extended bond type to the localized, tight-binding type bond, with an entire continuum of behavior in between these limits. Mathematically, the bond nature determines the spatial dispersion of a band, i.e. its dependence on the wave-vector; physically, this translates into the propagation velocity of the eigenmodes of the structure. This is an important factor to consider when designing a structure for a particular functionality. For example, to design a structure that possesses a large spectral gap within some frequency region, but otherwise quasi-linear dispersive behavior for propagating modes, we would likely choose a structure that is belongs to the extended lattice class. On the other hand, for a structure to possess multiple slow-group velocity modes, a tight-binding lattice is preferred. To the best of our knowledge, this classification of different structures has not yet been recognized
so the design of precious structures has not been guided nor optimized for the particular functionality. For example, in negative refraction, what has been commonly done is to pick the second band which is related to the 2\textsuperscript{nd} BZ as the negative refraction band. Depending on the band structure, one may or may not be able to have a complete region in the entire (w,k) space with only the desired negatively refracting bands, i.e. you might get undesired losses from mode mixing. There is not much control over the design of this propagation behavior in this sense. An additional complication arises from the fact that it is not always clear that a high order band immediately implies negative refractive behavior; we need to understand the details of the dynamic behavior of the eigenmodes to be able to verify this behavior.

To demonstrate a rational way of designing specific functionality in certain dispersion bands, i.e. to truly mold phonon propagation behavior, we need to demonstrate that we are able to specifically insert certain bands with characteristic propagation behavior and to be able, as well, to control their vector polarization. We first demonstrate this control using a 2D extended lattice of solid/air. We opt to control the flow of phonons in their full vector nature through the solid as opposed to structures where the solid phase forms only discrete perturbing scatterers, and the scalar fluid is the main propagating medium. We will first create a structure that possesses a large complete in-plane spectral gap of \(\sim 80\%\); it also possesses a complete spectral gap of 72\%, which is larger than what has been obtained in the literature currently, to the best of our knowledge.

Our EL design is implemented in a square lattice that possesses the maximal (for the square lattice) p4mm plane symmetry. By choosing to utilize only a single monolithic material, our
designs are amenable to scaling and not reliant on specific material combinations and rely only on the specific material geometry and are thus materials property tolerant.

![Diagram](image)

**Figure 4.10** Computed band structures of two structures with the same p4mm plane group symmetry, but with a deliberate change in the connectivity/topology between the two structures. Both structures belong to the extended lattice class, which is exemplified by their quasilinear dispersion bands, some of which are obscured by the avoided crossing by designed flat bands. In this work, we started deliberately with a structure with a large complete spectral gap (a), before we rationally induced pure negative refraction bands by increasing the
connectivity of the structure (b, inset). This has the net effect of "pulling" the 4th to 6th bands into the original gap position to form negative refracting bands. These negative refraction bands are distinct from conventional systems in that these negative refracting bands have low group velocities, by virtue of the way in which we induce them. The material is chosen to be amorphous silicon (E=156GPa, v=0.2152, ρ=2330kgm⁻³).

We start with structure (a), which possesses a complete in-plane spectral gap of 80%. The resonant scatterers are placed at the family of \{0.5a, 0.25a\} Wyckoff positions, on one set of mirror lines. The choice for the geometric motif maximizes the avoided crossing interaction.
Figure 4.11 Eigenmode plots showing the corresponding pairs of bands that interact to form the lowest spectral
gaps. For structure (a), the bands undergoing avoided crossing are the 13th(a,(i)) and the 6th(a,(ii)) bands. For
(b), the bands undergoing avoided crossing are the 8th(a,(i)) and the 3rd(a,(ii)) bands. It is a common mistake to
associate the corresponding bands by their band number, rather than their actual nature, which is given by the
dynamics of the eigenvector. In this case, the band numbers have changed because of the connectivity change
between the two structures, which introduces a number of extra flat bands in (a) that interact with the
"original" extended type bands (with quasi-linear dispersion), hence obscuring the band structure at first glance.
We note that the absolute method by which to identify the correct bands which undergo the avoided crossing
and hence, are responsible for the spectral gap formation is to classify them according to their irreducible
representations. In fact, it is clear from their eigen-modes that these two corresponding pairs of bands are the
same corresponding pairs of bands, with only the change in the connectivity perturbing the actual eigen-values
slightly. The effect of the change in the connectivity has much greater effect on the flat bands, or slow modes,
which is the purpose of this geometric connectivity change.

which is coupled to the Bloch Condition, hence it is resonant in nature, and leads to the large
interaction. For structure (a), this arises from the choice of the connected cylinders, which
creates a hotspot for localization of strain energy (see Fig4.11(a,i)), this has the effect of
lowering the eigenfrequency of the corresponding 3rd band for structure (a). The same
situation occurs for the upper band of the pair [Figure 4.11(a,ii)], with the higher band having
the same irreducible representations, and also having the strain energy localization
characteristics. The level splitting due to the avoided crossing stems from the topological
feature which provides the localization over the orthogonal corners.

Hence our choice of topography consisting of connected cylinders is to create the presence of
multiple low group velocity modes, i.e. relatively flat bands. The reason for this occurrence
Figure 4.12 Eigenmode plots showing the strain field evolution of the (a) 6th, (b) 5th and (c) 4th bands of structure (a) and (e) 6th, (f) 5th and (g) 4th bands of structure (b) as we increased the connectivity in order to create negative refractive bands. The color map indicates large (red) to zero (blue) displacement.
stems once again due to our introduction of topographical cuts to link the cylinders with orthogonal channels, which allows for multiple localized modes which serve to localize the strain energies at the free surfaces, as shown earlier in sections 3.3.

We then choose to geometrically induce a distortion by increasing the “connectivity” of the structure; this intuitively leads to an increase in group velocity in selected bands, forming our negative refracting bands; as previously shown, the mechanical connectivity is directly related to the resultant momentum flux and hence its spatial extent of (de)localization, which was discussed in some detail in the earlier sections; hence we have induced locally in space, a reinstatement of the connectivity to 4 once again. These negative refracting bands are also polarization specific, i.e., these are negatively refracting polarization bands. This approach is different from current approaches of “producing” negatively refracting phononic crystals, in that we first create a structure with a large complete spectral gap by utilizing an extended lattice structure. We then induce specific negative refractive bands into this spectral gap by geometrically increasing the connectivity of the structure. This maintains the size of the spectral gap while selectively modifying the behavior of specific bands. To be precise, we control their dispersion and hence make them negatively refracting. This ensures the formation of a “clean” negative refracting region, since we have formed these bands in a spectral gap. The ability to retain polarization persistence in the bands stems as well from our increase in connectivity of the structure while retaining specifically the point symmetry of the structure (4mm), this ensures that the increase in connectivity does not lead to mode-mixing, which would then destroy the polarization specificity. Intuitively, one notes that in structure (b), the
transverse and longitudinal modes “see” the same structural rigidity and hence do not mix to form new eigenmodes.

We note that these three negative refracting bands are physically derived from the originally low-lying bands 4 to 6, since the number of modes must be conserved. The only difference here is that we have increased the connectivity of the structure and the spatial (de)localization of the mode; this of course increases the group velocity of the bands as well. The polarization persistence is shown clearly here [Fig4.12].

We can visualize the physical process as follows. In (a), these flat bands were localized modes which effectively had zero group velocity and they are formally present due to the topology of the structure which induced the localized modes due to the presence of the extra boundaries. One notes that in (a), the three modes were respectively symmetric ((a),(c)) and antisymmetric (b) with respect to \( \sigma_x \). However, we note here that in (b), by increasing the connectivity of the structure, effectively will induce spatial dispersion to these very same modes (The interfaces for strong localization of energy cannot be sustained), one visualize this connectivity increase as the inclusion of addition mechanical bonds, hence leading to coherent extended modes. Another interesting point of note is that, this connectivity causes modes 4(c) and 6(a) to mix, forming the new modes (d) and (f) through bonding and anti-bonding combinations. This leads to the formation of polarization persistent negative refracting bands for transverse (antisymmetric) and longitudinal (symmetric) polarization phonons. This tailored method of inducing negative refracting bands allows for efficient coupling of incident beams into negative refracting channels for solid elastic waves, which is something that is not trivially achieved in considering structures with full vectorial fields. To date, there has been no rational way of
controlling the polarization persistence in solid phononic metamaterials, to our knowledge. In fact, due to the previous lack of knowledge as to how to actually deal with the vector phonon field that this control of polarization for individual bands has not been attempted or was not successful. Finally, to demonstrate that the 4th and 6th bands are indeed polarization persistent, we show the time evolution of these bands below [Figure 4.13].

![Figure 4.13](image_url)

Figure 4.13 Eigenmode plots showing the time evolution at (i) $t=0$, (ii) $t=\pi/2$, (iii) $t=\pi$, of the 4th and 6th negative refracting bands of structure (b). All of these plots were taken at $k=(0.3,0)$. It is clear that these two modes preserve their polarization generally as transverse-like (anti-symmetric) and longitudinal-like (symmetric) along the GX direction. This is only possible by controlling the starting symmetries of the two flat modes in structure(a) before increasing its propagation velocity by increasing the connectivity in a rational way to permit transport.
We demonstrated here a series of principles which we applied rationally in order to create a desired propagation behavior. By choosing the initial topology of four connected cylinders, we created a structure with a large spectral gap to start. More importantly, the choice of the connected topography was to induce multiple localized flat modes, which we will subsequently tailor. This is done by changing the dynamics of the phonon propagation by utilizing an increase in their bond connectivity. We recall that in solid-air systems, this connectivity shapes the bond nature of the lattice and hence, the associated propagation velocities. The net result of this is in the creation of three negative refracting bands, of which two are polarization specific negative refracting bands. To date, this is the first known rational design of polarization refractive bands in a solid phononic metamaterial. We follow this by introducing the design of a nonresonant metamaterial which is anisotropic in its long wavelength properties. In particular, we seemingly defy the common knowledge of a homogeneous medium limits, by creating a structure which has a higher transverse than longitudinal velocity along one direction but behaves normally in the other principle direction.
The two structures computed here belong to the second extrema of the lattice classification, that of the tight binding lattices (TBL). In this end of the classification scheme, we note that as is typical of tight binding lattices, that the dispersions of the bands are mostly flat (once the phonon modes can sample the structure, i.e. beyond the first two bands). Keeping the building blocks invariant, we geometrically perturb the structure by increasing the size of the connections, which translates essentially into increasing the mixing and interaction between the building blocks. Physically, the increase in the size of the connections implies an increase in the "mechanical" bond between the building blocks. Mathematically, the increases the non-locality, and hence by extension, the wave-vector $k$ dependence; this leads to a gradually

\( \text{(a)} \)

\( \text{(b)} \)
Figure 4.14 Computed band structures of the tight binding lattice structures. (a) possesses the largest known in-plane complete spectral gap of 105% (b) possesses a smaller complete in-plane spectral gap of ~ 60%. The material is chosen to be amorphous silicon (E=156GPa, v=0.2152, ρ=2330kgm⁻³).

quasilinear dispersion in the 5th and 6th bands. As the mechanical coupling has increased, the transport becomes less localized to the building blocks and delocalizes itself more significantly in the connections between the connecting blocks. We first examine this disparity by considering the corresponding pairs of bands that are involved in forming the spectral gap (fig 4.15). In this particular structure, the bounds of the gaps are indeed derived from the BZ boundaries, being given by the (5,8) and (6,10) pairs at X and (5,13) and (6,14) at the M point, as clearly shown [Figure 4.15]. However, we need to note here that, even so, the corresponding pairs of bands involved in the interaction processes belong to different pairs of bands at the X and M point respectively. At the X point, the interacting pairs of bands are (5,8) and (6,10). This second pair is not intuitively obvious because avoided crossing has occurred between bands 8 and 9 (at k~0.7π/a), hence 9 does not reach X with zero slope; instead the 10th band is the corresponding interacting band. This is lucid from their Irreps, by considering their symmetry with respect to a C₂ operation (which lies in the little group at the X point).

In comparison, at the M point, we note that the first 6 bands all have undergone avoided crossing at or near the M point; hence they enter M with zero slopes. This contrasts the situation along GX [Figure 4.14] where the first 4 bands join pair wise at X at non-zero slopes. Hence at the M point, the corresponding interacting band pairs are (5,13) and (6,14), because their Irreps are symmetric w.r.t to the mirror planes along GM. We see in all of these cases
how the Irreps of the eigenmodes are required to correctly classify the interactions leading to the spectral gap formations.

Figure 4.15 Eigenmode plots showing the corresponding pairs of bands that have undergone avoided crossing in order to create the complete spectral gap for structure (a) at the X and M points. The color map indicates large (red) to zero (blue) displacement.
To emphasize the role which the dynamic mechanical bond plays in controlling the dynamics of phonon propagation, we once again compare this with another structure whereby we introduced physically increased the coupling between the building blocks, hence making the original TBL more and more extended-like to verify this model. By comparing the band structures between the two structures [Figure 4.14], we witness the first changes in the 5th and 6th bands in (b) compared with (a), with the development of a more quasi-linear dispersion. That this is due to the increase in coupling between the building blocks can be observed from the eigenmodes again, not so much from their irreducible representations [Figure 4.16]. We show the eigenmodes at the Γ point for the pairs of bands (3,4) for (a) and (4,6) for (b) because these pairs of bands are the corresponding pairs for each structure. As we are at the Γ point, these eigenfrequencies are local, i.e. they are independent of $k$ (since $k=0$). We note here that for tight binding structures, as the name sounds, that we see that we may regard the pairs of bands highlighted here as bonding and anti-bonding combinations of the individual building blocks, or odd and even combinations of each other. It is also important to note that this method of “diagonalization” of eigenmodes for a two level Hamiltonian is only permissible where $k$ is not a parameter. Actually it is also strictly not valid in a lattice because of the discrete translational symmetry at the reciprocal lattice points as well; however in the weakly local limit of these two bands, this picture is semi-quantitative. In fact, the specific form of the eigenmodes exactly replicates this local, or tight-binding like nature. In comparison, for structure (b), the eigenmodes are markedly different in appearance. For structure (b), which has a larger coupling constant, we
Figure 4.16 Eigenmode plots comparing the 3rd and 6th bands at the $\Gamma$ point of structures (a) and structure (b) respectively. The color map indicates large (red) to zero (blue) displacement.
Figure 4.17 Eigenmode plots at the X point, for the same pairs highlighted in Figure 4.16. By comparing with the respective modes in Figure 4.16, we see that in (a) the tight-binding nature of the lattice type is apparent here from the decomposition of the eigenmodes into tight-binding like combinations of the building blocks. For (b), there is still significant mixing, which leads to the more spatially delocalized eigenmode profile.
see that the 6th mode is higher in energy than the 3rd mode because of the large displacement nodes at the connection points at the half unit cell positions. The increase in connectivity, or mechanical bond coupling (from the size of the connections) increase this interaction at the Γ point, hence leading to the larger splitting in the eigen-frequency, compared with the corresponding (3,4) pair in structure (a). What results from this as well is that the spectral gap size in structure (b) now depends on band 6 at the Γ point, compared to (a), which depended on band 6 at the X point and is essentially of totally different symmetric character. By now looking at the X point, we see that for structure (a), the building blocks form a degenerate pair, with different Irreps. Their degeneracy is not a coincidence but is rather instructive from considering this structure as a combination of two sub-lattices, displaced by (0.5a, 0.5a). The two modes are generated by considering eigenmodes that lie predominantly on each of the sub-lattices separately. That the two modes belong to different Irreps arise from the fact that there is essential no energy penalty when considering its symmetry/antisymmetry w.r.t to a $C_2$ operation. In contrast, the same is not true for structure (b) for the same two corresponding bands due to the increased coupling, which induces much more mixing between the building blocks. This evidently exhibits itself from the resultant eigenmodes, of which the 3rd to 6th bands have similar displacement fields, differing only subtly in terms of the Irreps; in the 4th and 6th bands showed, here, they differed in their (anti)symmetry w.r.t to a vertical glide plane, with the 4th (symmetric) and the 6th (antisymmetric) differing like so [Figure 4.16].
4.5 Conclusions

Our motivation in this chapter was to understand the relevant physical parameters involved in controlling the phonon dynamics in inhomogeneous media. The problem is interesting and frustrating at the same time, in that one has to consider the physical topography of the structure, the elastic contrasts, as well as the frequency ranges of interest, hence there are a lot of variables to consider. At the same time, because these variables are frequently coupled to, there is a lack of a sense of how to rationally treat combinations of these variables that makes the design transparent, and also physically accurate. We choose to consider the fundamental process of phonon flux through a general structure and recognize that the linear momentum (in our system), or impedance, is the relevant quantity of interest. In other words, given a particular frequency, we are concerned with the resultant trajectory of a phonon flux through the entire structure. This is essentially a variational extremization of the continuity equation, with the momentum flux being the quantity of interest. We found that the linear momentum/impedance serves as the relevant parameter for determining the dynamics of the phonons, taking into account as well the physical wavelength of the phonon in the medium. This is in contrast to other previous works, which separately considered contrasts in elastic constants, mass density etc, without being able to elucidate a general guiding principle that works in all cases. In contrast, the utilization of impedance contrast as the parameter holds valid, even under deliberately introduced conditions with different contrasts of the elastic constants and density. Hence, the impedance contrast is utilized as the first order physical parameter that determines the phonon dynamics, giving us the concept of the mechanical bond. The assignment of a bond type to a particular structure depends on the impedance
contrast, this is strictly dependent only on the materials involved, independent of the exact structure. The role of the physical topography comes in determining the matrix and the scatterer phase, from where we define the sign of the impedance contrast parameter value. In this sense, the assignment of the “matrix” or “scatterer” phase is only dependent on the geometric structure, not the particular set of materials. These two conditions then determine the dynamics of the phonons vis a vis the mechanical bond classification, hence giving a concrete grounding of types of material combinations and physical topography. We do not consider how these parameters affect the spectral gap opening tendencies because based on our general framework, this is not necessary. In a lot of the cases, the bounds of the gaps do not relate to the particular gap opening mechanism at work, as we have shown repeatedly throughout this and the previous chapters. Instead, it is more important to understand the dynamics which the phonons inherit based on these parameters, hence the concept of the mechanical bond. The dynamics, in our opinion, are more important in controlling the subsequent desired propagation behavior and realistically speaking, we can create complete spectral gaps irrespectively of what lattice class we are in. We subsequently generalize this approach also to solid-air structures and remapped the dynamical bond concept to rely on the geometry of the structure instead. We showed this bond type transition clearly from the EL to the TBL case using a general test case. Finally, we demonstrated full control by designing a structure with engineered polarization specific negative refracting bands using a starting EL lattice type. We subsequently also created a phononic structure, based on a TBL concept, that possesses an in-plane spectral gap of 102% and a combined total spectral gap of 88%. In the subsequent chapters (chapters 4,5), we demonstrate further the combinations of the general
design framework together with the phonon dynamics consideration to demonstrate a series of unique phononic metamaterials, utilizing only a single material platform, some with propagation behavior that has not been demonstrated before nor thought possible in phononics.
Chapter 5. Designing Dispersion Relations in Phononic Metamaterials I: Avoided Crossings

5.1 Introductory Remarks

The previous chapters sought to outline the governing physical principles of classical elastodynamics (Chapter 2), transitioning from discrete lattice dynamics into the continuum regime. This allowed us to view elastic waves as broken symmetry modes, both globally, which led to the formation of the transverse and longitudinal modes which we are familiar with, as well as the classical Rayleigh (edge) and Stoneley (interfacial) type modes, which is derived from symmetry breaking in a specific spatial region, analogous to surface plasmons. We took care to outline the different scenarios pertaining to bulk systems with induced discrete translational periodicities of different dimensionality as well as the connection of the bulk response of a medium and its interfaces in a general context of symmetry breaking and we were able to expound the role that group symmetry plays in tracking the actual eigen-modes of the phonons in a structure, which associated the entire details of each eigenmode’s polarization field as having to conform to the symmetry representation of the mode, dictated by the little group of the respective k-vector. At the expense of being seemingly too general, the purpose was to highlight the most fundamental conserved quantities that are present in a dynamical process that takes place at a general interface. This is crucial to help distinguish the governing equations (which conserve the relevant system under which the evolution of the phonons occur) from the constitutive relations (elastic constants coefficients, mass density), which is
somewhat more phenomenological and pertains directly to the material system being studied. This clear distinction is necessary in order to prevent one classification from being obfuscated with the other and subsequently, missing potential governing principles otherwise overlooked.

As we seek governing principles that are universal and hence are to a large extent, material system independent, this clear distinction and isolation is very important. This led to the development of a concrete mathematical structure (Chapter 3) that illustrated both the global as well as local principles of group theoretical and variational methods in order to control the band structure of a generic AS. It was also here where the concept of avoided crossings in the context of spectral gap formation was first outlined.

In this chapter, we generalize the requirements for the formation of spectral gaps in both phononic “metamaterials” and “crystals” by identifying what are the irreducible requirements for the formation of the spectral gaps in all cases. We will show that the fundamental requirements here, are the i) correct plane group symmetry, because they govern the allowed symmetry representations each dispersion bands can adopt, as well as ii) controlling the avoided crossing, which leads to the spectral gap formation. We subsume the current working knowledge tools by identifying their physical model as one of the possibilities in the generalized framework. We then illustrate how the generalized framework, by identifying the necessary and sufficient guiding principles, enable us to create both metamaterials and crystals (as defined in the current literature), using only a single elastic material. In fact, our design framework fully utilizes and accounts automatically the dispersion of the bands, i.e. their non-locality, hence the physical basis for the design principle for the band structure is assumption-
free. This is in contrast to conventional working knowledge for phononic metamaterials, which is inherently quasi-static in nature, and hence ignores the effect of the lattice in a cavalier fashion. Through this process, we remove the artificial distinction between what constitutes a phononic metamaterial and what constitutes a crystal. This is demonstrated through two examples, the first being a AS which possess both a complete sub-wavelength gap and a crystalline like gap, hence straddling the metamaterial and crystal regime. Importantly, this structure was designed utilizing only a single material platform, hence only explicit knowledge is made use of the plane group symmetry. The second example also builds on this theme, except that in this instance we create a structure which possesses meso-scale gaps, specifically a sub-wavelength gap for transverse modes and a crystalline gap for longitudinal modes. We call this a mesoscale polarization specific phononic metamaterial.

To the best of our knowledge, these are the first demonstrations of such behavior in phononic structures. More interestingly, these unique classes of behavior are achievable using only a single monolithic material platform. In addition, these designs are largely material independent; hence they are achievable using a significantly wide range of materials, ranging from polymer all the way to metals. This validates the value and utility of approaching the design of these structures from as global a perspective as possible. We now proceed to demonstrate these different forms of phonon propagation behavior, highlighting the governing principle in each demonstration.
5.2 From Crystals to “Resonant” Meta-materials

5.2.1 Untruths

As briefly mentioned, the conventional distinction between a resonant metamaterial and a crystal lies in the wave-length regime in which the spectral gap forms, together with their associated negative index bands. Another inherent assumption for metamaterials is the resonant response of the building blocks determines the behavior of the material, and hence the exact arrangement, i.e. lattice class doesn’t matter; this is somewhat linked to an erroneous interpretation of the effective medium approach [71], also commonly known as the locality approximation. The typical form of a metamaterial is shown [Figure 5.1a], strongly resembling a mechanical spring model. In these situations, typically three materials are needed, to take the role of the mechanical mass and springs. The associated signature is that of the typical dispersion relation as shown [Figure 5.1b], where the interaction occurs between the resonant mode and the “effective-medium” mode, leading to the formation of a spectral gap, which is deeply sub-wavelength. The exact position of this gap depends on the material properties, which follows the model that the spring resonance scales inversely with the static mass [55].

There are a few points of note here. First is that the formation of the spectral gap comes from the avoided crossing between the said two modes, hence the uniqueness of the property is linked to the building blocks and not so much the lattice, or that is at least the conventional explanation. This is untrue and can be regarded as somewhat over misinterpreted due to the
choice of the building blocks in this case. In the pioneering work of Liu et al [55], their choice of the large contrast of the mechanical spring, had a much larger impedance than the coupling

![Figure 5.1](image)

Figure 5.1 (a) Experimental Schematic of a resonant metamaterial, consisting of the lead sphere, surrounded by a soft rubber, with a stiffer epoxy matrix. (b) Computed band dispersion of the structure, which is a simple cubic lattice. Note that the reason for the dispersion bands being so flat is due to the extremely soft rubber acting as the soft spring. Taken from Ref [55]

Rubber (the elastic constants have a ratio of $\sim 10^5$, and an incompressible rubber), hence this leads to the fact that the resonances of the mechanical spring is only weakly coupled through the lattice; we gave a two-dimensional analog of this system earlier in section 3.4 where we discussed the role of nonlocality explicitly in the development of band structures. Hence, the response is very weakly-nonlocal, i.e. the locality is a result of the material parameters choice and not a general mechanism, as it was purported to be. The second point is that the avoided crossing is occurring at a small, BUT still finite wave vector, which naturally implies non-locality;
this is further reinforced by the fact that by definition, the avoided occurs between two modes with like-symmetries, since we know that the eigenmodes can only adopt representations belonging to the isotropy group of the particular wave vector (chapter 3.3), this implies immediately that the eigenmodes encompass information about the lattice lies in. This implies that in resonant metamaterials, the dispersion is non-local in general [71]; any perceived locality is due to particular choices of the material components. One should not mistake the latter for the general case, as has been mistakenly done, for both electromagnetic and acoustic metamaterials [73]. This was illustrated very clearly in section 3.4 where we took a common canonical structure of a 2D resonant metamaterial and plot the corresponding eigenmodes across the avoided crossing point, at various material parameters. One sees clearly that all the displacement fields maintain the symmetry of the isotropy group and not that of the isolated resonances.

Hence, we now formally cast the necessary condition for opening a spectral gap, regardless of whether we are dealing with a metamaterial or a conventional crystal, as the respective avoided crossing with the correct symmetries. The perceived key distinction between a metamaterial and a crystal is then the wavelength at which this avoided crossing occurs. In contrast to conventional working knowledge, while this is common but not always so, we do not regard the spectral gap formation of crystal to be due to the discrete translational symmetry; there are numerous examples that show that many bounds of the spectral gaps are not at the Brillouin zone boundaries [77]; hence we subsume the periodicity as translational Bloch symmetry and as but one of the possible symmetries that cause avoided crossings; this was shown in sections 3.4.
To summarize then, the present state of the art suffers from several issues, mostly fundamental in nature of i) what are the usual and actual constraints when creating a spectral gap ii) what is actually controlling the symmetry of the response functions and (iii), what are the true requirements for a dynamic negative susceptibility. Moreover, the problem of the choice of the optimal space and plane group symmetry and the subsequent symmetry of the response actually entail more than just the naïve issue of reducing the size of the IRBZ, for both crystals. The spatial non-locality, or wave-vector dependence of the AS response is inherently present and is meso-scale because it encompasses, in general, all the relevant length scales in the response through the irreducible representation of a particular band.

5.2.2 Truth: Avoided Crossings
To remove the artificial classifications of resonant type meta-materials and the classical phononic crystal, we recast the concept of spectral gap formation into a framework which is scale-invariant, i.e. does not require an intrinsic length scale to interpret. In this sense, we may now identify phononic crystals as structures which possess spectral gaps primarily based on avoided crossings due to the Bloch symmetry, whereas for phononic metamaterials, spectral gaps occurs due to avoided crossings between low-lying resonance modes and the longer nonlocal linearly dispersive bands of the medium. We thus remove the artificial distinction between what is a crystal and what is a metamaterial and classify them all within the same category of metamaterial from here on. Within this approach, we now identify the requirement of the low-lying mechanical resonance as a geometrical structuring of the material to have a low-lying resonant eigenmodes with the same irreducible representation as the long wavelength linear modes in order to create the sub-wavelength avoided crossing. The actual
Figure 5.2 (a) (i) Structure of the original honeycomb unit cell (Area fraction=56%). The black region represents solid material and the grey region air/vacuum. It possesses C3v point symmetry at the Γ point if we take a two-cylinder motif. (ii) Structure of the deformed honeycomb unit cell (ICS) (Area fraction=55%). The black region represents solid material and the grey region air/vacuum. It possesses C2v point symmetry at the Γ point. (b) (i) Corresponding Band Diagram for the in-plane polarization of the original honeycomb lattice (ii) Corresponding
Band Diagram for the in-plane polarization of the deformed honeycomb lattice. Calculations here utilized amorphous/polycrystalline silicon for the material. Note that the deformation opens a narrow sub-wavelength complete gap as well as enlarging the corresponding crystalline gap. The material is chosen to be amorphous silicon ($E=156\text{GPa}, v=0.2152, \rho=2330\text{kgm}^{-3}$).

mimicking of a mechanical spring is no longer necessary. In addition, by controlling the types of these resonances, we can selectively induce different dynamic negative mass density, modulus, and even shear modulus.

We start with a conventional honeycomb lattice [Figure 5.2a (i)], with the computed band structure as shown [Figure 5.2b(i)]. It is clear from the band structure that the spectral gap opening in this case is bounded by the band pairs (3,4) at the $\Gamma$ point, giving a gap size of about 52\% (as defined earlier). However, we note here that the avoided crossing actually occurs between the 3rd and the 8th band and the actual plane group of the system is $p6mm$ still; we associate the motif to be the two cylinders as is typical for a honeycomb lattice. Recalling our discussion in section 3.4, we note that because in symmorphic symmetry groups, we may carry out the factor group decomposition on the infinite plane group, that for considerations of the dispersion relations, it suffices for us to consider only the relevant isotropy group of $k$ being considered; this is our normal subgroup which we are interested in. Hence, reduction in point group symmetry is not as traumatizing as was originally purported to be!

We now wish to induce an avoided crossing between bands 2 and 3 along both $\Gamma M$ and $\Gamma K$ directions, while not diminishing the spectral gap size if possible. The way to do this is to reduce the symmetry of the isotropy group along these two directions, in order to have these two bands adopt the same irreducible representations. We accomplish this by lowering the
plane group symmetry of an initially p6mm honeycomb lattice into a lower symmetry p2mm lattice by breaking the symmetry of the motif [Figure 5.2a (i,ii)]; the associated volume fraction change here is approximately about 5%. The net result of this leads to the creation of a new sub-wavelength gap in addition to an increase of the Bragg Gap from 52% to 70% [Figure 5.2b (i) vs (ii)], which is roughly a 40% increase; we have created a phononic metamaterial possessing both sub-wavelength and crystalline gaps, utilizing only nonlocality by changing the global plane group symmetry and variationally controlling the interaction strengths through the local spatial changes in the motifs. Let us now examine these mechanisms in details.

Figure 5.3 (a) Modes 2 and 3 along ΓM for the honeycomb lattice, (b) Modes 2 and 3 along ΓM for the ICS lattice, (c) Mode 3 at the Γ point for the honeycomb lattice, (d) Mode 3 at the Γ point for the ICS lattice.
We first note that the creation of the sub-wavelength spectral gaps require avoided crossings between the 2nd and the 3rd bands along both ΓM, and ΓK directions, as well as at the K points. In order to retain the crystalline gap, we need to ensure that the modification to the structure must not be too drastic to diminish this original gap. The only way in which we may achieve symmetry breaking along the ΓM direction and K point is by distorting the honeycomb motif. The point double degeneracy at the K point is distinctive to the honeycomb lattice, due to the particular symmetric arrangement of the cylindrical voids; hence breaking this honeycomb arrangement would be sufficient to lift this K,K' point degeneracy. A mirror plane exists along ΓM, as exemplified clearly by the two eigenmodes lying on the 2nd and 3rd bands respectively [Figure 5.3(a,i),(b,i)], which are symmetric and antisymmetric with respect to to it and hence are allowed to cross. Hence, this mirror plane symmetry needs to be broken, while not diminishing the gap size. We see mode 3 at the Γ point [Figure 5.3(c,i)], which possesses a node in the middle of the honeycomb motif. Finally, we realize that along the ΓK direction, the isotropy group for the honeycomb only consists of {E, m} and we wish to retain this mirror plane because we don’t want to increase the size of the IRBZ too much. Hence our consideration of structural modifications become restricted to the p2mm class, because p6mm lattices have a second “equivalent” p2mm lattice, hence by only considering the p2mm lattices choices, we are allowed to still retain the same effective IRBZ size. Because the system is solid-air/vacuum, most of the elastic waves propagate through the solid structure, hence dynamically, we may alter the symmetry of the eigenmodes through this consideration on the mechanical connectivity; this particularly pertains to transport along the ΓK direction as the isotropy group for p6mm and p2mm lattices are the same along this direction!
All of these considerations are rather restrictive, allowing one to consider only changes that break the mirror symmetry along $\Gamma M$ while retaining $C2v$ point symmetry at the $\Gamma$ point. The result of this is the modified honeycomb structure shown [Figure 5.2(a,ii)], which we labeled the I-comb structure (ICS). This change in the motif fulfills all of our stated requirements. First of all, this symmetry reduction in the point group forces the dispersion bands in the deformed honeycomb (with maximal $C2v$ symmetry (at $\Gamma$)) to only adopt the identity representation that along the $\Gamma M$ direction since the mirror plane is lost, as shown [Figure 5.3(a),(b)].

This first point is responsible for the general avoided crossing in the sub-wavelength regime along the $\Gamma M$ direction, which will be enforced since there is only one possibility of the identity representation, as we went from $\{E,m\}$ down to $\{E\}$ for the isotropy group.

What is more crucial and not so straight-forward is the situation along the $\Gamma K$ direction, which actually still permits both representations which are anti-symmetric (AnS) or symmetric (S) about the mirror plane. Naturally, transverse-like eigenmodes associate to the former and the longitudinal-like eigenmodes the latter. Here we made use of the variational arguments by reducing the mechanical connectivity along the $\Gamma K$ direction by introduce a topographical cut which now connects the two void cylinders; this lowers the associated “resonant-like” modes[Figure 4,3(d)] while simultaneously interchanging the AnS and S modes, as shown [Figure 5.4(a),(b)]. This is physically intuitive from the standpoint of the cut impeding symmetric.
Figure 5.4 Eigenmodes of (a) Modes 2 and 3 along ΓK for the honeycomb lattice, (b) Modes 2 and 3 along ΓK for the ICS lattice.
propagation while actually promoting antisymmetric propagation by removing the physical node in the middle of the original honeycomb. Here, the particular choice of the geometric cut is important because while there exist a multitude of ways to reduce the symmetry, we have to induce the right change in order to be able to interchange the AnS and S modes! We note there that we are also essentially creating a medium that in the longer wavelength limits, has a faster “transverse-like” wave velocity, compared to the “longitudinal-like” wave velocity, counter to homogeneous materials. However, this is perfectly legitimate because these are velocities induced from the dynamics of propagation in the microstructure, in this casea solid-air or, equivalent for finite-element modeling, solid-free surface, i.e. at the interfaces we experience symmetry breaking, hence the effective medium approximation in the conventional quasi-static limit needs to be modified [73]. The combination of these considerations, together with the symmetry reduction, finally allows us to then induce a complete sub-wavelength gap, as is shown [Figure 5.2 b (i), (ii)].

The secondary effect of this is in augmenting the fundamental “crystalline“ gap, compared with the original honeycomb lattice, from 52% to 70% for the in-plane gap. There are also two more points of note here with regards to the crystalline gap and the symmetry reduction. First is the fact that we note that in comparison with the honeycomb lattice, where the bounds of the crystalline gap are at the Γ points; for the deformed honeycomb lattice, the upper and lower bounds are now at the Γ and the K point, respectively. In fact, this is quite common in band structures, which renders the Bragg scattering concept at best a first order estimate for predicting band gaps, or for systems where the gap formation is strongly depending on strongly scattering media, like colloidal-based systems, for example [67,74]. The final point we wish to
note is that the p6mm and p2mm lattices have the same IRBZ, because we retained the same lattice basis; this leads to the same Wigner Seitz (WS) cell size. We have verified that this band structure is correct when recalculating around using the associated p2mm lattice basis set.

To conclude here, we have created a metamaterial that has two-scale complete gaps, one sub-wavelength gap and one crystalline gap, using only a single monolithic elastic material with a geometric perturbation that changes the “connectivity” of the medium and lowers its symmetry utilizing the global and local variational principle outlined in chapter 3. This completely generalizes requirements for generating sub-wavelength gaps which are “metamaterial”, and by creating both classes of complete spectral in-plane gaps, we have hopefully established to the reader that a strict division between metamaterials and crystals is artificial, unnecessary and can be counterproductive for engineering the dispersion relations for devices and applications. It is also important to reiterate here that in our design of such a material, that we have shown that the process of generating these gaps depends strongly on non-locality. In fact, in this demonstration, we utilize the full extent of the non-locality in the bands, clear from their dispersion to create the resultant band structure. This is distinct in execution from the classical method, which is based on a locality approximation, as discussed in section 3.4.

Finally, we note that in order to create a negative index band, the initial motivation for metamaterial applications in order to achieve negative refraction, in an elastic material is considerable more complicated than creating such a band in an acoustic medium; this is mathematically a classical analog to what is known as a more general case of induced transparency, except here we are more interested in the induced dispersion relation than the
phenomenon of tuning that transparency, i.e. we are more interested in the formation of the bands with desired dispersion rather than the dynamics of tuning this transparency.

5.3 Meso-Scale Phononic Meta-Crystal: Polarization specific spectral gaps

In this section, we illustrate our design process using structures that specifically retain a square lattice and p4mm symmetry. This is complementary to section 5.2 where we reduced the plane group symmetry in order to enforce avoided crossings. In this approach, we induce avoided crossings by utilizing the mechanical connectivity and hence variational principles to control the positions of the avoided crossings. The first part of the work involves choosing a structure which possesses a complete crystalline-scale spectral gap at the lattice-scale, and by connecting sub-elements of the structure to induce the formation of a meta-material which possesses polarization-specific spectral gaps at both the lattice-scale and the sub-wavelength scale.

This topographical change involves a simple increase in the connectivity of the structure along the <11> directions, which one would normally associate with increased channels for propagation and hence, a reduction in the propensity for forming complete spectral gaps. Note that this change preserves the 4mm point symmetry of the structure at the gamma point and involves a volume fraction change from 39% to 51.5% [Figure 5.5 (a) (i),(ii)].
Figure 5.5 a) (i) Derivative Metamaterial Structure with p4mm plane group symmetry (Area fraction= 51.5%). The point symmetry at the Γ point retains C4v. (ii) Parent Crystal Structure with p4mm plane group symmetry (Area fraction= 39%). The point symmetry at the Γ point is C4v. (b) (i) Corresponding BandDiagram for the in-plane polarization of the high connectivity p4mm structure in (a, i) (ii) Corresponding Band Diagram for the in-plane polarization of the original parent p4mm structure in (a, ii) Calculations here utilized amorphous/polycrystalline silicon (E=156GPa, v=0.2152, p=2330kgm⁻³) for the material. The increase in connectivity increases the fundamental t1 mode velocity, allowing for the avoided crossing to create the sub-wavelength transverse gap.

As noted, the original parent structure possesses a complete in-plane normalized gap-width of approximately 80%. The origin of this quite large gap here can be traced to the condition where the building block dimension in this case optimizes the Bloch type avoided crossing process, similar to the situation described in section 3.3.

In this case, while the origin of the spectral gap opening is due to the discrete Bloch symmetry, commonly known as Bragg scattering, this occurs between the third and sixth dispersion bands, both of which have the same irreducible representations [Figure 5.5 (b), (iii)]. However, it is also clear that the spectral gap is set by the third and fourth bands; this situation is commonly the case where the limiting factor is typically not the strength of the so-called Bragg scattering, but the location of the other bands. This is also clear from the observing the eigenmodes, which possess the same irreducible representations, which possess the same symmetries between the third and the sixth bands. The Bragg nature of this spectral gap is also confirmed by its canonical normalized frequency of 0.5, which corresponds to the edge of the first BZ in k-space.
The topographical modification physically diminishes the size of the absolute band gap but it presents an interesting situation. Two polarization-specific complete spectral gaps are now created, of two different natures, if we follow the common convention. The higher complete spectral gap is a polarization specific gap that blocks only longitudinal modes, formed between
Figure 5.6  (a) Displacement Field for the t1 mode, as marked in Figure 4.4(b, i)  (b) Displacement Field for the t2 mode, as marked in Figure 4.4(b, i)  (c) Displacement Field for the l1 mode, as marked in Figure 4.4(b, i)  (d) Displacement Field for the l2 mode, as marked in Figure 4.4(b, i). Note here that even though strictly speaking, the modes are not transverse or longitudinal, we physically can design the displacement field to make it as “transverse-like” or “longitudinal-like”. Along the RX direction, this naturally is separated into the modes which are AS or S with regards to the horizontal mirror.

The third and fifth bands. The sub-wavelength gap, formed between the first and second bands, only blocks transverse modes, as clearly shown [Figure 5.6]. Once again, we note that it is difficult to identify the bands involved in creating a spectral gap without elucidation of the details of their eigenmodes profiles. Clearly, the presence of a two different gaps, which are strongly polarization specific and exists at two different length scales, is rather unexpected when only a single monolithic structure is employed. Perhaps more puzzling is the fact that the use of only a single elastic material can lead to a transverse sub-wavelength gap begets the question, where is the mechanical resonance required for the opening of the sub-wavelength gap? In some senses, the distinction of a crystal, which relies on the coherent scattering on the scale of the lattice, and a meta-material, which relies on a resonance phenomenon, is artificial.

With the notable exception of one study [75], this fact has not been addressed much in phononics as well. We state that by utilizing the generalized framework [76], that spectral gaps that occur due to the Bragg-like scattering and that due to sub-wavelength resonances can both be classified as avoided crossings between the interacting bands, as a result of their like symmetry. In the former case, the relevant symmetry is involved is that due to Bloch’s
Theorem, mathematically actually a manifestation of discrete translational symmetry. In fact, it is more accurate to state here that Bloch’s theorem is but a special case of a more general case of avoided crossing in the formation of spectral gaps in periodic crystals for both scalar and vector fields; this is especially true and extremely important for cases of dimensionality $n > 1$. In the one dimensionally periodic case for isotropic building blocks, the only symmetry present is due to Bloch symmetry, which is why this more fundamental reason has been concealed [77]. Now the case for the sub-wavelength gap that only blocks transverse modes is a very example of this more general avoided crossing [Fig5.5(a),(b)]. The avoided crossing position sets the length-scale dependence, with the size of the spectral gap depends on the interaction strength, this latter fact may depend on the length scale at which the avoided crossing occurs. Ultimately, the only requirement for the avoided crossing and hence for the spectral gap to form, is that the two interacting bands possess the same irreducible representations corresponding to the little group, or the isotropy group of the relevant wave vector considered (We shall use isotropy group for all cases from now on). In this situation, as the isotropy group in both the [10] and [11] directions is C1h, the first two bands both possess the $A''$ representation, anti-symmetric about the respective mirror planes, hence effecting the avoided crossing. This avoided crossing is tied fundamentally to the symmetry of the system, and may take place at any length-scale, or frequency. In this situation, it has occurred at the sub-wavelength scale and would be commonly identified with the sub-wavelength resonance type spectral gap.

For the case of the longitudinal gap, the avoided crossing occurs at the X and M points respectively, recovering the well-known Bragg condition. In this case, the avoided crossing also
occurs as a result of the like-symmetry [Fig5.6(c),(d)], although the signature of the Bloch symmetry stems from the non-locality of the bands. It is important to note once again in this case, that the size of the longitudinal gap is not diminished by the presence of the intermediate fifth band, which is actually strongly transverse in nature and hence is ‘deaf’, so to speak, to longitudinal excitation. Thus our simple topographical modification has created two distinct polarization complete gaps, a sub-wavelength transverse gap and a Bragg-like longitudinal gap.

By increasing the connectivity of the structure along the <11> presents similar environments for the propagating modes along both the [10] and [11] directions. This has the additional effect of reducing the mixing of the polarization of the displacement fields; because we note that in the limit of purely transverse and longitudinal modes, they still fulfill the symmetry requirements of the structure, which is anti-symmetric(transverse) and symmetric (longitudinal) with respective to the horizontal mirror plane. It is this very realization that has enabled the creation of this polarization specific two-scale spectral gap material.

5.4 Conclusions

We utilized here fully the non-locality and the dispersion of the bands, through selective geometric perturbations, to control specifically the positioning of several dispersion bands in order to enforce avoided crossings, resulting in the creation of spectral gaps in the frequency range that is desired. In the first example, we utilized symmetry reduction in order to enforce the avoided crossing and in this situation, we created two scale complete spectral gaps in a deformed version of the honeycomb lattice. Crucial to this realization was that we introduced a geometric perturbation that interchanged the transverse-like and longitudinal-like mode, this
was critical to enforce the avoided crossing in the desired frequency range. In the second example, we retained the plane and point symmetry of the system but this time we adopted the opposite approach and increased the connectivity to push the transverse-like mode to higher velocities, this allows the avoided crossings to occur at the sub-wavelength frequency range, in additional to the fundamental crystalline gap, enabling us to generate the meso-scale polarization specific spectral gaps. We summarize here that all these are based on the simple realization of what are the critical components for controlling the band structure of the structure and purely by utilizing geometric structuring; we are able to achieve quite a series of unique band structures without any reliance on specific material properties. This is to the best of our knowledge, the first demonstration of this general mechanism for controlling the band structures of any periodic structure, not just for phonons.
Chapter 6. Designing Dispersion Relations Phononic Metamaterials II: A Polychromatic Nonsymmorphic Phononic Crystal

6.1 Introductory Remarks

In this second part to the design of dispersion relations in phononic metamaterials, we here utilize a different approach, previously unemployned, in order to create a nonsymmorphic phononic crystal that possesses multiple complete spectral gaps. Instead of using avoided crossings which has been the default mechanism for creating spectral gaps and negative index bands, we utilize a complementary approach from the variational perspective. In particular, we create multiple complete in-plane high frequency gaps, by not making use of any avoided crossings. In fact, here we make use of both global and local principles to design such an AS. By recognizing that the relevant eigenmodes of the phonons obeys the allowed Irreps corresponding to the isotropy group, we are able to control and treat the vector nature of the phonons as before by only considering the global plane group symmetry.

However, instead of employing avoided crossings, here we utilize the local variational principles by shaping of the building blocks of the AS structure; this allows us to control the eigenfrequencies at the $\Gamma$ point. Together with the choice of the particular TBL lattice class, we control the evolution of the bands in k-space, forcing them to be quasi-flat. This results in a natural two-scale splitting of eigenfrequencies at the $\Gamma$ point, first due to the (anti)symmetry with respect to a mirror plane parallel to the k-vector direction considered, and then the (anti)symmetry with respect to the primary $C_4$ rotation operation. Together with the choice of the lattice class, which controls the transport dynamics, and the global plane group symmetry,
we are able to control both the positions of the eigenfrequencies and their evolution in k-space. This entire suite of tools, developed in chapter 3, allows us to design a phononic structure possessing multiple complete in-plane spectral gaps (6), spanning a total normalized gap width, 

$$\Delta \omega = \sum_n \frac{\omega_{\text{upp}} - \omega_{\text{low}}}{\omega_{\text{mid}}}$$

of over 100. The creation of phononic metamaterials possessing multiple complete spectral gaps is very interesting, both from a fundamental and applications perspective, allowing for the study of nonlinear phonon-phonon interaction processes [78] to development as a structural material for shaping and molding nonlinear waves such as solitons and shockwaves [14].

6.2 Global Symmetry: Nonsymmorphicity and Sticking Bands

In addition to the previous illustrations on the utilization of the generalized avoided crossing, we hinted of the final governing principle which aids our universal framework by linking the global constraints with the local design principles highlighted in the previous two sections. Simply stated, it is an adiabatic perturbation theory in wave-vector space which has its origins in the compatibility relations in group theory. Traditionally, this has been utilized for identifying the irreducible representations (Irreps) in the individual bands in electronic structure calculations. The perturbation can be fundamentally traced to a group-subgroup decomposition of the Irreps as we progress along a particular trajectory in k-space, for example the Gamma Point to a generic position along the GX direction. We remark that that this entire band can be joined and treated in this manner is not obvious, or easily proved [79,80,81] but we are able to trace as a series of equivalence transformations as we adiabatically vary the
wave-vector along some direction in $k$-space. For the time being, we will accept that this procedure works well and is well verified. The elegance of this perturbation theory is that once again, it is scale-invariant, i.e. takes care intrinsically of the non-locality of the bands and inherently conforms to the symmetry requirements along the trajectory in $k$-space. What we observe is the fact that this “analyticity” of the bands only sets together the possible connections in $k$-space in terms of symmetry requirements, but it enables us still full freedom in choosing how and where in the reciprocal space do the bands choose to evolve across. This controls, to a very large extent, how the size of the gaps may evolve. In fact, this allows the possibility of a new paradigm in designing spectral gaps, for example by controlling the position of eigenfrequencies at the Gamma point, which is local($k=0$), and then controlling the evolution of the bands across the rest of reciprocal space such that, for example, to create polychromatic complete spectral gaps. To achieve this, we need to control (i) the allowed dispersion of the bands as well as (ii) their allowed energies. This is because control over both these two features, in principle, allows us to have unprecedented freedom and control over where the dispersion bands exist in frequency, as well as their curvatures. Broadly speaking, in order to realize multiple complete gaps in a single structure, we want to reduce the dispersion of the bands as much as possible while at the same time create large spectral gaps, this requires control over both the curvature as well as the spectral positions of multiple bands as well as their evolution throughout the reciprocal space.

A combination of a global constraint and local design principle is utilized to achieve this purpose. Broadly outlining the steps we shall undertake, the global constraint utilizes group theoretical principles [59] and casts the underlying mathematical structure onto the linearized
elastic wave equation; this provides a framework within which to operate and engineer the
band structure. The “local” design principle takes into account the propagation behavior of the
classical phonon and identifies the category of geometrical structure of the phononic crystal
which we need in order to control the relative placement of energy eigenvalues of the
dispersion bands.

We choose to do this, of course for the in-plane two-dimensional linearized elastic wave
equation, given by:

\[
\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial}{\partial x_i} \left[ \lambda \left( \frac{\partial u_i}{\partial x_i} \right) \right] + \frac{\partial}{\partial x_k} \left[ \mu \left( \frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right) \right]
\]

\(\rho\) is the density
\(\lambda, \mu\) are the Lame coefficients
\(u_i\) are the displacement components.

The elastic wave, or phonon, possesses in general, three degrees of freedom; in two-
dimensions, the in-plane polarizations (two) are coupled with the final, out-of-plane
polarization decoupled from the system, it is the former case which we are solving for now.
Surprisingly, the nature of the field which we are trying to design, offers no more complication
in the global constraint framework, once we have properly identified their rank (i.e; vector,
scalar). In general, the definition of a transverse or longitudinal phonon loses meaning in an
inhomogeneous medium and the phonon eigenmodes possess a non-trivial displacement field
with mixed polarization, consisting of both transverse and longitudinal character. While the
details of the displacement field may differ greatly, depending on the normalized length scale
of the medium inhomogeneity (over the wavelength of the wave we are considering), a general
rule remains: The eigenmodes will possess the relevant symmetries of the system [63, 61];
whether the symmetries are dynamic, static or time-varying, this principle holds true. In phononic crystals, the eigenmodes hence must obey the discrete symmetries of the space (3D)/plane (2D) group of the system. Group theoretical principles have been utilized mainly as a powerful analysis tool [59,64]; we here apply it as a global constraint principle. While on its own, group theory cannot be utilized to design a particular structure, its elegance and power lies in its ability to cast the governing equation of a physical problem into a concrete mathematical structure that states the possibilities the solutions may take, i.e. its invariants; in our case, group theory is able to dictate for us the allowed possibilities for the band structure, which is physically realized through our choice of the symmetry group of the phononic crystal. In the design of phononic crystals, one main challenge has been the control the dispersion of bands along general directions i.e. low symmetry directions; this is especially important when one wishes to optimize complete spectral gaps. Hence, in order to create multiple complete spectral gaps, we need to have a way of controlling or reducing band curvatures along these low symmetry directions. We choose to employ band-sticking [60, 66,65], discussed earlier in section 3.3, which enforces bands to exist at least as double degenerate pairs along entire Brillouin zone (BZ) faces (3D) and edges(2D) that typically have low symmetries. In particular, band sticking occurs in structures possessing non-symmorphic
Figure 6.1 (i) Band Diagram of the Tight-Binding Lattice (TBL) (ii) Band Diagram of the Lower fill-fraction Lattice (SL) (insets show the corresponding geometrical structure and the BZ convention) The corresponding bands 11 and 12 are colored green and red respectively for both structures to illustrate the different mechanisms involved in controlling the band dispersion in the two lattices. Calculations here utilized amorphous/polycrystalline silicon (E=156GPa, ν=0.2152, ρ=2330kgm⁻³) for the material. Area fractions are: for the TBL (36.8%) and SL (59.5%)

plane/space groups, along certain BZ faces/boundaries or edges. In two-dimensional systems, only 4 (p4gm, p2gg, p2gm, pmg) out of the possible 17 plane groups are non-symmorphic and hence possess this property; among the 4, we chose the one with the highest point symmetry, the p4gm plane group [Fig6.1 (insets)]. We note here that not all the non symmorphic plane groups will possess sticking bands; the strict requirement is that along the particular BZ boundary of interest, that there are two commuting symmetry elements with their invariant axes perpendicular to one another; for the p4mg plane group, these are the glide-planes and 2 fold axes and happen to lie on the XM BZ face which we need to control. The reader may also
recall that for comparison, a p2gg structure has band sticking along two BZ boundaries, the XM and MY faces, as we showed earlier in section 3.5xx? Although initially discussed for electronic systems, band sticking is rather general and exists for vector fields as well, since it relies only on the symmetry of the structure. The group theoretical principle is a powerful global constraint because it is valid regardless of the nature of the field or its dimensionality. This is clearly shown in the series of theoretical in-plane band dispersions calculated for different fill fractions of structures possessing the same p4gm plane group symmetry [figure6.1]. The dispersion bands exist solely as degenerate pairs along the XM BZ boundary at all fill fractions, as they all maintain p4gm symmetry demonstrating that the sticking bands are a robust signature of the plane group symmetry (see section 3.5 for discussion). Hence, the global constraint has helped cast our wave equation with a concrete mathematical structure, bearing in mind that all of our allowed eigenmodes conform to the symmetries of the little group of the relevant wave vector.

6.3 Local Variational Principles: The Tight Binding Lattice (TBL) Class

It is important to note that while the global constraint is certainly useful in classifying the possibilities or the spaces to search for potential candidate structures, it does not allow active control over the details of the band structure, clear from the computed band structures over different fill fractions [Figure 6.1, (i) and (ii)]. In our case these details are the spectral positions of our bands, which require the details of the phonon propagation dynamics. It is important to note that the parameter of fill fraction is not so useful in the actual design of a phononic crystal, or any periodic structure for that matter although it is indeed useful from a fabrication
standpoint as a practical tuning parameter. The issues lies in the fact that it is potentially misleading when utilized as an actual design parameter when exploring for ideal structures from a fundamental standpoint; i.e. what structures we should be looking at for the properties which we want. We shall end with the remark that the crucial design parameter is to identify the category of geometric lattice structure that is desired before considering the fill fraction of the building blocks within the correct category.

This leads us now to the local design principles which we base on variational arguments [section 3.3]. As our purpose is to create structures with multiple complete spectral gaps, we
wish to reduce the curvature of our bands, indeed to flatten them as much as possible across
the XM BZ boundary, if at all possible. In addition, we also need to be able to control the band
dispersions in order to maximize the complete spectral gaps. This is achieved through the
phononic analogue of the tight-binding lattice (TBL) class in the extreme sense [chapter 4]. By
choosing solid building blocks which have very specific anisotropic eigenmodes and then
connecting them through weak “mechanical” bonds, we create bands with very small
curvatures, i.e. almost flat, across the XM boundary edges. Effectively, we have designed a
lattice such that the eigen-values are nearly degenerate at the X and M point, which belong to
two different isotropy groups.

Our TBL enforces a series of constraints on the allowed frequencies and their subsequent
evolution across k-space. First of all, due to the weak coupling between building blocks, the
dispersion bands now become ‘local’ in nature; a signature of this is exhibited their relatively
flat dispersions, as well as the fact that the displacement fields of the eigenmodes show
considerable localization [Figure 6.2]. This is crucial because most of the variational control of
the frequency spectrum can now be achieved by considering the spectral distribution primarily
at the Gamma point, $\Gamma$. As the little group at the $\Gamma$ point is $C_{4v}$, there exists the possibility of
doubly degenerate frequencies ($E$ representation) and four possible single frequencies
($A_1, A_2, B_1, B_2$). Hence, the TBL automatically ensures that the doubly-degenerate bands will
evolve across the entire BZ as nearly-flat bands, as is clearly the case [Figure 6.1(a)]. Note that
this is distinctly absent in the smaller fill-fraction (SL) [Figure 6.1(b)], which does not behave as
a TBL.
The final design consideration is in controlling the positions of the energy bands. In order to achieve multiple sizeable spectral gaps requires us to control the evolution of the remaining bands from the $\Gamma$ point to the respective sticking points at the X and M points such that the coalescing pairs of bands (from $\Gamma$ to X or M) are separated by smaller spectral widths, preferably between adjacent bands; this is usually not the case, as is demonstrated by comparing bands 9 to 11 between the TBL and the EL [Figure 6.1(a),(b)]. This is exactly where we are able to utilize the vector nature of the phonon to our advantage. As previously mentioned, the displacement fields of each eigen-mode possess in general, a complicated mixed profile [figure 6.2] and transverse and longitudinal modes strictly lose meaning. However, as the degrees of freedom remain conserved; within the phononic structure, each eigenmode obeys the symmetry of the relevant isotropy group, taking the form of an irreducible representation of the little group. The original two degrees of freedom (DOF) (two polarization modes) have hence been mapped into the irreducible representations of the isotropy group. From group compatibility relations in evolving from $\Gamma$ to X or M($C_\nu$ to $C_{\nu'}$) [79,65,81,59], we know that the bands coalescing to the sticking point need to NOT both be either symmetric($A_1,B_1$) or antisymmetric ($A_2,B_2$) at the $\Gamma$ point. This naturally establishes the desired criterion for how the symmetries of the eigenmodes should be arranged at each wave vector $k$. This is readily accomplished in our TBL through the choice of making the building blocks highly anisotropic, coupled with the fact that there are two DOF due to the vector nature, creates two orders of splitting in the energy eigenvalues at the $\Gamma$ point. The larger, first order energy splitting is with respect to symmetrization or anti-symmetrization with respect to the mirror plane [Figure 6.1 and Figure 6.2(i) (a) vs (c)]. The smaller, second order splitting, is with respect to symmetrization (A) or
anti-symmetrization (B) with respect to a four-fold rotation. (This is the distinction, for a C\textsubscript{4v} point group, for the naming of the A and B representations respectively). The shape anisotropy of the building blocks and their coupling over weak mechanical bonds makes it much less energetically costly to anti-symmetrize the displacement field of adjacent building blocks [Figure 6.2(i), (a) and (b)] as compared to the mirror plane [Figure 6.2(i), (a) and (c)]. Hence this automatically groups (A\textsubscript{1}, B\textsubscript{2}) and (A\textsubscript{2}, B\textsubscript{1}) type bands adjacently, enabling us to finally arrive at the desired pair-wise coalescing from \Gamma to X and M. Note that this two-energy scale splitting method is unique to our choice of geometrical structure in the TBL class, which is crucial to deriving the eventual band structure and is quickly lost once we move to structures that do not belong in this regime. A clear example is the SL [Figure 6.1(b) inset] which does not provide such a band structure because the building blocks are more strongly connected to each other, and hence there is stronger mixing in the nature of the bands [Figure 6.2(ii), (e),(f),(g),(h)]. No paired bands exist in this case and one is not able to obtain the multiple spectral gap band structure. It is interesting to note here as well that sticking bands coalesce at the X point at \textit{non-zero slope}, since there is no point degeneracy at the X and M points.

Our final criterion is that we would require that the bands remain essentially flat across the XM face as part of the design criterion to maximize the sizes of the multiple spectral gaps; this is fulfilled with our combination of the choice of the global plane group symmetry (p4gm), the TBL lattice and most importantly, the building blocks. Our choice of p4gm, the highest symmetry nonsymmorphic group ensures that we only need to match the energy eigenvalues at the X and M points, since bands only exists pairwise degenerate along XM. In order to ensure the persistence of the gaps, we need to ensure that the bands evolve from the X to the M point flat,
i.e., they do not cross in the XM region. This is distinct from sticking bands, since non-symmorphicity merely ensures that points at X and M are now double degenerate, it does not prevent the bands from crossing one another along XM. An example of this is in the evolution of band pairs (3, 4) of the SL[Figure 6.1(ii)] across XM, or that of (7,8) and (9,10) which cross close to the M point.

To do this, we have to design accidentally degenerate eigenmodes at the corresponding X, and M points. For the p4gm group, the isotropy groups at both the X and M points are C_{2v}, hence by utilizing our TBL, the eigenfrequencies are determined strongly by the geometry of the unit cell, and hence the building blocks. Earlier on we mentioned that our building blocks were anisotropic; this has the additional advantage of not introducing any additional self-symmetries in the building blocks themselves and this enabled the corresponding eigenfrequencies to be essentially close to being degenerate at the corresponding X and M points, as is clear from their displacement fields. [Figure 6.3] The band sticking across the XM face and the compatibility relations subsequently ensure that the bands evolve as desired, arriving at the final band structure which was desired[Figures 6.1(i)]. One notes also the fact that the tight-binding nature of the lattice helps ensure the coalescence of the odd-even pairs of bands because of the low energy requirement in switching the displacement fields between the two parities in the tight-binding regime.

195
Figure 6.3 Displacement Fields at X point for TBL for mode (a) 12, (b) 11, (c) 10, (d) 9, and at M point for TBL for mode (a') 12, (b') 11, (c') 10, (d') 9. Note that for modes (a), (a') and (b), (b'), the displacement fields are nearly identical whereas for modes (c), (c') and (d), (d'), they are very slightly offset (Figure 1(i) and (ii)). The color map indicates large (red) to zero (blue) displacement. The vector field represents the total displacement vector.
6.4 Conclusions

By utilizing these two general design principles, one governing the global properties and one
governing the local wave interactions of phonons within the structure, we demonstrate that it
is indeed possible to impose controls over spectral gaps in a rational fashion and even control
the band curvature.

By first considering how the plane group symmetry of the crystal manifests itself in the global
constraints placed on the dispersion relation of the crystal, we describe design principles for
controlling the allowed evolution of the eigenmodes of the phononic crystal, this led us to
choose a p4gm plane group for our starting structure, which ensures band sticking along low
symmetry BZ edges. This global principle determines the irreps of each eigenmode by defining
specific site symmetry representations via the isotropy groups along various direction in k-
space, giving a very useful and tractable handle towards controlling the eventual band
dispersion. This directed the specific approach we should exploit in controlling the
eigenfrequencies from a variational viewpoint, which was our local design principle. Finally,
building on earlier work (chapter 4), we recognize that the actually dynamics, and hence
dispersion and curvature of the bands hinges crucially on the lattice class of the structure,
 hence our final choice of a tight-binding lattice class completed our design process, allow us to
design a phononic crystal to have polychromatic spectral gaps utilizing a relatively simple
geometric structure. Beyond its tremendous importance as a analysis tool in understanding
certain selection rules in scattering processes and to examine spin-orbit coupling processes [59,
60, 61], the imprint of the symmetry of the system on the eigenmodes affords a powerful alternative to its usage as a tool to guide design of phononic crystals, cavities and waveguides etc. Importantly, in this work, symmetry has allowed us to make sense of how to most completely deal with the vectorial nature of the in-plane elastic waves/phonons vis a vis our local design principles, to achieve our desired phononic structure. While the entire design principle might seem involved, we note there that the salient point here is that the global symmetry principles determined the entire framework and language in an unambiguous manner, to allow us to ‘microscopically’, or locally alter the dispersion relation in a coherent and controlled fashion. Symmetry has proven here, more than in the previous chapter, its power as an elegant language with which to design, not just analyze the dispersion relations because it laid the foundations with which to apply all the subsequent design principles which we’ve had to invoke to arrive at our final design.
Chapter 7. Conclusions and Future Work

7.1 Summary of Work

In this thesis, we developed a generalized framework for the design of Artificial Structures (AS) that control phonons, or elastic waves. Our approach differs from others because we focused on the fundamental physical limits of phonon propagation in structured materials, reducing the governing principles into an identifiable minimal set. We call this the science of designing structures for manipulating phonons. By focusing on our own understanding of the propagation of phonons in structured materials, we believe that we will be able to develop a coherent understanding of phonon propagation that is valid across the meso-scales and is independent of the dimensionality and size of the structure.

More importantly, we believe that the current lack of a deterministic framework with which to guide the design of surfaces, waveguides and finite structures is due to the fact that technological concerns have been sometimes misinterpreted as scientific principles! One such instance is the reliance of fill fraction as a design parameter. Although a practical engineering parameter, fill fraction actually affects a multiplicity of issues in phonon propagation. These usually obscure the causal behavior of $\omega(k)$ when fill fraction is viewed as a primary design parameter from the engineering perspective. Instead we take inspiration instead from both a “more is different” [82] but at the same time, reductionist approach of paying care to the fundamental symmetries and develop our framework by building on symmetries and conservation principles. Our framework utilizing group theory places the design of various phononic structures, crystals, metamaterials and plates on the same footing. Importantly, this
point of view directly elucidates the vector nature of the phonon in a solid structure, an issue that has prevented the current scientific community from being able to identify the true underpinnings of the principles governing phonon propagation in Artificial Structures.

Our framework is surprisingly simple, in that it relies primarily only on two fundamental principles. One of these was the global group symmetry, which governs the allowed degeneracies of the eigenfrequencies at specific positions and along specific directions vis a vis the plane group and point group symmetry. The global symmetry imparts on the structure the second principle, namely the eigenmodes are classified by a set of irreducible representations. The irreducible representation confers significant physical insight: they are the actual classification of the polarization states of every eigenmode in any structure, just like the transverse and longitudinal modes, which we are familiar with, in bulk homogeneous systems. Moreover, the irreducible representations govern the possibility of interactions between different eigenmodes (scattering, resonant couplings etc...), shaping the dispersion relations and forming the spectral gaps which result from avoided crossings of bands with the same irreducible representation. Furthermore, the irreducible representations, when viewed from a variational perspective, help interpret the relative positioning of the eigenfrequencies. For example, we utilized this to our advantage when designing the polychromatic phononic metamaterial (chapter 5), by controlling the positioning of eigenfrequencies in specific (anti)symmetric-symmetric pairs as a function of the energetics. This variational perspective of viewing the propagation of phonons is complimentary to the conventional microscopic method of tracing the time evolution of the equations of motion. It automatically incorporates all the
interactions governing the final trajectory of the propagation into the set of possible $\omega(k)$ solutions for the structure.

The two symmetry principles control the possibility of interactions and provide the framework and importantly, the *language* which we utilize to design the dispersion relations. To realize the final design of a phononic structure, we further developed concepts, in our “symmetry” language, that govern the physical propagation of phonons within the structure. This is derived from conservation and continuity principles, enabling us to develop the concept of the dynamic mechanical bond and our lattice classification of the topology of the phononic structures.

From the viewpoint of the continuity and flux equations (chapter 2), the variational perspective of flux flow in a inhomogeneous medium allowed us to uncover a simple material and geometric parameter in classifying the type of dynamics which the propagating phonons possess in artificial structures, leading to the concept of a dynamic mechanical bond and the classification of different structures, with different combinations (solid-solid, solid-air) into different lattice classes. This helped to reconcile a long-standing argument with regards to the optimal physical topography for a phononic crystal. Crucial to this was the recognition that one needs to separate the geometric definitions of the matrix and scattering phase from the material choices for each phase. This method of classification was able to identify and reconcile the observed phonon dynamics within these structures in a coherent fashion and properly subsumes previous results within this new lattice classification scheme. As a result, we are able to create phononic AS with a wide and even *new* set of properties, ranging from phononic materials with complete and polarization specific meso-scale in plane gaps, to polychromatic

201
gaps and to large single gaps that are a significant improvement over the current state of the art (~2 to 3 fold), all by utilizing the same set of governing principles to deliberately design these properties. Many of these designs show a significant advancement over the current state of the art. Some of these, including the polychromatic band structure (Chapter 6), have never been previously realized or thought possible and offer very interesting new routes towards the control of phonon-phonon interactions and even the molding of nonlinear elastic waves. This new design paradigm for artificial structures allows new technologically useful properties via molding phonon flow. The technological requirements and metrics become constraints and inputs for the realization of unique devices that exhibit novel behavior enabled by the unique physics.

7.2 Technological Applications of Phononic Networks

The pursuit of a universal design framework to control the flow of phonons, photons and other vector/scalar waves through rational design of artificial structures affords an extremely interesting way to greatly further the reach of materials science and engineering. As outlined in the beginning of the thesis, the conception of phoXonic crystals and metamaterials has contributed greatly to the development of classes of interesting devices, such as compact negative refractive lenses, broadband filters, super-couplers and even possibly cloaks. Our approach to the science of manipulating phonons avoided potential pitfalls of adopting empirical design rules often arising from engineering constraints and instead concentrated on the fundamental symmetry principles to control phonon propagation behavior. We now make some suggestions and speculations on how one may apply some of this work to several
technological applications of relevance, including X_1oX_2onics: phononics, photonics and
magnonics (X_1=p, m and X_2=n,t).

In the work of this thesis, we demonstrated the possibility of creating artificial structures with
various unique band diagrams, from those having extremely large single complete spectral
gaps, to those having multiple complete in-plane spectral gaps. Such structures offer unique
opportunities for exploring the control of nonlinear wave propagation and wave interactions.
In the dispersion relations in the linear phonon regime, we noted the ability to create multiple
frequency spectral gaps also implies the ability to control the interactions between phonons of
different frequencies, i.e. phonon-phonon interactions. While the phonon-phonon scattering
process is inelastic and often times nonlinear, the intrinsic material nonlinearities, which govern
the phonon-phonon scattering processes are embodied in the material constitutive relations
(chapter 2) and hence do not alter the fundamental continuity and flux equation starting points.
Hence, even in the linear regime, our designed phononic structures offer a valid starting point
as well as a framework on which to build on the development and understanding of these
nonlinear processes. Some of the most promising applications that come to mind include i)
improving the ZT of thermoelectric materials by engineering the thermal conductivity to ii)
PhoXonic Metamaterials for breaking up the propagation of high energy nonlinear pulses, such
as shock waves and solitons. We offer here some speculation and possible future directions for
technological considerations for phononic structures.
7.2.1 Thermoelectrics and Engineering Thermal Conductivity

Figure 7.1 a) Map of ZT vs Temperature for state of the art thermoelectric materials [87]. b) Progress Map tracing the evolution of ZT performance of various thermoelectric materials over the years [88]. c) Map of ZT vs Temperature for various state of the art commercial bulk thermoelectric materials as well as those utilized and developed by NASA for space thermoelectric power generation [6].

Recent interest in the search for improved renewable and sustainable energy sources has highlighted the need for new technologies for harvesting energy; thermoelectric (TE) devices currently play a very minor role – mostly TE devices are employed in portable refrigeration units or as coolers for electronic equipment. However, with further research and exploitation, TE has a large future potential for major contribution to practical energy technologies since thermoelectrics can harvest energy from waste heat present in all technological processes. TEs thus provide the opportunity of an essentially ‘zero cost’ source of either electrical power or
cooling. At the same time, it is a well known fact that controlling heat flow or phonon flow is a very challenging problem. The history of thermoelectric materials performance has exhibited essentially no change for nearly 40 years until the dramatic upswing in the figure of merit (ZT) in the past decade [Figure. 1]. This sudden jump in progress can be attributed, in no small part, to the development of fabrication and characterization methods that allow manipulation of materials on the nano-scale.

The efficiency of a thermoelectric device can be summarized with the following figure of merit (FOM):

$$ZT = \frac{S(T)^2 T}{\rho (\kappa_e + \kappa_l)}$$

$T =$ temperature, $S(T) =$ Seebeck Coefficient, $\rho =$ electronic resistivity, $\kappa_e =$ electronic thermal conductivity, $\kappa_l =$ lattice thermal conductivity

The efficiencies of both thermoelectric power generation as well as Peltier cooling depend on $ZT$. Hence, the higher the FOM, the more efficient a thermoelectric device and hence its potential to be an alternative energy source. The main strategy has been to increase the Seebeck coefficient while at the same time reducing the electrical resistivity and thermal conductivity of the material system. The Seebeck coefficient, which corresponds to the voltage developed per unit temperature difference across the device, can be improved by controlling the electronic structure of the material, by engineering either the electronic density of states or the electronic transport properties of the material [83, 5]. At the same time the thermal conductivity (more specifically, the lattice contribution to the thermal conductivity) can be
reduced by impeding phonon transport in the material. There have been many approaches for reducing the thermal conductivity, divided broadly into (1) bulk material composition approaches [83] and (2) artificial structuring of the material [84,85]. It is the latter approach that we focus on.

Structuring of the thermoelectric material includes use of nano-composites [5], superlattices [42] and nanowires [85]. All these approaches aim to increase phonon scattering, by increasing the density of scattering surfaces/interfaces for the phonons by either geometrical confinement effects (nanowires, superlattices (in-plane propagation)) or introducing inhomogenities in the structures (nanograin size composites, superlattice (out-plane)). Figure 7.1(a) shows the effect of this ‘phonon-engineering’ approach in the enhancement of the FOM in the Bi-Te and Pb-Te alloy based systems, compared with the parallel development of bulk complex thermoelectric materials [Figure 7.1(c)] that are available commercially as well as under development at NASA.

These approaches can be unified into the notion of fabricating materials with correct compositions and appropriate length scale structures, such that electrons and phonons will interact with the materials at their respective physical length scales, to produce the desired thermoelectric power generation or cooling effects. Appropriate length scales straddle the sub-nm to sub-micron regime and hence, were not easily accessible until recently with the development of nanofabrication equipment -- indeed, this explains the sudden jump in FOM via nanoscale breakthroughs over the past decade [Fig7.1(b)]. Moreover it appears that there has not yet been a clear focus toward a design strategy of an optimal thermoelectric material; theoretical approaches have explored only the available materials processing platforms or
focused on computations for simple structures which have already been built. The structures
considered have mostly been limited to superlattices; only recently have TE investigations been
extended to nanostructures such as nanowires and nano-composites. From a more
fundamental perspective, current theoretical methods have not yet been able to make
quantitative predictions on the thermal conductivity of nano-structured thermoelectric
materials. Hence, while experimental capabilities have managed to allow access to these
nanoscale dimensions, there are several fundamental notions on thermal transport and
thermoelectric efficiency which have not been fully understood. It is important to note here
that quantitative methods of predicting thermal conductivity would open the avenues not just
to more efficient methods of designing optimal thermoelectrics, but also to the question of
finally being able to control thermal management of structures and materials over the meso-
scale, something that is crucial to device performance and reliability. For example, dielectric
structures (films, multilayers) with high thermal conductivities are desired in order to rapidly
dissipate heat on dense electronic device platforms [86], while structures with low thermal
conductivities are required to enhance the efficiency of thermoelectrics. Theoretical methods
that can quantitatively calculate and predict the conduction of heat at these small scales
become crucial in the development of novel electronic and thermoelectric devices [45]. While
the strategies and routes towards the nanoengineering of composite materials have been
diverse, there remains a need for a series of rational design principles to help guide the
realization of optimal structures for controlling thermal emission and thermal flow and phonon
and photon propagation in general. A TE device that was structured as a phononic crystal
would effectively reduce the thermal conductivity of the material while maintaining good
electronic conductivity. This is possible because the physical de-Broglie wavelengths of phonons and electrons are very different, hence by structuring the materials at the correct length scales, we can selectively control the phonon behavior and for example, increase the FOM by reducing thermal conductivity, while keeping the electron resistivity largely unaffected. For example, by adding inclusions (e.g. voids), we reduce both the electrical conductivity and the thermal conductivity by reducing the effective cross section (purely geometrical effect), but most importantly by designing the inclusion feature size and spacing to be on the order of the average phonon wavelength for the temperature of the material, we can greatly influence the phonon scattering by creating the set of interfaces between the two materials having quite different mechanical impedances and hence reduce the thermal conductance. Heat transport is nonlinear and is inherently coupled to the intrinsic material parameters of surface and interface roughness and compositional purity, which strongly impacts the mean free path and coherency of the phonons as well. Our design framework allows us a coherent platform to probe the dynamics of phonon-phonon interaction because of our ability to correct classify the polarization states of the different phonon eigenmodes and hence the subsequent phonon-phonon interactions. This enables finding selection rules for the vector phonon-phonon interactions, something that has not been dealt with much so far [46]. From a scientific perspective, phonon-phonon interactions belong to the extremely rich realm of many-body physics. The control of the linear dispersion and most importantly, the polarization states, offer a promising route with which one may now design these AS to replicate many-body behavior in a more-controlled manner, i.e. dealing with particular frequency regimes. While manipulating thermal conductivity points certainly to an immediate technological area of relevance, the
possibilities of being able to rationally control the degree of (non)linearity in the interactions between phonons offers promise for the development of new thermal management materials and has implications for other phonon-Xonon interactions.

7.2.2 PhoXonic Metamaterial Networks and Information Processing

The development of a complete theoretical tool-box operating with a universal set of design principles for the design of structures and devices with arbitrary application requirements would significantly open up technical applications and shorten the search for promising candidates for the desired device application before prototyping and subsequent experimental characterization. As previously mentioned, a direct extension of this current work is the desire to enable wave propagation control using a structure with a form factor significantly more compact than that utilizing “scattering”; this was one of the touted considerations leading to the development of metamaterials, although this remains somewhat immature in its development. From a technological and device standpoint, it is important to be able to include form factor requirements in the development of devices that can exploit these unique phonon dynamics. Some of these questions include, how does one go about designing a finite device, based on the theoretical infinite systems in order to achieve the optimal level of performance possible in the required form factor? Producing entire classes of structures with unique opportunities for controlling the flow of photons and phonons within a wide window of frequencies/wavelengths, with the additional advantage of having a compact form factor (up to 1 to 2 orders of magnitude smaller compared to the wavelength of interest). Furthermore,
by being able to create structures with different dispersion relations out of a single monolithic material, one will be able to design an entire network of structures that may almost arbitrarily mold, deflect and shape incident (non)linear elastic vector and acoustic scalar waves in a wide variety of applications, ranging from absorption to even information processing.

To extend the work further, the generality of our framework is transitive from phonons to photons, spin waves as well as coupling interactions in inelastic processes. The proviso is to understand and classify the different waves into the correct lattice classes with respect to the structure we decide on. What is of potential interest is the application of this current framework to the parallel fields of photonics and magnonics to pursue the discovery of new and perhaps better classes of photonic and magnonic structures.

7.3 Current and Future Work: Xoxonics?

The concepts of broken symmetry are general and can also apply to broken symmetries at an internal interface or free boundary. In bulk media, there are the well known Stoneley modes and Rayleigh modes [4], as we previously discussed [Figure 7.2]. Figure 7.1(a) shows a semi-infinite medium, with one free surface. As the symmetry is broken along this surface, a new mode, the Rayleigh mode appears. This Rayleigh mode is an edge or surface mode, analogous to surface waves. In comparison, when we compare with a finite slab, as before in the classical Lamb plate [Figure 7.1(b)], the mirror symmetry and the presence of two symmetric boundaries, causes symmetry to be broken at two spatial locations, leading to two broken symmetry modes. In this case, the mirror plane forces the Rayleigh-like modes to be coupled at
both boundaries, forming, symmetric and anti-symmetric irreducible representations with respect to the mirror plane.

Figure 7.2 Eigenmode plots. (a) a single edge mode in a semi-infinite medium (the lower bound extends to infinity) of which we show a section near the surface (b) the antisymmetric coupled surface Rayleigh mode and (c) the symmetric coupled surface Rayleigh of a Lamb plate, or a finite slab. The color map indicates large (red) to zero (blue) displacement.
This simple problem is exactly analogous to the situation of surface modes of phononic metamaterials. Current work in the community suffers from a lack of a governing principle with which to design a surface of an otherwise bulk volume phononic or photonic metamaterial. The design of the surface is extremely important for devices because the interface between the device and the external (interacting) environment, governs the propagation and hence distribution of information within the metamaterial. Once again, the link between this demonstration of broken symmetry leading the presence of a surface, interface or edge mode and that of surface, edge and interface modes lies once again in the length scale of the propagating waves and the artificial structure inhomogeneity [89].

To reiterate, the eventual goal of this approach is, to borrow from PW Anderson’s [82] famous words, that “more is different”, to understand complexity from a set of simple principles. In a somewhat analogous approach, we have focused on only utilizing the underlying symmetries of the system to deduce the possible eigenmodes of phonons. Moreover, our framework is not restricted to phonons, but works for all fields, vector or scalar, with the only proviso that we correctly identify the relevant length scales. This suggests that this approach would enable design of efficient multi-functional phononic-photonic-magnonic (XoXonic) networks that the different kinds of waves with one another at specific spatial locations because our design rules are not based on artificial requirements of infinite periodicity and may treat interfaces, boundaries and the bulk alike.

It is interesting to contemplate Nature’s various phononic networks, the auditory systems of all living organisms. From the complexity and meso-scale multiple sensing auditory system of insects [90] to the compact yet broadband auditory systems of humans, it will be interesting to
determine if Nature exploits symmetries to develop an efficient auditory systems, subject to
the needs of various situational awareness and of course, the constraint of the available
constituent materials found in all living forms.
A ‘complex’ system can be described by a few ‘simple” fundamental principles, just like how a
complicated phononic band structure can be described and dictated by a few governing rules.
To truly realize a multi-functional Xoxonic (X=m, t, n, for photonics, phononics and magnonics)
metamaterial network, this same set of underlying simple principles will provide a tractable
way for us to realize fully functional integrated material platforms and extend the materials
design and performance paradigm and to be able to control complexity with simplicity.
Bibliography

2. Love AEH, *A Mathematical Treatise of Elasticity*, University of Michigan (1906)
47. Lax M, “Multiple Scattering of Waves”, Rev. Mod. Phys, 23, 287(1951)
75. Ao XY, Chan CT, “Complex Band Structure and effective medium descriptions of periodic acoustic systems”, PRB, 80, 235118 (2009)