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Photonic band structure calculations for 2D and 3D photonic crystals

Aaron Vincent Morton
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PHOTONIC BAND STRUCTURE CALCULATIONS FOR 2D AND 3D
PHOTONIC CRYSTALS

A Thesis

Presented to

The Faculty of the Department of Physics

San Jose State University

In Partial Fulfillment

of the Requirements for the Degree

Master of Science

by

Aaron Vincent Morton

August 2002

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ABSTRACT

PHOTONIC BAND STRUCTURE CALCULATIONS FOR 2D AND 3D PHOTONIC CRYSTALS

by

Aaron Vincent Morton

Photonic crystals are dielectric materials containing a periodicity in dielectric constant. The periodic dielectric constant can create a range of forbidden frequencies for electromagnetic waves called a photonic band gap. Photonic band structure calculations are performed for several two-dimensional and three-dimensional photonic crystal geometries. Using a plane wave expansion, Maxwell's equations are solved numerically using a frequency-domain computational method that takes the vector nature of the electromagnetic field into account. Photonic band gaps are found to exist for both two-dimensional and three-dimensional photonic crystal geometries. Specifically, Photonic band gaps are confirmed for both the triangular lattice in two dimensions and for the diamond lattice in three dimensions. For the diamond lattice of spheres of low-dielectric constant embedded in a background of high-dielectric constant, the effects of packing fraction and dielectric constant on photonic band gap width are investigated.

To my wife Brenda.

Acknowledgments

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Contents

List of Figures	ix
1 Introduction	1
1.1 Photonic Crystals	3
1.2 Two-Dimensional Photonic Crystals	5
1.2.1 Square Lattice Photonic Crystals	6
1.2.2 Triangular Lattice Photonic Crystals	7
1.3 Three-Dimensional Photonic Crystals	8
1.3.1 fcc Lattice Photonic Crystals	8
1.3.2 Diamond Lattice Photonic Crystals	9
1.4 Photonic Band Structure	9
1.5 Potential Applications of Photonic Crystals	12
1.6 Comparison with Electronic Band Structure	15
1.7 Scope and Outline	19
2 Theoretical Framework	21
2.1 Maxwell's Equations	21
2.2 Maxwell's Equations and Photonic Crystals	23
2.3 Plane Wave Expansion of Maxwell's Equations	25
2.4 Two-Dimensional Photonic Crystals	31
2.4.1 The Square Lattice of Dielectric Columns	33
2.4.2 The Triangular Lattice of Dielectric Columns	39
2.5 Three-Dimensional Photonic Crystals	42
2.5.1 The fcc Lattice of Dielectric Spheres	43
2.5.2 The Diamond Lattice of Dielectric Spheres	49
3 Numerical Methodology	54
3.1 Frequency-Domain Computational Method	54
3.1.1 Numerical Method in Two Dimensions	55
3.1.2 Numerical Method in Three Dimensions	57

3.2	Convergence of the Frequency Eigenvalues	59
4	Two-Dimensional Results	60
4.1	The Square Lattice of Dielectric Columns	61
4.2	The Square Lattice of Air Columns	62
4.3	The Triangular Lattice of Dielectric Columns	63
4.4	The Triangular Lattice of Air Columns	65
5	Three-Dimensional Results	68
5.1	The fcc Lattice of Dielectric Spheres	68
5.2	The fcc Lattice of Air Spheres	70
5.3	The Diamond Lattice of Dielectric Spheres	71
5.4	The Diamond Lattice of Air Spheres	72
5.4.1	Effect of Packing Fraction on Gap Width	75
5.4.2	Effect of Background Dielectric on Gap Width	75
5.4.3	Effect of Different Sphere Dielectrics on Gap Width	76
6	Conclusions	79
6.1	Summary of Results	80
	Bibliography	83
A	MATLAB Code.	86
A.1	2D Photonic Band Structure Code	86
A.2	3D Photonic Band Structure Code	96

List of Figures

1.1	(a) The two-dimensional square lattice of columns of high-dielectric ϵ_a (shown in blue) in a background of low-dielectric constant ϵ_b . (b) The square lattice of columns of low-dielectric constant ϵ_a (shown in white) in a background of high-dielectric constant ϵ_b	6
1.2	(a) The two-dimensional triangular lattice of columns of high-dielectric constant ϵ_a (shown in blue) in a background of low-dielectric constant ϵ_b . (b) The triangular lattice of columns of low-dielectric constant ϵ_a (shown in white) in a background of high-dielectric constant ϵ_b	7
1.3	(a) The three-dimensional fcc lattice of spheres of high-dielectric constant ϵ_a (shown in blue) in a background of low-dielectric constant ϵ_b . (b) The fcc lattice of spheres of low-dielectric constant ϵ_a (shown in white) in a background of high-dielectric constant ϵ_b	8
1.4	(a) The three-dimensional diamond lattice of spheres of high-dielectric constant ϵ_a in a background of low-dielectric constant ϵ_b . (b) The diamond lattice of spheres of low-dielectric constant ϵ_a in a background of high-dielectric constant ϵ_b	9
2.1	(a) The real-space representation of the two-dimensional square lattice of columns of high-dielectric constant ϵ_a (shown in blue) in a background of low-dielectric constant ϵ_b . (b) The reciprocal-space representation of the two-dimensional square lattice of columns of high-dielectric constant ϵ_a in a background of low-dielectric constant ϵ_b . (c) The reciprocal-space representation of the two-dimensional square lattice shown in (b) with the square Brillouin zone highlighted (in grey). The triangular irreducible portion of the Brillouin zone is shown in the upper right corner of the Brillouin zone (in yellow).	34

2.2	An expanded view of the Brillouin zone (in grey) for the two-dimensional square lattice. The triangular irreducible portion of the Brillouin zone is shown in the upper right corner of the Brillouin zone (in yellow). The $\mathbf{k}$ -space points of high symmetry $\bar{X}$, $\bar{\Gamma}$, and $\bar{M}$ define the irreducible Brillouin zone.	35
2.3	Schematic illustration of the unit cell construction for the 2D square lattice of dielectric columns. Shown in the figure are the inverse dielectric functions for the unit cell dielectric background ($f_b^0 = \frac{1}{\epsilon_b}$) and the dielectric column ($f_a^0 = \frac{1}{\epsilon_a}$)	37
2.4	(a) The real-space representation of the two-dimensional triangular lattice of columns of high-dielectric constant ϵ_a (shown in blue) in a background of low-dielectric constant ϵ_b . (b) The reciprocal-space representation of the two-dimensional triangular lattice of columns of high-dielectric constant ϵ_a in a background of low-dielectric constant ϵ_b . (c) The reciprocal-space representation of the two-dimensional triangular lattice shown in (b) with the hexagonal Brillouin zone highlighted (in grey). The triangular irreducible portion of the Brillouin zone is shown in the upper right corner of the Brillouin zone (in yellow). . . .	40
2.5	An expanded view of the Brillouin zone (in grey) for the two-dimensional triangular lattice. The triangular irreducible portion of the Brillouin zone is shown in the upper right corner of the Brillouin zone (in yellow). The $\mathbf{k}$ -space points of high symmetry $\bar{\Gamma}$, $\bar{M}$, and $\bar{K}$ define the irreducible Brillouin zone.	41
2.6	The reciprocal-space representation of both the three-dimensional fcc and diamond lattices. The Brillouin zone is highlighted (in grey). The irreducible portion of the Brillouin zone is highlighted (in yellow). The $\mathbf{k}$ -space points of high symmetry $\bar{X}$, $\bar{\Gamma}$, $\bar{U}$, $\bar{W}$, $\bar{L}$ and $\bar{K}$ define the irreducible Brillouin zone.	44
2.7	Schematic illustration of the unit cell construction for the three-dimensional fcc lattice of dielectric spheres. Shown in the figure are the inverse dielectric functions for the unit cell dielectric background ($f_b^0 = \frac{1}{\epsilon_b}$) and the dielectric sphere ($f_a^0 = \frac{1}{\epsilon_a}$).	47
2.8	Schematic illustration of the unit cell construction for the three-dimensional diamond lattice of dielectric spheres. Shown in the figure are the inverse dielectric functions for the unit cell dielectric background ($f_b^0 = \frac{1}{\epsilon_b}$) and the dielectric spheres ($f_a^0 = \frac{1}{\epsilon_a}$).	51

4.1	The photonic band structure for the two-dimensional square lattice of dielectric columns. The transverse magnetic (TM) polarized modes are shown in blue in the figure. The transverse electric (TE) polarized modes are shown in red. The square lattice of dielectric columns possesses a photonic band gap for the TM polarized modes but not for the TE polarized modes.	62
4.2	The photonic band structure for the two-dimensional square lattice of air columns. The transverse magnetic (TM) polarized modes are shown in blue in the figure. The transverse electric (TE) polarized modes are shown in red. The square lattice of air columns does not possess a photonic band gap for either the TM or TE modes.	64
4.3	The photonic band structure for the two-dimensional triangular lattice of dielectric columns. The transverse magnetic (TM) polarized modes are shown in blue in the figure. The transverse electric (TE) polarized modes are shown in red. The triangular lattice of high-dielectric columns in an air background does not possess a photonic band gap for either TM or TE polarized modes.	66
4.4	The photonic band structure for the two-dimensional triangular lattice of dielectric columns. The transverse magnetic (TM) polarized modes are shown in blue in the figure. The transverse electric (TE) polarized modes are shown in red. The triangular lattice of air columns in a high-dielectric background does possess a complete photonic band gap for both TM and TE modes. The photonic band gap is indicated in the figure by a yellow bar, showing the range of forbidden frequencies.	67
5.1	The photonic band structure for the three-dimensional fcc lattice of dielectric spheres. A photonic band gap does not exist for this photonic crystal geometry.	70
5.2	The photonic band structure for the three-dimensional fcc lattice of air spheres. A photonic band gap does not exist for this photonic crystal geometry.	72
5.3	The photonic band structure for the three-dimensional diamond lattice of dielectric spheres. A photonic band gap exists for this photonic crystal geometry. The photonic band gap is indicated in the figure by a yellow bar, showing the range of forbidden frequencies.	73
5.4	The photonic band structure for the three-dimensional diamond lattice of air spheres. A photonic band gap exists for this photonic crystal geometry. The photonic band gap is indicated in the figure by a yellow bar, showing the range of forbidden frequencies.	74

5.5	The photonic band gap width as a function of packing fraction for the three-dimensional diamond lattice of low-dielectric spheres. The dielectric constant of the spheres ($\epsilon_a = 1$) and the dielectric constant of the background ($\epsilon_b = 13$) are fixed.	76
5.6	The photonic band gap width as a function of the dielectric constant of the background for the three-dimensional diamond lattice of low-dielectric spheres. The dielectric constant of the spheres ($\epsilon_a = 1$) and the packing fraction ($P_f = 0.34$) are fixed.	77
5.7	The photonic band gap width as a function of the dielectric constant of a single sphere of the two-sphere basis of the the three-dimensional diamond lattice of low-dielectric spheres. The dielectric constant of the first sphere ($\epsilon_{a1} = 1$), the dielectric constant of the background ($\epsilon_b = 13$), and the packing fraction ($P_f = 0.34$) are fixed.	78

Chapter 1

Introduction

The topic of this thesis is the calculation of photonic band structures for two-dimensional and three-dimensional periodic dielectric structures, so-called photonic crystals. In particular, the thesis focuses on band gaps that can form in the photonic band structures of the photonic crystals considered.

Photons have several advantages over electrons. One of the greatest advantages is that photons can travel in a dielectric material at a much greater speed than electrons in a metallic wire. Another advantage is that the bandwidth of dielectric materials is larger than that of metals. For example, in conventional fiber-optic communications systems the bandwidth is typically of the order of one terahertz, while the bandwidth of electronic systems such as those in the telecommunications industry have bandwidths of only a few hundred kilohertz. In addition, photons are not as strongly interacting as electrons, which therefore helps to substantially reduce

the energy losses in practical systems [1].

Semiconductor materials have played a huge role in virtually all aspects of everyday life since their discovery over 50 years ago. The drive towards miniaturization and high-speed performance of highly-integrated electronic circuits has stimulated tremendous research efforts in both academia and industry. However, some of the unfortunate consequences of electronic circuit miniaturization are increased resistance and increased power dissipation. Furthermore, higher circuit speeds lead to increased sensitivity to signal synchronization. Research is therefore beginning to turn towards the use of photons instead of electrons as the primary information carrier [1].

Photonic crystals are dielectric materials that contain a periodicity in dielectric constant. The periodic contrast in static dielectric constant can create a range of forbidden frequencies called a photonic band gap. Electromagnetic modes with energies lying within a band gap cannot propagate through the photonic crystal and are therefore forbidden.

In recent years [1][2], there has been a great interest in determining the photonic band structures, also known as dispersion curves, for electromagnetic waves propagating in various two-dimensional and three-dimensional photonic crystals. The goal of these investigations has been to determine whether the photonic band structures formed by the branches of these dispersion curves are separated by any photonic band gaps. To be useful, the photonic band gaps must exist for all wave vector values in the Brillouin zone for the photonic crystal under study.

Periodic dielectric structures have for years played an important role in many branches of physics. For example, interference coatings have become indispensable in the field of wave optics. The interference coatings are actually layered dielectric structures that have a quarter wavelength periodicity in their index of refraction. This dielectric periodicity creates a photonic band gap in the electromagnetic dispersion curves for those electromagnetic waves that propagate perpendicular to the layers. This one-dimensional photonic band gap makes these one-dimensional periodic dielectric structures valuable as highly ideal reflective mirrors. An example of a popular device that takes advantage of this one-dimensional photonic band gap is the Fabry-Perot resonator. The prospect of similarly useful device applications has provided tremendous motivation to create both two-dimensional and three-dimensional photonic crystals in which there exists a photonic band gap. Photonic crystals therefore offer the possibility of allowing for unprecedented control and manipulation of light.

1.1 Photonic Crystals

The exciting potential of photonic crystals is the ability to have unprecedented control over the properties of light within the photonic crystal. Yablonovitch [3] and John [4] were the first to suggest the idea of designing materials that might affect the properties of photons analogous to the way that ordinary semiconductor crystals

affect the properties of electrons. It was suggested that structures that were periodic in dielectric constant could dictate which electromagnetic modes might exist.

There is a strong analogy between photonic crystals and semiconductor crystals. An electron propagating through a semiconductor crystal sees a periodic potential created by the atomic lattice. Because of Bragg-like diffraction from the atoms in the semiconductor crystal lattice, a gap in allowed electron energies opens up. Electrons with energies in this forbidden range cannot propagate in the semiconductor crystal in any direction. In a photonic crystal the analogous periodic potential, (the mechanism causing the Bragg-like diffraction), is due to a lattice of periodic dielectric contrast. An example is a periodic arrangement of dielectric columns in two dimensions or of dielectric spheres in three dimensions. If the dielectric constants of the columns or spheres are different enough from the dielectric constant of the background crystal then Bragg-like scattering off of the dielectric interfaces can produce many of the same phenomena for photons as the atomic potential of a semiconductor crystal creates for electrons. Therefore, a photonic band gap in a photonic crystal may be viewed as the optical analogue of the electronic band gap in a semiconductor.

In an electronic crystal the periodic potential and lattice constant are fixed, so any resulting energy gap will be fixed. However, in a photonic crystal one can design a crystal with any lattice constant and equivalent periodic potential, thereby allowing the gap to be controlled. On the other hand, in an electronic crystal the potential is strong enough to result in a gap for many types of crystal lattices, whereas in

photonic crystals the existence of a photonic band gap is highly dependent on the lattice geometry and dielectric contrast. As a result, there are fewer examples of three-dimensional photonic crystals which possess photonic band gaps.

A photonic crystal might therefore be engineered to possess a photonic band gap for a specific range of frequencies for which electromagnetic waves are forbidden to exist within the crystal. The electromagnetic modes would be forbidden in a perfectly periodic photonic crystal. However, if there is a defect in the otherwise perfectly periodic crystal, localized photonic states could exist within the photonic band gap. A point defect within an otherwise perfectly periodic photonic crystal might act like a microcavity, a line defect might act like a waveguide, and a planar defect might act like a perfect mirror [1].

1.2 Two-Dimensional Photonic Crystals

There have been several previous studies [2][5], of the photonic band structures of both two-dimensional and three-dimensional photonic crystals. A variety of such photonic crystals are considered. A two-dimensional photonic crystal is periodic along two of its axes and homogeneous along the third. Two classes of two-dimensional photonic crystal are considered. The first is a photonic crystal formed by a square lattice of dielectric columns of dielectric constant ϵ_a in a different dielectric background of dielectric constant ϵ_b . The second is a photonic crystal made by arranging

the dielectric columns in a triangular lattice.

1.2.1 Square Lattice Photonic Crystals

Figure 1.1(a) illustrates the first class of two-dimensional photonic crystals to be studied, namely, the square lattice of columns of high-dielectric constant ϵ_a in a background of low-dielectric constant ϵ_b . Figure 1.1(b) shows the square lattice of columns of low-dielectric constant ϵ_a in a background of high-dielectric constant ϵ_b .

The square lattice structure consists of a periodic array of parallel dielectric columns of circular cross section and dielectric constant ϵ_a whose intersections with a perpendicular plane form a square lattice. The dielectric columns are embedded in a dielectric material whose dielectric constant is ϵ_b .

Figure 1.1: (a) The two-dimensional square lattice of columns of high-dielectric ϵ_a (shown in blue) in a background of low-dielectric constant ϵ_b . (b) The square lattice of columns of low-dielectric constant ϵ_a (shown in white) in a background of high-dielectric constant ϵ_b .

1.2.2 Triangular Lattice Photonic Crystals

The second class of two-dimensional photonic crystals to be considered is illustrated in Figure 1.2. Figure 1.2(a) shows a two-dimensional photonic crystal that is comprised of a triangular lattice of columns of high-dielectric constant ϵ_a in a background of low-dielectric constant ϵ_b . Figure 1.2(b) shows the triangular lattice of columns of low-dielectric constant ϵ_a in a background of high-dielectric constant ϵ_b .

The triangular lattice structure consists of a periodic array of parallel dielectric columns of circular cross section and dielectric constant ϵ_a whose intersections with a perpendicular plane form a triangular lattice. The dielectric columns are embedded in a dielectric material whose dielectric constant is ϵ_b .

The square lattice and triangular lattice photonic crystals are of interest because dielectric structures with these symmetries are now being fabricated for experimental studies of photonic band structures [5].

Figure 1.2: (a) The two-dimensional triangular lattice of columns of high-dielectric constant ϵ_a (shown in blue) in a background of low-dielectric constant ϵ_b . (b) The triangular lattice of columns of low-dielectric constant ϵ_a (shown in white) in a background of high-dielectric constant ϵ_b .

1.3 Three-Dimensional Photonic Crystals

A three-dimensional photonic crystal is periodic along all three axes. Two classes of three-dimensional photonic crystals are studied. The first is the fcc lattice photonic crystal. The second is the diamond lattice photonic crystal.

1.3.1 fcc Lattice Photonic Crystals

Figure 1.3(a) illustrates the first class of three-dimensional photonic crystals to be studied, namely, the fcc lattice of spheres of high-dielectric constant ϵ_a in a background of low-dielectric constant ϵ_b . Figure 1.3(b) shows the fcc lattice of spheres of low-dielectric constant ϵ_a in a background of high-dielectric constant ϵ_b .

Figure 1.3: (a) The three-dimensional fcc lattice of spheres of high-dielectric constant ϵ_a (shown in blue) in a background of low-dielectric constant ϵ_b . (b) The fcc lattice of spheres of low-dielectric constant ϵ_a (shown in white) in a background of high-dielectric constant ϵ_b .

1.3.2 Diamond Lattice Photonic Crystals

Figure 1.4 illustrates the second class of three-dimensional photonic crystals to be studied. Figure 1.4(a) shows the diamond lattice of spheres of high-dielectric constant ϵ_a in a background of low-dielectric constant ϵ_b . Figure 1.4(b) shows the diamond lattice of spheres of low-dielectric constant ϵ_a in a background of high-dielectric constant ϵ_b .

Figure 1.4: (a) The three-dimensional diamond lattice of spheres of high-dielectric constant ϵ_a in a background of low-dielectric constant ϵ_b . (b) The diamond lattice of spheres of low-dielectric constant ϵ_a in a background of high-dielectric constant ϵ_b .

1.4 Photonic Band Structure

The analogy between photonic crystals and semiconductor crystals is more easily seen when one considers the so-called master equation for photonic crystals. In the absence of external currents and sources, Maxwell's equations can be re-written, (as

is done in chapter 2), in the following simple form that is very similar in appearance to the Schrödinger equation. This equation for photonic crystals is given as,

$$\nabla \times \frac{1}{\epsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) = \left(\frac{\omega}{c}\right)^2 \mathbf{H}(\mathbf{r}) \quad (1.1)$$

Where $\mathbf{H}(\mathbf{r})$ is the magnetic field of the photon, ω is its frequency, c is the speed of light and $\epsilon(\mathbf{r})$ is the macroscopic dielectric function describing the photonic crystal. Equation 1.1 represents a linear Hermitian eigenvalue problem. The eigenvalues, or eigenfrequencies, are determined entirely by the macroscopic dielectric function $\epsilon(\mathbf{r})$. If $\epsilon(\mathbf{r})$ is perfectly periodic, as in a perfect photonic crystal, the solutions are characterized by a wave vector $\mathbf{k}$ and a band index n . The collection of eigenfrequency dispersion curves as a function of the wave vector, usually taken in the first Brillouin zone, is referred to as the photonic band structure.

The photonic band structure depends on the lattice constant, a , the radius of the dielectric column in two dimensions, or sphere in three dimensions, and the dielectric contrast between the cylinder or sphere relative to the material making up the background of the photonic crystal. One of the key differences between the study of photonic band structure and electronic band structure is that in the study of photonic crystals, (through Maxwell's equations), there is no fundamental length scale [1]. In the study of semiconductor crystals, (using Schrödinger's equation), the potentials have a fundamental length scale on the order of the Bohr radius. Therefore crystals that differ only in their absolute length scale will have very different electronic band

structures. The situation is quite different with photonic crystals, where solutions at different length scales differ by a simple scale factor. Therefore, the solution for the photonic band structure at one length scale determines the photonic band structure at all other length scales. A comparison of photonic band structure calculations with electronic band structure calculations is discussed in section 1.6.

Photonic band gaps may exist for a variety of photonic crystals. The gap is a region of frequencies for which no electromagnetic modes may exist within the photonic crystal for any value of the wave vector $\mathbf{k}$ within the Brillouin zone. The band above a photonic band gap is commonly referred to as the air band and the band below a photonic band gap is commonly referred to as the dielectric band. These photonic band structure terms are analogous with the use of the terms conduction band and valence band for the electronic band structure of semiconductor crystals.

Since electromagnetic modes with frequencies that are within the photonic band gap are forbidden, spontaneous emission will be forbidden in cases in which the photonic band gap overlaps the electronic band edge. This suppression of spontaneous emission can dramatically improve the performance of many optical and electronic devices [5]. It is therefore desirable to obtain a photonic band structure with a photonic band gap, within which the propagation of electromagnetic waves is forbidden for all wave vectors $\mathbf{k}$ within the Brillouin zone.

Early theoretical studies of the propagation of electromagnetic waves in photonic crystals were based upon the scalar-wave approximation [6] in which the vector nature

of the electromagnetic field is ignored. These calculations did not give correct results for the band structure [2]. Recent theoretical studies of photonic crystals [1][2][7], therefore rely on the fully vectorized electromagnetic field.

The translational symmetry of a photonic crystal is broken by addition of a dielectric defect. This is essentially a change in the dielectric constant of a specific region within the otherwise perfectly periodic photonic crystal. These dielectric defects may result in defect states within the photonic band gap, permitting a localized mode to exist about the defect within the crystal. Dielectric defects result in defect states within the photonic band gap just below the air band, while air defects result in defect states just above the dielectric band of the photonic band structure [1][8]. These are similar to the impurity levels in semiconductors.

1.5 Potential Applications of Photonic Crystals

Spontaneous emission plays a fundamental role in limiting the performance of semiconductor lasers, hetero-junction bipolar transistors, and solar cells. If a three-dimensional photonic crystal has a photonic band gap that overlaps the electronic band edge then spontaneous emission can be significantly reduced or even forbidden. Entirely optical circuits have yet to be commercially available on a large scale despite the numerous advantages of photons over electrons. Several hybrid opto-electronic circuits have been produced that have significantly improved the performance of elec-

tronic circuits. However the difficulties in designing an optical component analogous to the electronic transistor have severely hindered the spread of entirely optical systems [1]. Photonic crystals may hold the key towards the continued progress towards entirely optical integrated circuits [2].

A two-dimensional photonic crystal that has a transverse magnetic (TM) band gap but no transverse electric (TE) band gap, (or vice versa), for a certain range of frequencies could be used to act as a polarizer for electromagnetic waves in the frequency range of the photonic band gap. In addition, photonic crystals that have a photonic band gap for a certain range of frequencies could act as notch filters for those frequencies, and could be useful in various microwave communications applications.

A line defect in an otherwise perfect photonic crystal gives rise to a novel type of optical waveguide. Photonic crystal waveguides provide the means to efficiently guide optical light through narrow channels of air or low-dielectric constant. If the frequency of the guided electromagnetic mode lies within the photonic band gap then the mode will be forbidden to penetrate into the bulk of the photonic crystal. Therefore the most significant source of loss can only be the reflection of the light back out the entrance to the photonic crystal waveguide, and suggests that it is possible to guide light around sharp corners [9]. The basic idea is to carve a path through an otherwise perfect photonic crystal. Light with a frequency within the photonic band gap of the crystal is confined to propagate within the waveguide. A photonic crystal optical waveguide is truly a novel mechanism for guiding light. Traditional

fiber-optic waveguides can guide light without significant losses. However, fiber-optic cables rely on total internal reflection. If a fiber-optic cable curves too tightly then the angle of incidence will become too large for total internal reflection to occur and as a result light escapes at the sharp bends and corners and is lost. Photonic crystal optical waveguides on the other hand, can continue to confine light even around tight corners and bends [2][9]. This could be tremendously useful in the fields of optical communications and optical computing.

A point defect in an otherwise perfect photonic crystal can act like an optical cavity that can trap light at the defect point within the crystal. Point defects involve changing the dielectric constant in a local region of the crystal somewhere deep within its bulk. An example would be to modify a single dielectric sphere within the bulk of a photonic crystal that was made up of a diamond lattice of air spheres as shown in Figure 1.4. Modifications might include changing the size of the sphere, changing the dielectric constant of the sphere, or removing it entirely from the photonic crystal. If the defect introduced into the photonic crystal involves the removal of dielectric then the cavity mode will evolve from the dielectric band, and is known as a so-called air defect because of the newly introduced vacancy. Similarly, if the defect involves the addition of dielectric material then the cavity mode will evolve from the air band, and is known as a so-called dielectric defect [2][10]. These properties of defects make photonic crystals a very attractive medium for the design of novel types of filters, polarizers, couplers, lasers, and light-emitting diodes [9]. For the case of either laser

or light-emitting diode cavities, photonic crystals can provide unique capability to control spontaneous emission.

Recent studies have also been carried out to develop methods to dynamically tune the photonic band gap [11][12]. For example, Leonard *et al* [11] have investigated the photonic band gap of a two-dimensional photonic crystal that was continuously tuned using the temperature dependent refractive index of a liquid crystal. The liquid crystal had been infiltrated into the air pores of a photonic crystal made by arranging a triangular lattice of air columns similar to the photonic crystal shown in Figure 1.2 (b). The goal of these photonic band gap tunability studies is to develop an optical analogue of the transistor, or an optical switch.

1.6 Comparison with Electronic Band Structure

The electronic band structure is obtained by solving the Schrödinger equation with the periodic potential of the crystal. The photonic band structure, on the other hand is obtained by solving Maxwell's equations for a crystal which is periodic in dielectric constant. Theoretical treatment to solve these equations is very similar. The field of photonic crystals has therefore inherited much of the terminology and theorems from electronic band structure calculation. This section presents a brief comparison of standard techniques and terminology used to calculate electronic band structures in semiconductor crystals with those used to calculate photonic band structures in

photonic crystals.

For the case of electrons, the scalar wave function $\Psi(\mathbf{r}, t)$ describes the properties of the electrons within the semiconductor crystal. The usual condition is that $\Psi(\mathbf{r}, t)$ must be normalizable. The time dependence of the wave function $\Psi(\mathbf{r}, t)$ is typically separated out by expanding it in a set of energy eigenstates, or normal modes $\Psi_E(\mathbf{r})$ as follows,

$$\Psi(\mathbf{r}, t) = \sum_E c_E \Psi_E(\mathbf{r}) e^{iEt/\hbar} \quad (1.2)$$

$\Psi_E(\mathbf{r})$ satisfies the time independent Schrödinger equation given by,

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \Psi_E(\mathbf{r}) = E \Psi_E(\mathbf{r}) \quad (1.3)$$

$V(\mathbf{r})$ is the crystal potential and E corresponds to the electron energy eigenvalues.

For the case of photonic crystals one can consider either the transverse electric or transverse magnetic vector field of the photon. However, because of mathematical simplicity, one usually solves for the magnetic field $\mathbf{H}(\mathbf{r}, t)$ of the photon, and then from Maxwell's equations one can find the electric field. The electric field form of the problem can be derived as well, but the result is a generalized eigenvalue problem that is much more difficult to solve numerically [2]. The time dependence of the magnetic vector field is removed through a similar expansion in a set of harmonic modes $\mathbf{H}_\omega(\mathbf{r})$ as follows,

$$\mathbf{H}(\mathbf{r}, t) = \sum_{\omega} c_{\omega} \mathbf{H}_{\omega}(\mathbf{r}) e^{i\omega t} \quad (1.4)$$

where $\mathbf{H}_{\omega}(\mathbf{r})$ satisfies the Maxwell wave equation,

$$\nabla \times \frac{1}{\epsilon(\mathbf{r})} \nabla \times \mathbf{H}_{\omega}(\mathbf{r}) = \left(\frac{\omega}{c} \right)^2 \mathbf{H}_{\omega}(\mathbf{r}) \quad (1.5)$$

Note that the operator on the right-hand side of equation 1.5 is Hermitian. Therefore, the value $\left(\frac{\omega}{c} \right)^2$ corresponds to the frequencies of the allowed modes for the magnetic vector field $\mathbf{H}_{\omega}(\mathbf{r})$.

For the case of the electron, the potential $V(\mathbf{r})$ in equation 1.3 is due to the periodic arrangement of the atoms on the crystal lattice. Therefore, it has the periodicity of the crystal lattice with the form,

$$V(\mathbf{r}) = V(\mathbf{r} + \mathbf{R}) \quad (1.6)$$

for all of the lattice vectors $\mathbf{R}$. As a result, one can write the wave function $\Psi_E(\mathbf{r})$ in the Bloch form,

$$\Psi_E(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} \quad (1.7)$$

where,

$$u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) \quad (1.8)$$

is also a periodic function having the periodicity of the crystal lattice for all of the lattice vectors $\mathbf{R}$.

The periodicity in photonic crystals arises from a macroscopic periodicity in the dielectric contrast throughout the crystal lattice. This periodicity in dielectric, $\epsilon(\mathbf{r})$, takes the following form,

$$\epsilon(\mathbf{r}) = \epsilon(\mathbf{r} + \mathbf{R}) \quad (1.9)$$

for all of the lattice vectors $\mathbf{R}$.

In a similar way, the translational symmetry of the periodic dielectric, $\epsilon(\mathbf{r})$, allows us to write the harmonic modes $\mathbf{H}_\omega(\mathbf{r})$ in Bloch form [13] as a periodic function $\mathbf{u}_\mathbf{k}(\mathbf{r})$ modulated with a plane wave component of wave vector $\mathbf{k}$ as follows,

$$\mathbf{H}_\mathbf{k}(\mathbf{r}) = \mathbf{u}_\mathbf{k}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \quad (1.10)$$

The allowable values for the wave vector $\mathbf{k}$ again lie in the Brillouin zone of the reciprocal space for the crystal under study [13][14].

The eigenvalues, $E_n(\mathbf{k})$, describe the electron energies of the allowed eigenstates or normal modes for the semiconductor crystal, where n is the band index and $\mathbf{k}$ is the wave vector. The physical origin of the band structure is due to coherent scattering of electron wave vectors from the different periodic potential regions in the crystal [13][14]. When a gap appears in the electronic band structure, no propagating electrons regardless of wave vector are allowed to exist in that energy range. This is

commonly known as an electronic band gap. Similarly, the eigenvalues $\omega_n(\mathbf{k})$ describe the frequencies of the allowed eigenstates, (or harmonic modes), for the photonic crystal, where n is the band index and $\mathbf{k}$ is the wave vector. The physical origin of the photonic band gap is due to coherent scattering of electromagnetic fields at the interfaces between different periodic dielectric regions in the photonic crystal. When a gap appears in the photonic band structure no electromagnetic modes, regardless of wave vector, can exist in that frequency range. This is commonly referred to as a photonic band gap.

1.7 Scope and Outline

Chapter 2 discusses the theoretical framework used to study photonic crystals. This chapter begins with an overview of Maxwell's equations and the approximations used. The so-called master equation for photonic crystals is derived, and the subsequent plane-wave expansion of this equation is carried out. The chapter concludes by discussing in detail both the real and reciprocal space representations of the two classes of two-dimensional and three-dimensional photonic crystals studied.

Chapter 3 describes the computational approach adopted. The chapter begins by discussing the frequency-domain computational method used. Details specific to the application of the method in both two and three dimensions are also discussed. The chapter concludes by addressing the issue of eigenvalue convergence in all of the

calculations carried out.

Chapter 4 presents the results of the application of the computational method to two types of two-dimensional photonic crystals. Specifically, the square and triangular lattices of columns of dielectric constant ϵ_a embedded in a dielectric background of dielectric constant ϵ_b are examined.

Chapter 5 presents the results of the application of the computational method to two types of three-dimensional photonic crystals. Specifically, the fcc and diamond lattices of spheres of dielectric constant ϵ_a embedded in a dielectric background of dielectric constant ϵ_b are examined.

Chapter 6 presents the conclusions, and Appendix A presents the Matlab code used for both the two-dimensional and three-dimensional calculations.

Chapter 2

Theoretical Framework

The description of electromagnetic waves in a photonic crystals involves the solution of Maxwell's equations. One of the appealing aspect of Maxwell's equations is that they can be solved exactly. Another appealing aspect of Maxwell's equations is that there is no fundamental length scale. The only assumption is that the periodic dielectric system, (the photonic crystal), is macroscopic. If the dielectric is not considered to be a function of frequency, then a photonic crystal designed at one length scale will have the same fractional photonic band gap as the same photonic crystal at any other length scale [1].

2.1 Maxwell's Equations

Maxwell's well known [2][15] equations, (in Gaussian units), are given by,

$$\nabla \cdot \mathbf{D} = 4\pi\rho \quad (2.1)$$

$$\nabla \cdot \mathbf{B} = 0 \quad (2.2)$$

$$\nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} \quad (2.3)$$

$$\nabla \times \mathbf{H} = \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t} + \frac{4\pi}{c} \mathbf{J} \quad (2.4)$$

The components of $\mathbf{D}$ and $\mathbf{E}$ are related to one another through the following constitutive relation [2][15],

$$D_i = \sum_j \epsilon_{ij} E_j + \sum_k k\chi_{ijk} E_j E_k + O(E^3) \quad (2.5)$$

Several assumptions [2] are made. The first assumption is that the field strengths are small so that only the linear terms in equation 2.5 contribute. The second assumption is that the dielectric material is macroscopic and isotropic, so that $\mathbf{E}$ and $\mathbf{D}$ are then related by a scalar dielectric constant $\epsilon(\mathbf{r})$. The third assumption is that the dielectric constant is independent of frequency. The fourth assumption is that only low-loss dielectrics are considered so that $\epsilon(\mathbf{r})$ can be assumed to be purely real. Together these assumptions lead to the following relation between $\mathbf{E}$ and $\mathbf{D}$ [15].

$$\mathbf{D} = \epsilon(\mathbf{r})\mathbf{E} \quad (2.6)$$

$\mathbf{B}$ and $\mathbf{H}$ are related to one another through a constitutive relation as follows,

$$\mathbf{B} = \mu \mathbf{H} \quad (2.7)$$

For most dielectric materials of practical interest [2] the magnetic permeability μ is equal to unity. It is therefore assumed that the following relation between $\mathbf{B}$ and $\mathbf{H}$ holds,

$$\mathbf{B} = \mathbf{H} \quad (2.8)$$

If it is further assumed that there is no free electric charge ρ or current J , Maxwell's equations, equations 2.1-2.4 reduce to,

$$\nabla \cdot \mathbf{D} = 0 \quad (2.9)$$

$$\nabla \cdot \mathbf{B} = 0 \quad (2.10)$$

$$\nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{H}}{\partial t} \quad (2.11)$$

$$\nabla \times \mathbf{H} = \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t} \quad (2.12)$$

2.2 Maxwell's Equations and Photonic Crystals

The so-called master equation used in the study of photonic crystals is really a simplified form of Maxwell's equations where it is assumed that there is no free electric charge ρ or current J .

From equations 2.6 and 2.12 we have,

$$\nabla \times \mathbf{H} - \frac{1}{c} \frac{\partial}{\partial t} (\epsilon(\mathbf{r}) \mathbf{E}) = 0 \quad (2.13)$$

For mathematical convenience we may write the harmonic mode as a field pattern times a complex exponential as follows,

$$\mathbf{H}(\mathbf{r}, t) = \mathbf{H}(\mathbf{r}) e^{i\omega t} \quad (2.14)$$

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}(\mathbf{r}) e^{i\omega t} \quad (2.15)$$

substitution of equations 2.14 and 2.15 into equations 2.11 and 2.13 yields,

$$\nabla \times \mathbf{E}(\mathbf{r}) + i \left(\frac{\omega}{c} \right) \mathbf{H}(\mathbf{r}) = 0 \quad (2.16)$$

$$\nabla \times \mathbf{H}(\mathbf{r}) - i \left(\frac{\omega}{c} \right) \epsilon(\mathbf{r}) \mathbf{E}(\mathbf{r}) = 0 \quad (2.17)$$

Dividing by $\epsilon(\mathbf{r})$ on both sides of equation 2.17 and then taking the curl we find,

$$\nabla \times \frac{1}{\epsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) - i \left(\frac{\omega}{c} \right) \nabla \times \mathbf{E}(\mathbf{r}) = 0 \quad (2.18)$$

using equation 2.16 we obtain,

$$\nabla \times \frac{1}{\epsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) - \left(\frac{\omega}{c} \right)^2 \mathbf{H}(\mathbf{r}) = 0 \quad (2.19)$$

rearranging this equation gives the so-called master equation for photonic crystals,

$$\nabla \times \frac{1}{\epsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) = \left(\frac{\omega}{c}\right)^2 \mathbf{H}(\mathbf{r}) \quad (2.20)$$

This is an electromagnetic eigenvalue problem. The left-hand side of equation 2.20 can be treated as an operator Θ , operating on $\mathbf{H}(\mathbf{r})$. This simple change in notation makes the rearranged form of Maxwell's equations look explicitly like an eigenvalue problem,

$$\Theta \mathbf{H}(\mathbf{r}) = \left(\frac{\omega}{c}\right)^2 \mathbf{H}(\mathbf{r}) \quad (2.21)$$

This magnetic field form of the master equation is typically [2][7] used since it results in an ordinary eigenvalue problem. The electric field form of the problem could have been derived as well, but the result is a generalized eigenvalue problem that is much more difficult to solve numerically [2].

2.3 Plane Wave Expansion of Maxwell's Equations

In order to solve the special form of Maxwell's equations, the so-called master equation of photonic crystals, (equation 2.20), we write,

$$\mathbf{H}(\mathbf{r}) = \sum_{\mathbf{k}, \lambda} \hat{e}(\mathbf{k}, \lambda) h(\mathbf{k}, \lambda) e^{i\mathbf{k} \cdot \mathbf{r}} \quad (2.22)$$

where $\hat{e}(\mathbf{k}, \lambda)$, $\lambda = 1, 2$, are unit polarization vectors for a given plane wave vector $\mathbf{k}$. For transverse fields we therefore have,

$$\mathbf{k} \cdot \hat{e}(\mathbf{k}, \lambda) = 0 \quad (2.23)$$

Let,

$$f(\mathbf{r}) = \frac{1}{\epsilon(\mathbf{r})} \quad (2.24)$$

Since $\epsilon(\mathbf{r})$ is a periodic function of the position vector $\mathbf{r}$, $f(\mathbf{r})$ will necessarily be periodic with $\mathbf{r}$ as well. We may therefore expand it in terms of reciprocal lattice vectors $\mathbf{G}$ as follows,

$$f(\mathbf{r}) = \sum_{\mathbf{G}} f(\mathbf{G}) e^{i\mathbf{G} \cdot \mathbf{r}} \quad (2.25)$$

substitution of equations 2.22 and 2.25 into equation 2.20 yield,

$$\begin{aligned} \sum_{\mathbf{k}, \lambda, \mathbf{G}} (\mathbf{k} + \mathbf{G}) \times f(\mathbf{G}) [\mathbf{k} \times \hat{e}(\mathbf{k}, \lambda)] h(\mathbf{k}, \lambda) e^{i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{r}} \\ = - \left(\frac{\omega}{c} \right)^2 \sum_{\mathbf{k}, \lambda} \hat{e}(\mathbf{k}, \lambda) h(\mathbf{k}, \lambda) e^{i\mathbf{k} \cdot \mathbf{r}} \end{aligned} \quad (2.26)$$

Fourier transformation of equation 2.26 proceeds by multiplying both sides of equation 2.26 by $\hat{e}(\mathbf{k}', \lambda') e^{-i\mathbf{k}' \cdot \mathbf{r}}$ and then integrating over all space to obtain,

$$\begin{aligned} \sum_{\mathbf{k}, \lambda, \mathbf{G}} (\mathbf{k} + \mathbf{G}) \times f(\mathbf{G}) [\mathbf{k} \times \hat{e}(\mathbf{k}, \lambda)] \cdot \hat{e}(\mathbf{k}', \lambda') h(\mathbf{k}, \lambda) \delta_{\mathbf{k}', \mathbf{k} + \mathbf{G}} \\ = - \left(\frac{\omega}{c} \right)^2 \sum_{\mathbf{k}, \lambda} \hat{e}(\mathbf{k}, \lambda) \cdot \hat{e}(\mathbf{k}', \lambda') h(\mathbf{k}, \lambda) \delta_{\mathbf{k}', \mathbf{k}} \end{aligned} \quad (2.27)$$

further reducing equation 2.27 yields,

$$\begin{aligned} \sum_{\lambda, \mathbf{G}} \mathbf{k}' \times f(\mathbf{G})[(\mathbf{k}' - \mathbf{G}) \times \hat{e}(\mathbf{k}' - \mathbf{G}, \lambda)] \cdot \hat{e}(\mathbf{k}', \lambda') h(\mathbf{k}' - \mathbf{G}, \lambda) \\ = - \left(\frac{\omega}{c} \right)^2 \sum_{\lambda} \hat{e}(\mathbf{k}', \lambda) \cdot \hat{e}(\mathbf{k}', \lambda') h(\mathbf{k}', \lambda) \end{aligned} \quad (2.28)$$

noting that $\hat{e}(\mathbf{k}', \lambda) \cdot \hat{e}(\mathbf{k}', \lambda') = \delta_{\lambda, \lambda'}$ we obtain,

$$\begin{aligned} \sum_{\lambda, \mathbf{G}} \mathbf{k}' \times f(\mathbf{G})[(\mathbf{k}' - \mathbf{G}) \times \hat{e}(\mathbf{k}' - \mathbf{G}, \lambda)] \cdot \hat{e}(\mathbf{k}', \lambda') h(\mathbf{k}' - \mathbf{G}, \lambda) \\ = - \left(\frac{\omega}{c} \right)^2 \sum_{\lambda} \delta_{\lambda, \lambda'} h(\mathbf{k}', \lambda) \end{aligned} \quad (2.29)$$

simplifying the right-hand side of equation 2.29 we obtain,

$$\begin{aligned} \sum_{\lambda, \mathbf{G}} \mathbf{k}' \times f(\mathbf{G})[(\mathbf{k}' - \mathbf{G}) \times \hat{e}(\mathbf{k}' - \mathbf{G}, \lambda)] \cdot \hat{e}(\mathbf{k}', \lambda') h(\mathbf{k}' - \mathbf{G}, \lambda) \\ = - \left(\frac{\omega}{c} \right)^2 h(\mathbf{k}', \lambda') \end{aligned} \quad (2.30)$$

let, $\mathbf{k}' \rightarrow \mathbf{k} + \mathbf{G}'$,

$$\begin{aligned} \sum_{\lambda, \mathbf{G}} (\mathbf{k} + \mathbf{G}') \times f(\mathbf{G})[(\mathbf{k} + \mathbf{G}' - \mathbf{G}) \times \hat{e}(\mathbf{k} + \mathbf{G}' - \mathbf{G}, \lambda)] \cdot \hat{e}(\mathbf{k} + \mathbf{G}', \lambda') h(\mathbf{k} + \mathbf{G}' - \mathbf{G}, \lambda) \\ = - \left(\frac{\omega}{c} \right)^2 h(\mathbf{k} + \mathbf{G}', \lambda') \end{aligned} \quad (2.31)$$

let, $\mathbf{G}' - \mathbf{G} \rightarrow \mathbf{G}''$,

$$\begin{aligned}
& \sum_{\lambda, \mathbf{G}''} [\hat{e}(\mathbf{k} + \mathbf{G}', \lambda') \cdot (\mathbf{k} + \mathbf{G}')] \times f(\mathbf{G}' - \mathbf{G}'') [(\mathbf{k} + \mathbf{G}'') \times \hat{e}(\mathbf{k} + \mathbf{G}'', \lambda)] h(\mathbf{k} + \mathbf{G}'', \lambda) \\
& = - \left(\frac{\omega}{c} \right)^2 h(\mathbf{k} + \mathbf{G}', \lambda')
\end{aligned} \tag{2.32}$$

let, $\mathbf{G}' \rightarrow \mathbf{G}$, and $\mathbf{G}'' \rightarrow \mathbf{G}'$. In addition, rename $\lambda \rightarrow \lambda'$, and $\lambda' \rightarrow \lambda$. This variable renaming is done so that the final form of the expansion matches the result that is quoted in the literature [2][7].

We then obtain,

$$\begin{aligned}
& \sum_{\lambda', \mathbf{G}'} [\hat{e}(\mathbf{k} + \mathbf{G}, \lambda) \cdot (\mathbf{k} + \mathbf{G})] \times f(\mathbf{G} - \mathbf{G}') [(\mathbf{k} + \mathbf{G}') \times \hat{e}(\mathbf{k} + \mathbf{G}', \lambda')] h(\mathbf{k} + \mathbf{G}', \lambda') \\
& = - \left(\frac{\omega}{c} \right)^2 h(\mathbf{k} + \mathbf{G}, \lambda)
\end{aligned} \tag{2.33}$$

using the vector identity [16],

$$\mathbf{A} \cdot (\mathbf{B} \times \mathbf{C} \times \mathbf{D}) = (\mathbf{A} \times \mathbf{B}) \cdot (\mathbf{C} \times \mathbf{D}) \tag{2.34}$$

we may rewrite the following,

$$\begin{aligned}
& [\hat{e}(\mathbf{k} + \mathbf{G}, \lambda) \cdot (\mathbf{k} + \mathbf{G})] \times [(\mathbf{k} + \mathbf{G}') \times \hat{e}(\mathbf{k} + \mathbf{G}', \lambda')] \\
& = [\hat{e}(\mathbf{k} + \mathbf{G}, \lambda) \times (\mathbf{k} + \mathbf{G})] \cdot [(\mathbf{k} + \mathbf{G}') \times \hat{e}(\mathbf{k} + \mathbf{G}', \lambda')]
\end{aligned} \tag{2.35}$$

$$[\hat{e}(\mathbf{k} + \mathbf{G}, \lambda) \cdot (\mathbf{k} + \mathbf{G})] \times [(\mathbf{k} + \mathbf{G}') \times \hat{e}(\mathbf{k} + \mathbf{G}', \lambda')]$$

$$= -[(\mathbf{k} + \mathbf{G}) \times \hat{e}(\mathbf{k} + \mathbf{G}, \lambda)] \cdot [(\mathbf{k} + \mathbf{G}') \times \hat{e}(\mathbf{k} + \mathbf{G}', \lambda')] \quad (2.36)$$

substituting this result into equation 2.33 we obtain,

$$\begin{aligned} \sum_{\lambda', \mathbf{G}'} [(\mathbf{k} + \mathbf{G}) \times \hat{e}(\mathbf{k} + \mathbf{G}, \lambda)] \cdot [(\mathbf{k} + \mathbf{G}') \times \hat{e}(\mathbf{k} + \mathbf{G}', \lambda')] f(\mathbf{G} - \mathbf{G}') h(\mathbf{k} + \mathbf{G}', \lambda') \\ = \left(\frac{\omega}{c}\right)^2 h(\mathbf{k} + \mathbf{G}, \lambda) \end{aligned} \quad (2.37)$$

Using a plane wave expansion, we have therefore obtained a system of linear equations [2],

$$\sum_{\lambda, \mathbf{G}, \lambda', \mathbf{G}'} \Theta_{(\lambda, \mathbf{G}, \lambda', \mathbf{G}')}^{\mathbf{k}} h(\mathbf{k} + \mathbf{G}, \lambda') = \left(\frac{\omega}{c}\right)^2 h(\mathbf{k} + \mathbf{G}, \lambda) \quad (2.38)$$

where, the $\mathbf{k}$ dependent matrix Θ is given as follows,

$$\Theta_{(\lambda, \mathbf{G}, \lambda', \mathbf{G}')}^{\mathbf{k}} = [(\mathbf{k} + \mathbf{G}) \times \hat{e}(\mathbf{k} + \mathbf{G}, \lambda)] \cdot [(\mathbf{k} + \mathbf{G}') \times \hat{e}(\mathbf{k} + \mathbf{G}', \lambda')] f(\mathbf{G} - \mathbf{G}') \quad (2.39)$$

For a given $\mathbf{k}$ and N reciprocal lattice vectors $\mathbf{G}_{1,2,3,\dots,N}$, the fully vectorized, three-dimensional, linear, Hermitian matrix Θ will be of dimension $2N \times 2N$ and have the following general structure,

$$\begin{pmatrix} \Theta_{(\lambda_1, \mathbf{G}_1, \lambda_1, \mathbf{G}_1)}^{\mathbf{k}} & \Theta_{(\lambda_1, \mathbf{G}_1, \lambda_2, \mathbf{G}_1)}^{\mathbf{k}} & \Theta_{(\lambda_1, \mathbf{G}_1, \lambda_1, \mathbf{G}_2)}^{\mathbf{k}} & \Theta_{(\lambda_1, \mathbf{G}_1, \lambda_2, \mathbf{G}_2)}^{\mathbf{k}} & \cdots & \Theta_{(\lambda_1, \mathbf{G}_1, \lambda_2, \mathbf{G}_N)}^{\mathbf{k}} \\ \Theta_{(\lambda_2, \mathbf{G}_1, \lambda_1, \mathbf{G}_1)}^{\mathbf{k}} & \Theta_{(\lambda_2, \mathbf{G}_1, \lambda_2, \mathbf{G}_1)}^{\mathbf{k}} & \Theta_{(\lambda_2, \mathbf{G}_1, \lambda_1, \mathbf{G}_2)}^{\mathbf{k}} & \Theta_{(\lambda_2, \mathbf{G}_1, \lambda_2, \mathbf{G}_2)}^{\mathbf{k}} & \cdots & \Theta_{(\lambda_2, \mathbf{G}_1, \lambda_2, \mathbf{G}_N)}^{\mathbf{k}} \\ \Theta_{(\lambda_1, \mathbf{G}_2, \lambda_1, \mathbf{G}_1)}^{\mathbf{k}} & \Theta_{(\lambda_1, \mathbf{G}_2, \lambda_2, \mathbf{G}_1)}^{\mathbf{k}} & \Theta_{(\lambda_1, \mathbf{G}_2, \lambda_1, \mathbf{G}_2)}^{\mathbf{k}} & \Theta_{(\lambda_1, \mathbf{G}_2, \lambda_2, \mathbf{G}_2)}^{\mathbf{k}} & \cdots & \Theta_{(\lambda_1, \mathbf{G}_2, \lambda_2, \mathbf{G}_N)}^{\mathbf{k}} \\ \Theta_{(\lambda_2, \mathbf{G}_2, \lambda_1, \mathbf{G}_1)}^{\mathbf{k}} & \Theta_{(\lambda_2, \mathbf{G}_2, \lambda_2, \mathbf{G}_1)}^{\mathbf{k}} & \Theta_{(\lambda_2, \mathbf{G}_2, \lambda_1, \mathbf{G}_2)}^{\mathbf{k}} & \Theta_{(\lambda_2, \mathbf{G}_2, \lambda_2, \mathbf{G}_2)}^{\mathbf{k}} & \cdots & \Theta_{(\lambda_2, \mathbf{G}_2, \lambda_2, \mathbf{G}_N)}^{\mathbf{k}} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \Theta_{(\lambda_2, \mathbf{G}_N, \lambda_1, \mathbf{G}_1)}^{\mathbf{k}} & \Theta_{(\lambda_2, \mathbf{G}_N, \lambda_2, \mathbf{G}_1)}^{\mathbf{k}} & \Theta_{(\lambda_2, \mathbf{G}_N, \lambda_1, \mathbf{G}_2)}^{\mathbf{k}} & \Theta_{(\lambda_2, \mathbf{G}_N, \lambda_2, \mathbf{G}_2)}^{\mathbf{k}} & \cdots & \Theta_{(\lambda_2, \mathbf{G}_N, \lambda_2, \mathbf{G}_N)}^{\mathbf{k}} \end{pmatrix}$$

In two dimensions, we may separate the problem into two polarizations of the electromagnetic waves. These polarizations are the transverse magnetic (TM) polarization where the electric field vector is parallel to the columns, and transverse electric (TE) polarization where the magnetic field vector is parallel to the columns. The TM and TE polarizations are relative to the plane of periodicity of the photonic crystal. The separation into TM and TE polarized modes allows us to make several simplifications to the $\mathbf{k}$ dependent matrix Θ given in equation 2.39. As is shown in [5], the simplified forms of the Θ matrix for TM and TE polarizations in two dimensions are given by,

$$\Theta_{TM}^{\mathbf{k}}(\mathbf{G}, \mathbf{G}') = |\mathbf{k} + \mathbf{G}| |\mathbf{k} + \mathbf{G}'| f(\mathbf{G} - \mathbf{G}') \quad (2.40)$$

and,

$$\Theta_{TE}^{\mathbf{k}}(\mathbf{G}, \mathbf{G}') = (\mathbf{k} + \mathbf{G}) \cdot (\mathbf{k} + \mathbf{G}') f(\mathbf{G} - \mathbf{G}') \quad (2.41)$$

In the following sections, we use equations 2.39 to find the eigenvalues for three-dimensional photonic crystals and equations 2.40 and 2.41 to find the eigenvalues for two-dimensional photonic crystals.

2.4 Two-Dimensional Photonic Crystals

In two dimensions, because of the presence of a mirror symmetry in the plane perpendicular to the dielectric columns, it is possible to decouple the electromagnetic modes into transverse magnetic (TM) and transverse electric (TE) field polarizations with respect to the plane normal to the dielectric columns.

The general rule presented by Joannopoulos in [2] is that TM band gaps are favored in a lattice of isolated regions of high-dielectric constant, and that TE band gaps are favored in a connected lattice of high-dielectric regions [2]. Joannopoulos' rule can be used to design a two-dimensional photonic crystal that has a photonic band gap for both TE and TM modes. The design requires a photonic crystal that attempts to combine lattice features which favor both TM and TE band gaps. Such a crystal will therefore have high-dielectric constant regions that are almost entirely isolated (favoring TM band gaps) but which are still connected by narrow high-dielectric constant veins (favoring TE band gaps). The triangular lattice of columns of low-dielectric constant ϵ_a in a background of high-dielectric constant ϵ_b is an example of such a photonic crystal. The remnants of high-dielectric between the columns can be

considered to be the isolated regions of high-dielectric constant required for TM band gaps. If the columns are slightly smaller than the maximum packing would allow, then narrow veins of high-dielectric constant will connect the mostly isolated regions and allow for TE band gaps to exist as well.

The dielectric columns of dielectric constant ϵ_a are assumed to be parallel to the z axis. The intersections of the axes of these columns with the xy -plane form a two-dimensional lattice (square or triangular) whose sites are given by the vector,

$$\mathbf{r} = l\mathbf{a}_1 + m\mathbf{a}_2 \quad (2.42)$$

The vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are the two primitive translation vectors of the lattice, and l and m are any two integers.

For the square lattice of lattice constant a , the primitive lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are,

$$\mathbf{a}_1 = a \begin{bmatrix} 1, 0 \end{bmatrix} \quad (2.43)$$

$$\mathbf{a}_2 = a \begin{bmatrix} 0, 1 \end{bmatrix} \quad (2.44)$$

For the triangular lattice of lattice constant a , the primitive lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are,

$$\mathbf{a}_1 = a \left[\frac{\sqrt{3}}{2}, \frac{1}{2} \right] \quad (2.45)$$

$$\mathbf{a}_2 = a \left[-\frac{\sqrt{3}}{2}, \frac{1}{2} \right] \quad (2.46)$$

The dielectric constant of this composite system is therefore position dependent, and is denoted by $\epsilon(\mathbf{r})$. The area of the primitive unit cell of this lattice is equal to $A_u = |\mathbf{a}_1 \times \mathbf{a}_2|$.

2.4.1 The Square Lattice of Dielectric Columns

Real-Space Representation

Shown in Figure 2.1(a) is the real-space representation of the two-dimensional square lattice of columns of high-dielectric constant ϵ_a (shown in blue) in a background of low-dielectric constant ϵ_b .

Reciprocal-Space Representation

Shown in Figure 2.1(b) is the reciprocal-space representation of the two-dimensional square lattice of columns. The reciprocal-space representation of the two-dimensional square lattice shown in (b) with the square Brillouin zone highlighted (in grey). The triangular irreducible portion of the Brillouin zone is shown in the upper right corner of the Brillouin zone (in yellow).

Figure 2.1: (a) The real-space representation of the two-dimensional square lattice of columns of high-dielectric constant ϵ_a (shown in blue) in a background of low-dielectric constant ϵ_b . (b) The reciprocal-space representation of the two-dimensional square lattice of columns of high-dielectric constant ϵ_a in a background of low-dielectric constant ϵ_b . (c) The reciprocal-space representation of the two-dimensional square lattice shown in (b) with the square Brillouin zone highlighted (in grey). The triangular irreducible portion of the Brillouin zone is shown in the upper right corner of the Brillouin zone (in yellow).

Figure 2.2 shows an expanded view of the Brillouin zone (in grey) for the two-dimensional square lattice. The triangular irreducible portion of the Brillouin zone is shown in the upper right corner of the Brillouin zone (in yellow).

The $\mathbf{k}$ -space points of high symmetry $\bar{X}$, $\bar{\Gamma}$, and $\bar{M}$ define the irreducible Brillouin zone, and are given as,

$$\bar{\Gamma} = \frac{2\pi}{a} \begin{bmatrix} 0, 0 \end{bmatrix} \quad (2.47)$$

$$\bar{M} = \frac{2\pi}{a} \begin{bmatrix} \frac{1}{2}, \frac{1}{2} \end{bmatrix} \quad (2.48)$$

Figure 2.2: An expanded view of the Brillouin zone (in grey) for the two-dimensional square lattice. The triangular irreducible portion of the Brillouin zone is shown in the upper right corner of the Brillouin zone (in yellow). The $\mathbf{k}$ -space points of high symmetry $\bar{X}$, $\bar{\Gamma}$, and $\bar{M}$ define the irreducible Brillouin zone.

$$\bar{X} = \frac{2\pi}{a} \left[\frac{1}{2}, 0 \right] \quad (2.49)$$

The irreducible portion of the Brillouin zone defines the $\mathbf{k}$ -space trajectory to be followed when calculating the photonic band structure. The band structure for all other $\mathbf{k}$ -space points outside the irreducible portion of the Brillouin zone can be found by taking advantage of the symmetry of the Brillouin zone.

Reciprocal Space Representation of $f(\mathbf{r})$ for Square Lattice

Within each unit cell of the square lattice we have a single dielectric column.

Let,

$$f(\mathbf{r}) = \frac{1}{\epsilon(\mathbf{r})} \quad (2.50)$$

The position dependent dielectric function $\epsilon(\mathbf{r})$ is periodic with all lattice vectors $\mathbf{R}_i$. The real reciprocal of the dielectric function $f(\mathbf{r})$ will therefore be periodic, and we may write,

$$f(\mathbf{r}) = \sum_i f^0(\mathbf{r} + \mathbf{R}_i) \quad (2.51)$$

The function $f^0(\mathbf{r} + \mathbf{R}_i)$ corresponds to the unit cell located at $\mathbf{R}_i = [0, 0]$. The periodic real reciprocal dielectric function $f(\mathbf{r})$ may therefore be expanded in a Fourier series [13][17] in terms of lattice reciprocal vectors as follows,

$$f(\mathbf{r}) = \sum_{\mathbf{G}} f(\mathbf{G}) e^{i\mathbf{G} \cdot \mathbf{r}} \quad (2.52)$$

We may solve for the Fourier expansion coefficients $f(\mathbf{G})$ by taking the Fourier transform of equation 2.50 as follows,

$$f(\mathbf{G}) = \frac{1}{A} \int f(\mathbf{r}) e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^2 \quad (2.53)$$

$$f(\mathbf{G}) = \frac{1}{A} \sum_i \int_u f^0(\mathbf{r} + \mathbf{R}_i) e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^2 \quad (2.54)$$

where u denotes integration over a unit cell.

Substitution of variables gives,

Figure 2.3: Schematic illustration of the unit cell construction for the 2D square lattice of dielectric columns. Shown in the figure are the inverse dielectric functions for the unit cell dielectric background ($f_b^0 = \frac{1}{\epsilon_b}$) and the dielectric column ($f_a^0 = \frac{1}{\epsilon_a}$)

$$f(\mathbf{G}) = \frac{1}{A} \sum_i \int_u f^0(\mathbf{r} + \mathbf{R}_i) e^{-i\mathbf{G} \cdot (\mathbf{r} + \mathbf{R}_i)} d\mathbf{r}^2 \quad (2.55)$$

Using the fact that $e^{i\mathbf{G} \cdot \mathbf{R}_i} = 1$, we obtain,

$$f(\mathbf{G}) = \frac{N}{A} \int_u f^0(\mathbf{r}) e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^2 = \frac{1}{A_u} \int_u f^0(\mathbf{r}) e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^2 \quad (2.56)$$

where, $A_u = \frac{A}{N}$ is the area of the unit cell. Figure 2.3 illustrates the decomposition of $f^0(\mathbf{r})$ within the unit cell. We may therefore write,

$$f(\mathbf{G}) = \frac{1}{A_u} \int_u \frac{1}{\epsilon_b} e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^2 + \frac{1}{A_u} \int_c \frac{1}{\epsilon_a} e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^2 - \frac{1}{A_u} \int_c \frac{1}{\epsilon_b} e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^2 \quad (2.57)$$

$$f(\mathbf{G}) = \frac{1}{\epsilon_b} \delta_{\mathbf{G},0} + \frac{1}{A_u} \int_c \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^2 \quad (2.58)$$

Where the integral in equation 2.58 is over the circle c .

$$f(\mathbf{G}) = \frac{1}{\epsilon_b} \delta_{\mathbf{G},0} - \frac{1}{A_u} \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) \int_c e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^2 \quad (2.59)$$

The second term on the right hand side of equation 2.59 will also contain a $\mathbf{G} = 0$ term. We therefore write,

$$f(\mathbf{G}) = f(\mathbf{G} = 0) + f(\mathbf{G} \neq 0) \quad (2.60)$$

$$f(\mathbf{G} = 0) = \frac{1}{\epsilon_b} + \frac{1}{A_u} \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) \int_c dr^2 \quad (2.61)$$

$$f(\mathbf{G} = 0) = \frac{1}{\epsilon_b} + \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) \frac{\pi R^2}{A_u} \quad (2.62)$$

The $\frac{\pi R^2}{A_u}$ term corresponds to the packing fraction for the square lattice of dielectric columns. The packing fraction is given by,

$$P_f = \frac{A_c}{A_u} \quad (2.63)$$

where A_c is the cross-sectional area of the dielectric column.

$$f(\mathbf{G} = 0) = \frac{1}{\epsilon_b} + \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) P_f \quad (2.64)$$

$$f(\mathbf{G} \neq 0) = \frac{1}{A_u} \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) \int_c e^{-i\mathbf{G} \cdot \mathbf{r}} dr^2 \quad (2.65)$$

As is shown in [5] and [17], the integral on the right hand side of equation 2.65, evaluates to a relation involving a Bessel function of the first kind as follows,

$$\int_c e^{-i\mathbf{G}\cdot\mathbf{r}} d\mathbf{r}^2 = (\pi R^2) 2 \frac{J_1(GR)}{GR} = A_c 2 \frac{J_1(GR)}{GR} \quad (2.66)$$

substitution of this result into equation 2.65 yields,

$$f(\mathbf{G} \neq 0) = \frac{A_c}{A_u} \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) 2 \frac{J_1(GR)}{GR} = P_f \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) 2 \frac{J_1(GR)}{GR} \quad (2.67)$$

Note that $f(\mathbf{G} = 0)$ corresponds to the average dielectric constant for the photonic crystal, and $f(\mathbf{G} \neq 0)$ is responsible for scattering.

Summarizing, we have,

$$f_{square}(\mathbf{G}) = \begin{cases} \frac{1}{\epsilon_b} + \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) P_f & , \quad \mathbf{G} = 0 \\ P_f \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) 2 \frac{J_1(GR)}{GR} & , \quad \mathbf{G} \neq 0 \end{cases}$$

where P_f is the packing fraction for the square lattice of dielectric columns.

2.4.2 The Triangular Lattice of Dielectric Columns

Real-Space Representation

Shown in Figure 2.4(a) is the real-space representation of the two-dimensional triangular lattice of columns of high-dielectric constant ϵ_a (shown in blue) in a background of low-dielectric constant ϵ_b .

Figure 2.4: (a) The real-space representation of the two-dimensional triangular lattice of columns of high-dielectric constant ϵ_a (shown in blue) in a background of low-dielectric constant ϵ_b . (b) The reciprocal-space representation of the two-dimensional triangular lattice of columns of high-dielectric constant ϵ_a in a background of low-dielectric constant ϵ_b . (c) The reciprocal-space representation of the two-dimensional triangular lattice shown in (b) with the hexagonal Brillouin zone highlighted (in grey). The triangular irreducible portion of the Brillouin zone is shown in the upper right corner of the Brillouin zone (in yellow).

Reciprocal-Space Representation

Shown in Figure 2.4(b) is the reciprocal-space representation of the two-dimensional triangular lattice of columns. The reciprocal-space representation of the two-dimensional triangular lattice shown in (b) with the hexagonal Brillouin zone highlighted (in grey). The triangular irreducible portion of the Brillouin zone is shown in the upper right corner of the Brillouin zone (in yellow).

Figure 2.5 shows an expanded view of the Brillouin zone (in grey) for the two-dimensional square lattice. The triangular irreducible portion of the Brillouin zone is shown in the upper right corner of the Brillouin zone (in yellow).

The $\mathbf{k}$ -space points of high symmetry $\bar{\Gamma}$, $\bar{M}$, and $\bar{K}$ define the irreducible Brillouin

Figure 2.5: An expanded view of the Brillouin zone (in grey) for the two-dimensional triangular lattice. The triangular irreducible portion of the Brillouin zone is shown in the upper right corner of the Brillouin zone (in yellow). The $\mathbf{k}$ -space points of high symmetry $\bar{\Gamma}$, $\bar{M}$, and $\bar{K}$ define the irreducible Brillouin zone.

zone, and are given as.

$$\bar{\Gamma} = \frac{2\pi}{a} \begin{bmatrix} 0.0 \\ 0.0 \end{bmatrix} \quad (2.68)$$

$$\bar{M} = \frac{2\pi}{a} \begin{bmatrix} \frac{\sqrt{3}}{3}, 0 \end{bmatrix} \quad (2.69)$$

$$\bar{K} = \frac{2\pi}{a} \begin{bmatrix} \frac{\sqrt{3}}{3}, \frac{1}{3} \end{bmatrix} \quad (2.70)$$

The irreducible portion of the Brillouin zone defines the $\mathbf{k}$ -space trajectory to be followed when calculating the photonic band structure. The band structure for all other $\mathbf{k}$ -space points outside the irreducible portion of the Brillouin zone can be found

by taking advantage of the symmetry of the Brillouin zone.

Reciprocal Space Representation of $f(\mathbf{r})$ for Triangular Lattice

The reciprocal space representation of $f(\mathbf{r})$ for the triangular lattice of dielectric columns is same as that of the square lattice with the exception that the packing fraction P_f for the triangular lattice must be used. Summarizing, we have,

$$f_{triangular}(\mathbf{G}) = \begin{cases} \frac{1}{\epsilon_b} + \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) P_f & , \quad \mathbf{G} = 0 \\ P_f \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) 2 \frac{J_1(GR)}{GR} & , \quad \mathbf{G} \neq 0 \end{cases}$$

2.5 Three-Dimensional Photonic Crystals

Three-dimensional photonic crystals are periodic in three dimensions. Calculation of photonic band structures is much more complicated in three dimensions. It is no longer possible to decouple the electromagnetic modes into transverse magnetic (TM) and transverse electric (TE) field polarizations as was done in two dimensions. All polarizations must therefore be considered.

The dielectric spheres of dielectric constant ϵ_a form a three-dimensional lattice (fcc or diamond) whose sites are given by the vector,

$$\mathbf{r} = l\mathbf{a}_1 + m\mathbf{a}_2 + n\mathbf{a}_3 \quad (2.71)$$

The vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ are the three primitive translation vectors of the lattice

and l , m and n are any three integers.

For the fcc lattice $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ are,

$$\mathbf{a}_1 = a \left[\frac{1}{2}, \frac{1}{2}, 0 \right] \quad (2.72)$$

$$\mathbf{a}_2 = a \left[0, \frac{1}{2}, \frac{1}{2} \right] \quad (2.73)$$

$$\mathbf{a}_3 = a \left[\frac{1}{2}, 0, \frac{1}{2} \right] \quad (2.74)$$

For the diamond lattice $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ are the same as those for the fcc lattice. However, within each unit cell of the diamond lattice there are two dielectric spheres that are offset from the fcc lattice position by $\bar{\tau} = a \left[\frac{1}{8}, \frac{1}{8}, \frac{1}{8} \right]$, and $-\bar{\tau} = -a \left[\frac{1}{8}, \frac{1}{8}, \frac{1}{8} \right]$ as is shown in Figure 1.4.

The dielectric constant is therefore position dependent, and is denoted by $\epsilon(\mathbf{r})$. The volume of the primitive unit cell of this lattice is equal to $V_u = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|$.

2.5.1 The fcc Lattice of Dielectric Spheres

Real-Space Representation

Figure 1.3(a) illustrates the first class of three-dimensional photonic crystal to be studied, namely, the fcc lattice of spheres of high-dielectric constant ϵ_a in a background

Figure 2.6: The reciprocal-space representation of both the three-dimensional fcc and diamond lattices. The Brillouin zone is highlighted (in grey). The irreducible portion of the Brillouin zone is highlighted (in yellow). The $\mathbf{k}$ -space points of high symmetry $\bar{X}$, $\bar{\Gamma}$, $\bar{U}$, $\bar{W}$, $\bar{L}$ and $\bar{K}$ define the irreducible Brillouin zone.

of low-dielectric constant ϵ_b . Figure 1.3(b) shows the fcc lattice of spheres of low-dielectric constant ϵ_a in a background of high-dielectric constant ϵ_b .

Reciprocal-Space Representation

Shown in Figure 2.6 is the reciprocal-space representation for both the three-dimensional fcc and diamond lattices. The Brillouin zone is highlighted in grey. The irreducible portion of the Brillouin zone is highlighted in yellow. The $\mathbf{k}$ -space points of high symmetry $\bar{X}$, $\bar{\Gamma}$, $\bar{U}$, $\bar{W}$, $\bar{L}$ and $\bar{K}$ define the irreducible Brillouin zone. These

points are defined to be,

$$\bar{X} = \frac{2\pi}{a} \left[1, 0, 0 \right] \quad (2.75)$$

$$\bar{U} = \frac{2\pi}{a} \left[1, \frac{1}{4}, \frac{1}{4} \right] \quad (2.76)$$

$$\bar{\Gamma} = \frac{2\pi}{a} \left[0, 0, 0 \right] \quad (2.77)$$

$$\bar{L} = \frac{2\pi}{a} \left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right] \quad (2.78)$$

$$\bar{K} = \frac{2\pi}{a} \left[\frac{3}{4}, \frac{3}{4}, 0 \right] \quad (2.79)$$

$$\bar{W} = \frac{2\pi}{a} \left[1, \frac{1}{2}, 0 \right] \quad (2.80)$$

Reciprocal-Space Representation of $f(\mathbf{r})$ for the fcc Lattice

The reciprocal-space representation of $f(\mathbf{r})$ for the three-dimensional fcc lattice is found in a manner analogous to the method employed for the two-dimensional lattices of section 2.4. Within each unit cell of the fcc lattice we have a single dielectric sphere.

Proceeding similarly in three dimensions as we did for two dimensions in section 2.4, we have for the fcc lattice of dielectric spheres,

$$f(\mathbf{r}) = \frac{1}{\epsilon(\mathbf{r})} \quad (2.81)$$

The function $f(\mathbf{r})$ is periodic with all lattice vectors $\mathbf{R}_i$ and we may again write,

$$f(\mathbf{r}) = \sum_i f^0(\mathbf{r} + \mathbf{R}_i) \quad (2.82)$$

The periodic function $f(\mathbf{r})$ may be expanded in terms of lattice reciprocal vectors as follows,

$$f(\mathbf{r}) = \sum_{\mathbf{G}} f(\mathbf{G}) e^{i\mathbf{G} \cdot \mathbf{r}} \quad (2.83)$$

$$f(\mathbf{G}) = \frac{1}{V} \int f(\mathbf{r}) e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 \quad (2.84)$$

Taking the Fourier transform of equation 2.82 we obtain,

$$f(\mathbf{G}) = \frac{1}{V} \sum_i \int_u f^0(\mathbf{r} + \mathbf{R}_i) e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 \quad (2.85)$$

substitution of variables again gives,

$$f(\mathbf{G}) = \frac{1}{V} \sum_i \int_u f^0(\mathbf{r}) e^{-i\mathbf{G} \cdot (\mathbf{r} - \mathbf{R}_i)} d\mathbf{r}^3 \quad (2.86)$$

where u denotes integration over a unit cell.

Using the fact that $e^{i\mathbf{G} \cdot \mathbf{R}_i} = 1$, we obtain,

Figure 2.7: Schematic illustration of the unit cell construction for the three-dimensional fcc lattice of dielectric spheres. Shown in the figure are the inverse dielectric functions for the unit cell dielectric background ($f_b^0 = \frac{1}{\epsilon_b}$) and the dielectric sphere ($f_a^0 = \frac{1}{\epsilon_a}$).

$$f(\mathbf{G}) = \frac{V}{V_u} \int_u f^0(\mathbf{r}) e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 = \frac{1}{V_u} \int_u f^0(\mathbf{r}) e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 \quad (2.87)$$

where, $V_u = \frac{V}{N}$ is the volume of the unit cell. Figure 2.7 illustrates the decomposition of $f^0(\mathbf{r})$ within the unit cell. We may therefore write,

$$f(\mathbf{G}) = \frac{1}{V_u} \int_u \frac{1}{\epsilon_b} e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 + \frac{1}{V_u} \int_s \frac{1}{\epsilon_a} e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 - \frac{1}{V_u} \int_s \frac{1}{\epsilon_b} e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 \quad (2.88)$$

$$f(\mathbf{G}) = \frac{1}{\epsilon_b} \delta_{\mathbf{G},0} + \frac{1}{V_u} \int_s \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 \quad (2.89)$$

Where the integral in equation 2.89 is over the sphere s .

$$f(\mathbf{G}) = \frac{1}{\epsilon_b} \delta_{\mathbf{G},0} + \frac{1}{V_u} \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) \int_s e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 \quad (2.90)$$

The second term on the right hand side of equation 2.90 will also contain a $\mathbf{G} = 0$ term. We therefore write,

$$f(\mathbf{G}) = f(\mathbf{G} = 0) + f(\mathbf{G} \neq 0) \quad (2.91)$$

$$f(\mathbf{G} = 0) = \frac{1}{\epsilon_b} + \frac{1}{V_u} \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) \int_s dr^3 \quad (2.92)$$

$$f(\mathbf{G} = 0) = \frac{1}{\epsilon_b} + \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) \frac{4\pi R^3}{3V_u} \quad (2.93)$$

The $\frac{4\pi R^3}{3V_u}$ term corresponds to the packing fraction for the fcc lattice of dielectric spheres. The packing fraction is given by,

$$P_f = \frac{V_s}{V_u} \quad (2.94)$$

$$f(\mathbf{G} = 0) = \frac{1}{\epsilon_b} + \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) P_f \quad (2.95)$$

$$f(\mathbf{G} \neq 0) = \frac{1}{V_u} \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) \int_s e^{-i\mathbf{G} \cdot \mathbf{r}} dr^3 \quad (2.96)$$

Using spherical coordinates equation 2.96 becomes,

$$f(\mathbf{G} \neq 0) = \frac{1}{V_u} \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) \int_r \int_{\cos(\theta)} \int_{\phi} e^{-iGr \cos(\theta)} d(\cos(\theta)) d\phi r^2 dr \quad (2.97)$$

Carrying out the angle integration gives,

$$f(\mathbf{G} \neq 0) = \frac{4\pi}{V_u} \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) \int_r \left[\frac{\sin(Gr)}{G} \right] r dr \quad (2.98)$$

Integrating equation 2.98 by parts yields,

$$f(\mathbf{G} \neq 0) = \frac{4\pi}{V_u} \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) \left[\frac{\sin(GR)}{G^3} - \frac{R \cos(GR)}{G^2} \right] \quad (2.99)$$

which may be written in terms of the packing fraction as,

$$f(\mathbf{G} \neq 0) = 3P_f \left(\frac{1}{\epsilon_b} - \frac{1}{\epsilon_a} \right) \frac{1}{(GR)^3} [GR \cos(GR) - \sin(GR)] \quad (2.100)$$

Note that $f(\mathbf{G} = 0)$ corresponds to the average dielectric constant for the photonic crystal, and $f(\mathbf{G} \neq 0)$ is responsible for scattering.

Summarizing, we have,

$$f_{fcc}(\mathbf{G}) = \begin{cases} \frac{1}{\epsilon_b} + \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) P_f & , \quad \mathbf{G} = 0 \\ 3P_f \left(\frac{1}{\epsilon_b} - \frac{1}{\epsilon_a} \right) \frac{1}{(GR)^3} [GR \cos(GR) - \sin(GR)] & , \quad \mathbf{G} \neq 0 \end{cases}$$

where, P_f is the packing fraction for the fcc lattice of dielectric spheres.

2.5.2 The Diamond Lattice of Dielectric Spheres

Real-Space Representation of Diamond Lattice

Figure 1.4(a) illustrates the second class of three-dimensional photonic crystal to be studied, namely, the diamond lattice of spheres of high-dielectric constant ϵ_a in a

background of low-dielectric constant ϵ_b . Figure 1.4(b) shows the diamond lattice of spheres of low-dielectric constant ϵ_a in a background of high-dielectric constant ϵ_b .

Reciprocal Space Representation of Diamond Lattice

Shown in Figure 2.5 is the reciprocal space representation for both the three-dimensional fcc and diamond lattices. The Brillouin zone is highlighted in grey. The irreducible portion of the Brillouin zone is highlighted in yellow. The k-space points of high symmetry $\bar{X}$, $\bar{\Gamma}$, $\bar{U}$, $\bar{W}$, $\bar{L}$ and $\bar{K}$ define the irreducible Brillouin zone. These points are given by equations 2.75 - 2.80.

Reciprocal-Space Representation of $f(\mathbf{r})$ for the Diamond Lattice

Obtaining the reciprocal-space representation of $f(\mathbf{r})$ for diamond lattice proceeds in the same way as was done for the fcc lattice. However, within each unit cell of the diamond lattice we have two dielectric spheres that are offset from the fcc lattice position by $\bar{\tau} = a \left[\frac{1}{8}, \frac{1}{8}, \frac{1}{8} \right]$, and $-\bar{\tau} = -a \left[\frac{1}{8}, \frac{1}{8}, \frac{1}{8} \right]$, respectively.

Proceeding as we did for the fcc unit cell, we may write,

$$f(\mathbf{G}) = \frac{1}{V_u} \int_u f^0(\mathbf{r}) e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 \quad (2.101)$$

where, $V_u = \frac{V}{N}$ is the volume of the unit cell.

Figure 2.8 illustrates the decomposition of $f^0(\mathbf{r})$ within the unit cell. We may therefore write,

Figure 2.8: Schematic illustration of the unit cell construction for the three-dimensional diamond lattice of dielectric spheres. Shown in the figure are the inverse dielectric functions for the unit cell dielectric background ($f_b^0 = \frac{1}{\epsilon_b}$) and the dielectric spheres ($f_a^0 = \frac{1}{\epsilon_a}$).

$$f(\mathbf{G}) = \frac{1}{V_u} \int_u \frac{1}{\epsilon_b} e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 + \frac{1}{V_u} \int_s \frac{1}{\epsilon_{a1}} e^{-i\mathbf{G} \cdot (\mathbf{r} - \tilde{\tau})} d\mathbf{r}^3 + \frac{1}{V_u} \int_s \frac{1}{\epsilon_{a2}} e^{-i\mathbf{G} \cdot (\mathbf{r} - \tilde{\tau})} d\mathbf{r}^3 - \frac{1}{V_u} \int_s \frac{1}{\epsilon_b} e^{-i\mathbf{G} \cdot (\mathbf{r} - \tilde{\tau})} d\mathbf{r}^3 - \frac{1}{V_u} \int_s \frac{1}{\epsilon_b} e^{-i\mathbf{G} \cdot (\mathbf{r} - \tilde{\tau})} d\mathbf{r}^3 \quad (2.102)$$

where ϵ_{a1} and ϵ_{a2} are the dielectric constants for sphere 1 and sphere 2 respectively, within the unit cell of Figure 2.8. Assuming, as is done in the literature [2][6], that both spheres have the same dielectric constant, $\epsilon_{a1} = \epsilon_{a2} = \epsilon_a$, we may simplify equation 2.102 as follows.

$$f(\mathbf{G}) = \frac{1}{V_u} \int_u \frac{1}{\epsilon_b} e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 + 2 \cos(\mathbf{G} \cdot \tilde{\tau}) \frac{1}{V_u} \int_s \frac{1}{\epsilon_a} e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 - 2 \cos(\mathbf{G} \cdot \tilde{\tau}) \frac{1}{V_u} \int_s \frac{1}{\epsilon_b} e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 \quad (2.103)$$

$$f(\mathbf{G}) = \frac{1}{\epsilon_b} \delta_{\mathbf{G},0} + 2 \cos(\mathbf{G} \cdot \tilde{\tau}) \frac{1}{V_u} \int_s \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 \quad (2.104)$$

The second term on the right-hand side of equation 2.104 will also contain a $\mathbf{G} = 0$ term. We therefore write,

$$f(\mathbf{G}) = f(\mathbf{G} = 0) + f(\mathbf{G} \neq 0) \quad (2.105)$$

$$f(\mathbf{G} = 0) = \frac{1}{\epsilon_b} + P_f \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) \quad (2.106)$$

where, $P_f = 2\frac{V_s}{V_u}$ for diamond.

Comparing equation 2.104 with equation 2.96 we see that for the diamond lattice of identical dielectric spheres we have,

$$f(\mathbf{G} \neq 0) = 3P_f \cos(\mathbf{G} \cdot \bar{\tau}) \left(\frac{1}{\epsilon_b} - \frac{1}{\epsilon_a} \right) \frac{1}{(GR)^3} [GR \cos(GR) - \sin(GR)] \quad (2.107)$$

Summarizing, we see that for the diamond lattice of identical dielectric spheres we have,

$$f_{diamond}^{(\epsilon_{a1}=\epsilon_{a2})}(\mathbf{G}) = \begin{cases} \frac{1}{\epsilon_b} + P_f \left(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) & , \quad \mathbf{G} = 0 \\ 3P_f \cos(\mathbf{G} \cdot \bar{\tau}) \left(\frac{1}{\epsilon_b} - \frac{1}{\epsilon_a} \right) \frac{1}{(GR)^3} [GR \cos(GR) - \sin(GR)] & , \quad \mathbf{G} \neq 0 \end{cases}$$

where, P_f is the packing fraction for the diamond lattice of dielectric spheres.

If the two spheres in the diamond lattice unit cell have different dielectric constants $\epsilon_{a1} \neq \epsilon_{a2}$, then the following relation for $f(\mathbf{G})$ is found,

$$f(\mathbf{G}) = \frac{1}{\epsilon_b} \delta_{\mathbf{G},0} - 2 \cos(\mathbf{G} \cdot \bar{\tau}) \frac{1}{V_u} \int_s \frac{1}{\epsilon_b} e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3 + e^{-i\mathbf{G} \cdot \bar{\tau}} \frac{1}{V_u} \int_s \frac{1}{\epsilon_{a1}} e^{-i\mathbf{G} \cdot \mathbf{r}} d\mathbf{r}^3$$

$$+e^{i\mathbf{G}\cdot\bar{\mathbf{r}}}\frac{1}{V_u}\int_s\frac{1}{\epsilon_{a2}}e^{-i\mathbf{G}\cdot\mathbf{r}}d\mathbf{r}^3 \quad (2.108)$$

We may once again write,

$$f(\mathbf{G}) = f(\mathbf{G} = 0) + f(\mathbf{G} \neq 0) \quad (2.109)$$

For the diamond lattice of spheres of different dielectric constant we have,

$$f(\mathbf{G} = 0) = \frac{1}{\epsilon_b} + P_f \left(\frac{1}{2\epsilon_{a1}} + \frac{1}{2\epsilon_{a2}} - \frac{1}{\epsilon_b} \right) \quad (2.110)$$

$$f(\mathbf{G} \neq 0) = 3P_f \left(\frac{1}{\epsilon_b} \cos(\mathbf{G} \cdot \bar{\mathbf{r}}) - \frac{e^{-i\mathbf{G}\cdot\bar{\mathbf{r}}}}{2\epsilon_{a1}} - \frac{e^{i\mathbf{G}\cdot\bar{\mathbf{r}}}}{2\epsilon_{a2}} \right) \frac{1}{(GR)^3} [GR \cos(GR) - \sin(GR)] \quad (2.111)$$

It should be noted that equations 2.110 - 2.111 reduce to equations 2.106 - 2.107 when $\epsilon_{a1} = \epsilon_{a2}$.

Chapter 3

Numerical Methodology

The computational method used is a frequency-domain method. Maxwell's equations are expanded using a plane-wave basis. The approaches used for the calculation of photonic band structures for both two-dimensional and three-dimensional photonic crystals are very similar. The details of the computational method for both two-dimensional and three-dimensional photonic crystals is given in the following sections.

3.1 Frequency-Domain Computational Method

The special form of Maxwell's equations used for the study of photonic crystals, equation 2.20, can be solved through expansion using a plane-wave basis, as is described in section 2.3. The result of the plane-wave expansion is a set of linear equations. The eigenfrequencies for a given reciprocal-space trajectory can then be

solved for using standard Hermitian matrix-diagonalization methods [18], and the resulting photonic band structure plotted. The two-dimensional and three-dimensional photonic band structure code listed in Appendix A was written using the Matlab programming language. Matlab uses LAPACK routines to compute eigenvalues and eigenvectors. For a Hermitian matrix, the LAPACK ZHEEV routine is used [20].

3.1.1 Numerical Method in Two Dimensions

The first step is to define the real-space lattice vectors and lattice constant for the two-dimensional photonic crystal under investigation, either the square or triangular lattice. The second step is to define the various dielectric lattice parameters. This includes the dielectric constants of both the dielectric column, ϵ_a and dielectric background, ϵ_b . Next, the packing fraction is specified for the lattice under study, and the area of the primitive unit cell calculated. The radius of each dielectric column is taken to be a function of the specified packing fraction. The next step is to generate the primitive reciprocal-space lattice vectors for the photonic crystal under study. Once the primitive reciprocal-space lattice vectors have been determined, the reciprocal vectors, $\mathbf{G}$, to be used for the calculation are collected. The reciprocal vectors used belong to a discrete approximation to a circular region in $\mathbf{k}$ -space bounded by some maximum value. The maximum value is the norm of the largest reciprocal vector allowed for a desired number of plane waves. The number of plane waves used for a given calculation is chosen to guarantee eigenvalue convergence to within 3%. The

next step is to determine the required Fourier coefficients $f(\mathbf{G} - \mathbf{G}')$ for the inverse dielectric function $f(\mathbf{r})$.

For each photonic crystal studied, the reciprocal-space trajectory and number of steps along each $\mathbf{k}$ -space trajectory is defined. These trajectories trace out the irreducible portion of the Brillouin zone between the points of high symmetry and depend on the specific photonic crystal being considered. For the square lattice these points are the $\bar{X}$, $\bar{\Gamma}$, and $\bar{M}$ $\mathbf{k}$ -space points defined by equations 2.47 - 2.49. For the triangular lattice these points are the $\bar{K}$, $\bar{\Gamma}$, and $\bar{M}$ $\mathbf{k}$ -space points defined by equations 2.68 - 2.70.

The Hermitian matrices Θ_{TM} and Θ_{TE} given by equations 2.40 and 2.41 respectively are then obtained for each $\mathbf{k}$ -space point along each trajectory, and the eigenfrequencies for each $\mathbf{k}$ -space step are calculated. The collection of TM and TE eigenfrequencies as a function of $\mathbf{k}$ -space defines the photonic band structure. The $\mathbf{k}$ -space trajectory lengths are different and this is accounted for when plotting the photonic band structures.

The two-dimensional photonic band structure code, *pbs2D.m*, is listed in Appendix A.1. This code was used to generate the photonic band structures for both the square and triangular lattice photonic crystals.

3.1.2 Numerical Method in Three Dimensions

The application of the frequency-domain method in three dimensions is very similar to the application in two dimensions, however, there are some differences that make the calculation much more difficult. Specifically, the electromagnetic waves can no longer be split into TM and TE polarizations. The result is a much more complicated Θ matrix, as can be seen from equation 2.39. In addition, the Θ matrix to be diagonalized in three dimensions is twice as large as its Θ_{TM} or Θ_{TE} counterparts in two dimensions for a given number of plane waves.

The first step is to again define the real-space lattice vectors and lattice constant for the three-dimensional photonic crystal under investigation, either the fcc or diamond lattice. The second step is to define the various dielectric lattice parameters. This includes the dielectric constants of both the dielectric sphere and dielectric background. Next, the packing fraction is specified for the lattice under study, and the volume of the primitive unit cell calculated. The radius of each dielectric sphere is taken to be a function of the specified packing fraction. The next step is to generate the primitive reciprocal-space lattice vectors for the photonic crystal under study. Once the primitive reciprocal-space lattice vectors have been determined, the reciprocal vectors, $\mathbf{G}$, to be used for the calculation are collected. The reciprocal vectors used belong to a discrete approximation to a spherical region in $\mathbf{k}$ -space bounded by some maximum value. The maximum value is the norm of the largest reciprocal vector allowed for a desired number of plane waves. The number of plane waves used for

a given calculation is chosen to guarantee eigenvalue convergence to within 3%. The next step is to determine the required Fourier coefficients $f(\mathbf{G} - \mathbf{G}')$ for the inverse dielectric function $f(\mathbf{r})$.

The Brillouin zones for both the fcc and diamond lattice is given in Figure 2.5. The figure shows the irreducible portion of the Brillouin zone, highlighted in yellow. Also shown in the figure are the points of high symmetry that define the irreducible portion of the Brillouin zone. These points are the the $\bar{X}$, $\bar{U}$, $\bar{\Gamma}$, $\bar{L}$, $\bar{K}$, and $\bar{W}$ k-space points and defined by equations 2.75 - 2.80.

The k-space trajectory as well as the number of steps along each k-space trajectory is then defined. This trajectory traces out the irreducible portion of the Brillouin zone between the points of high symmetry.

The Hermitian Θ matrix, equation 2.39 is then obtained for each k-space step along each trajectory and the eigenfrequencies for each k-space step are calculated. The collection of eigenfrequencies as a function of k-space defines the photonic band structure. The k-space trajectory lengths are different and this is accounted for when plotting the photonic band structures.

The three-dimensional photonic band structure code, *pbs3D.m*, is listed in Appendix A.2. This code was used to generate the photonic band structures for both the fcc and diamond lattice photonic crystals.

3.2 Convergence of the Frequency Eigenvalues

The number of plane waves used in both the two and three dimensional calculations was varied until the eigenfrequencies differed by less than 3%. The Matlab code used to calculate the photonic band structures, given in Appendix A.1 and A.2, was run on a PC with a 1GHz Pentium III processor using the Windows NT operating system. The time to run the code depended on the number of $\mathbf{k}$ -space steps used to examine the irreducible Brillouin zone for a given reciprocal lattice. In two dimensions, the time to obtain the photonic band structure for 10 $\mathbf{k}$ -space steps along each of the 3 trajectories describing the irreducible Brillouin zone was approximately 30 minutes for a given photonic crystal. For a given photonic crystal geometry in three dimensions the time to obtain the photonic band structure for 10 $\mathbf{k}$ -space steps along each of the 6 trajectories describing the irreducible Brillouin zone was approximately 3 hours.

Chapter 4

Two-Dimensional Results

The computational method described in chapter 3 was applied in two dimensions for both the square and triangular lattice of dielectric columns with dielectric constant ϵ_a , embedded in a background dielectric material characterized by a dielectric constant ϵ_b . In two dimensions, the electromagnetic waves were assumed to propagate in a plane perpendicular to the columns. Two polarizations of these waves were considered. The first was the transverse electric, or TE polarization where the magnetic field vector is parallel to the columns. The second was the transverse magnetic, or TM polarization where the electric field vector is parallel to the columns. The eigenfrequencies were found for the corresponding $\mathbf{k}$ dependent matrices for these polarizations Θ_{TE} and Θ_{TM} as given by equations 2.46 and 2.47 respectively.

4.1 The Square Lattice of Dielectric Columns

The photonic band structure for the two-dimensional square lattice of dielectric columns is shown in Figure 4.1. The dielectric constant of the dielectric columns was taken to be $\epsilon_a = 13$, while the background dielectric was taken to be air, with a dielectric constant $\epsilon_b = 1$. The packing fraction was taken to be $P_f = 0.126$. This value of the packing fraction corresponded to columns of radius $R = 0.2a$ and allowed for comparison with similar results presented in [2]. The reciprocal vectors used in the calculation were chosen from all those reciprocal vectors contained within a circular region in $\mathbf{k}$ -space bounded by a maximum $|\mathbf{G}|$ that would ensure proper convergence of the eigenfrequencies. The circular region is a discrete estimate that improves as the number of reciprocal vectors is increased. A total of 373 plane waves were used in obtaining the resulting photonic band structure, and this number of $\mathbf{G}$'s ensured that the eigenfrequencies converged to within at least 2%. The value for ϵ_a was chosen to since it is approximately the static dielectric constant for GaAs, a reasonable dielectric choice for photonic crystals that might be manufactured for the microwave frequency range. As can be seen from Figure 4.1, the two-dimensional square lattice of dielectric columns has a photonic band gap for the TM modes (shown in blue) but not the TE modes (shown in red). The TM photonic band gap exists between the first and second band, and extends throughout the entire irreducible Brillouin zone. The TE modes have a large gap throughout most of the Brillouin zone, however, a photonic band gap is closed in the $\mathbf{k}$ -space region from $\tilde{X}$ to $\tilde{M}$.

Figure 4.1: The photonic band structure for the two-dimensional square lattice of dielectric columns. The transverse magnetic (TM) polarized modes are shown in blue in the figure. The transverse electric (TE) polarized modes are shown in red. The square lattice of dielectric columns possesses a photonic band gap for the TM polarized modes but not for the TE polarized modes.

4.2 The Square Lattice of Air Columns

The photonic band structure for the two-dimensional square lattice of air columns is shown in Figure 4.2. The dielectric constant of the dielectric columns was taken to be $\epsilon_a = 1$, while the background dielectric was taken to be GaAs, with a dielectric constant $\epsilon_b = 13$. The packing fraction was taken to be $P_f = 0.126$. This value of

the packing fraction corresponded to columns of radius $R = 0.2a$ and allowed for comparison with similar results presented in [2]. The reciprocal vectors used in the calculation were chosen from all those reciprocal vectors contained within a circular region in $\mathbf{k}$ -space bounded by a maximum $|\mathbf{G}|$ that would ensure proper convergence of the eigenfrequencies. The circular region is a discrete estimate that improves as the number of reciprocal vectors is increased. A total of 373 plane waves were used in obtaining the resulting photonic band structure, and this number of $\mathbf{G}$'s ensured that the eigenfrequencies converged to within at least 2%. As can be seen from Figure 4.2, the two-dimensional square lattice of dielectric columns does not have a photonic band gap for either the TM modes (shown in blue) or the TE modes (shown in red). The TM photonic band gap exists between the first and second band, and extends throughout the entire irreducible Brillouin zone. Both the TM and TE modes have a large gap throughout most of the Brillouin zone, however, a photonic band gap for both polarizations is closed in the $\mathbf{k}$ -space region from $\bar{X}$ to $\bar{M}$.

4.3 The Triangular Lattice of Dielectric Columns

The photonic band structure for the two-dimensional triangular lattice of air columns is shown in Figure 4.3. The dielectric constant of the dielectric columns was again taken to be $\epsilon_a = 13$, while the background dielectric was taken to be air, with a dielectric constant $\epsilon_b = 1$. The packing fraction was taken to be $P_f = 0.836$.

Figure 4.2: The photonic band structure for the two-dimensional square lattice of air columns. The transverse magnetic (TM) polarized modes are shown in blue in the figure. The transverse electric (TE) polarized modes are shown in red. The square lattice of air columns does not possess a photonic band gap for either the TM or TE modes.

This value of the packing fraction corresponded to columns of radius $R = 0.48a$. A total of 433 plane waves were necessary to obtain the resulting photonic band structure. This increased number of plane waves necessary to ensure that the calculated eigenfrequencies converged to within at least 2%. As can be seen from Figure 4.3, the two-dimensional triangular lattice of dielectric columns does not have a photonic

band gap for either the TM modes (shown in blue) or the TE modes (shown in red). The TM photonic band gap exists between the first and second band, and extends throughout the entire irreducible Brillouin zone. Both the TM and TE modes have a large gap throughout most of the Brillouin zone, however, a photonic band gap for both polarizations is closed in the $\mathbf{k}$ -space region from $\bar{X}$ to $\bar{M}$. For a sufficiently large, but rather impractical value of $\epsilon_a > 20$, both TM and TE modes will have photonic band gaps open up. However, the resulting TM and TE photonic band gaps will not be overlapping, and therefore a photonic band gap for both polarizations will not exist.

4.4 The Triangular Lattice of Air Columns

It is desirable to have a photonic crystal with a photonic band gap in a given range of frequencies for both TM and TE modes. To achieve this requires that the photonic crystal have high-dielectric regions that are practically isolated and linked by narrow veins [2]. The photonic band structure for the two-dimensional triangular lattice of air columns is shown in Figure 4.4. The dielectric constant of the air columns was again taken to be $\epsilon_a = 1$, while the background dielectric was taken to be GaAs, with a dielectric constant $\epsilon_b = 13$. The packing fraction was again taken to be $P_f = 0.836$, corresponding to columns of radius $R = 0.48a$. A total of 433 plane waves were again necessary to obtain the resulting photonic band structure, ensuring that the

Figure 4.3: The photonic band structure for the two-dimensional triangular lattice of dielectric columns. The transverse magnetic (TM) polarized modes are shown in blue in the figure. The transverse electric (TE) polarized modes are shown in red. The triangular lattice of high-dielectric columns in an air background does not possess a photonic band gap for either TM or TE polarized modes.

calculated eigenfrequencies converged to within at least 2%. As can be seen from Figure 4.4, the two-dimensional triangular lattice of air columns does indeed possess a photonic band gap for both the TM modes (shown in blue) and the TE modes (shown in red). The TM photonic band gap exists between the second and third TM band, and extends throughout the entire irreducible Brillouin zone. The TE photonic

band gap exists between the first and second TE band, and overlaps the TM photonic band gap throughout the entire irreducible Brillouin zone.

Figure 4.4: The photonic band structure for the two-dimensional triangular lattice of dielectric columns. The transverse magnetic (TM) polarized modes are shown in blue in the figure. The transverse electric (TE) polarized modes are shown in red. The triangular lattice of air columns in a high-dielectric background does possess a complete photonic band gap for both TM and TE modes. The photonic band gap is indicated in the figure by a yellow bar, showing the range of forbidden frequencies.

Chapter 5

Three-Dimensional Results

The computational method described in Chapter 3 was next applied in three dimensions for both the fcc and diamond lattices of dielectric spheres with dielectric constant ϵ_a , embedded in a background dielectric material characterized by a dielectric constant ϵ_b . In three dimensions, the electromagnetic waves cannot be assumed to propagate in any preferential plane, and therefore, cannot be separated into TM and TE polarization modes. All polarizations must therefore be considered. The eigenfrequencies were found for the corresponding $\mathbf{k}$ dependent matrix Θ , given by equation 2.45, for randomly polarized plane waves.

5.1 The fcc Lattice of Dielectric Spheres

The photonic band structure for the three-dimensional fcc lattice of dielectric spheres is shown in Figure 5.1. The dielectric constant of the dielectric spheres was

taken to be GaAs with dielectric constant $\epsilon_a = 13$, while the background dielectric was taken to be air, with a dielectric constant $\epsilon_b = 1$. The packing fraction was taken to be $P_f = 0.741$. This is the maximum value of the packing fraction for non-overlapping spheres and allowed for comparison with similar results presented in [2]. The reciprocal vectors used in the calculation were chosen from all those reciprocal vectors contained within a spherical region in $\mathbf{k}$ -space bounded by a maximum $|\mathbf{G}|$ that would ensure proper convergence of the eigenfrequencies. The spherical region is a discrete estimate of a sphere in $\mathbf{k}$ -space that improves as the number of reciprocal vectors is increased. A total of 283 plane waves were used in obtaining this photonic band structure, and this number of $\mathbf{G}$'s ensured that the eigenfrequencies converged to within at least 3%. As can be seen from Figure 5.1, the three-dimensional fcc lattice of dielectric spheres does not have a photonic band gap. A large gap does exist between bands two and three throughout most of the Brillouin zone in the $\mathbf{k}$ -space region from $\bar{L}$ to $\bar{\Gamma}$ to $\bar{X}$. However, Figure 5.1 shows that a photonic band gap is closed off in the $\mathbf{k}$ -space regions from $\bar{X}$ to $\bar{U}$ to $\bar{L}$ as well as from $\bar{X}$ to $\bar{W}$ to $\bar{K}$. There is no photonic band gap for the the fcc photonic crystal regardless of packing fraction and dielectric constants used [6].

Figure 5.1: The photonic band structure for the three-dimensional fcc lattice of dielectric spheres. A photonic band gap does not exist for this photonic crystal geometry.

5.2 The fcc Lattice of Air Spheres

The photonic band structure for the three-dimensional fcc lattice of air spheres is shown in Figure 5.2. The dielectric constant of the air spheres was taken to be $\epsilon_a = 1$, while the background dielectric was taken to be GaAs, with a dielectric constant $\epsilon_b = 13$. The packing fraction was again taken to be $P_f = 0.741$ for the fcc structure. A total of 283 plane waves were again used in obtaining this photonic

band structure, and ensured that the eigenfrequencies converged to within at least 3%. As can be seen from Figure 5.2, the three-dimensional fcc lattice of air spheres does not have a photonic band gap. Bands two and three again maintain a relatively large separation throughout most of the Brillouin zone in the $\mathbf{k}$ -space region from $\bar{L}$ to $\bar{\Gamma}$ to $\bar{X}$. However, Figure 5.2 shows that a photonic band gap is again inhibited in the $\mathbf{k}$ -space regions from $\bar{X}$ to $\bar{U}$ to $\bar{L}$ as well as from $\bar{X}$ to $\bar{W}$ to $\bar{K}$. There is no photonic band gap for the the fcc photonic crystal regardless of packing fraction and dielectric constants used [6].

5.3 The Diamond Lattice of Dielectric Spheres

The next photonic crystal examined was the diamond lattice of dielectric spheres. The photonic band structure for the three-dimensional diamond lattice of dielectric spheres is shown in Figure 5.3. The dielectric constant of the dielectric spheres was again taken to be $\epsilon_a = 13$, while the background dielectric was taken to be air, with a dielectric constant $\epsilon_b = 1$. The packing fraction was taken to be $P_f = 0.34$. This is the maximum value of the packing fraction for non-overlapping spheres in the diamond lattice and allowed for comparison with similar results presented in [2]. A total of 283 plane waves were used in obtaining this photonic band structure, and ensured that the eigenfrequencies converged to within at least 3%. As can be seen from Figure 5.3, the three-dimensional diamond lattice of dielectric spheres does indeed have a

Figure 5.2: The photonic band structure for the three-dimensional fcc lattice of air spheres. A photonic band gap does not exist for this photonic crystal geometry.

photonic band gap. A large gap. (highlighted in yellow), exists between bands two and three throughout the entire Brillouin zone.

5.4 The Diamond Lattice of Air Spheres

The final photonic crystal examined was the diamond lattice of air spheres. The photonic band structure for the three-dimensional diamond lattice of air spheres is

Figure 5.3: The photonic band structure for the three-dimensional diamond lattice of dielectric spheres. A photonic band gap exists for this photonic crystal geometry. The photonic band gap is indicated in the figure by a yellow bar, showing the range of forbidden frequencies.

shown in Figure 5.4. The dielectric constant of the air spheres was again taken to be $\epsilon_a = 1$, while the background dielectric was taken to be GaAs, with a dielectric constant $\epsilon_b = 13$. The packing fraction was again taken to be $P_f = 0.34$, corresponding to the maximum value of the packing fraction for non-overlapping spheres in the diamond lattice and allowed for comparison with similar results presented in [2]. A total of 283 plane waves were used in obtaining this photonic band structure, and ensured that the eigenfrequencies converged to within at least 3%. As can be seen

from Figure 5.4, the three-dimensional diamond lattice of air spheres does indeed possess a photonic band gap. The photonic band gap exists between bands two and three throughout the entire Brillouin zone. A photonic band gap will exist for this photonic crystal for dielectric contrasts as low as $\epsilon_b = 6.3$.

Figure 5.4: The photonic band structure for the three-dimensional diamond lattice of air spheres. A photonic band gap exists for this photonic crystal geometry. The photonic band gap is indicated in the figure by a yellow bar, showing the range of forbidden frequencies.

5.4.1 Effect of Packing Fraction on Gap Width

The effect of packing fraction, P_f , on gap width was examined for the three-dimensional diamond lattice of air spheres. The dielectric constants of the spheres were fixed at $\epsilon_a = 1$, and the background dielectric constant was fixed at $\epsilon_b = 13$. The packing fraction was then decreased from 100% of its maximum value, $P_f = \frac{\pi}{16}\sqrt{3}$, to 70% of its maximum value in 5% steps. As can be seen from Figure 5.5, the width of the photonic gap decreases approximately linearly with packing fraction. The photonic gap closes when the packing fraction reaches approximately $P_f = 0.25$, or 73.5% of the maximum packing fraction.

5.4.2 Effect of Background Dielectric on Gap Width

The effect of background dielectric, ϵ_b , on gap width was examined for the three-dimensional diamond lattice of air spheres. The packing fraction was fixed at its maximum value, $P_f = 0.34$, and the dielectric constant of the spheres was fixed at $\epsilon_a = 1$. The background dielectric was then decreased from $\epsilon_b = 13$ in 10% steps. As can be seen from Figure 5.6, the width of the photonic gap decreases with decreasing background dielectric. The photonic gap closes when the background dielectric reaches approximately $\epsilon_b = 6.25$.

Figure 5.5: The photonic band gap width as a function of packing fraction for the three-dimensional diamond lattice of low-dielectric spheres. The dielectric constant of the spheres ($\epsilon_a = 1$) and the dielectric constant of the background ($\epsilon_b = 13$) are fixed.

5.4.3 Effect of Different Sphere Dielectrics on Gap Width

For the two-sphere basis of the three-dimensional diamond lattice, the effect of non-identical sphere dielectric constants on gap width was examined. The packing fraction was fixed at its maximum value, $P_f = 0.34$, and the dielectric constant of the background was fixed at $\epsilon_b = 13$. The dielectric constant of a single sphere of

Figure 5.6: The photonic band gap width as a function of the dielectric constant of the background for the three-dimensional diamond lattice of low-dielectric spheres. The dielectric constant of the spheres ($\epsilon_a = 1$) and the packing fraction ($P_f = 0.34$) are fixed.

the two-sphere diamond basis was then increased from $\epsilon_{a2} = 1$ to $\epsilon_{a2} = 4$ in steps of 0.5. As can be seen from Figure 5.7, the width of the photonic gap decreases as the dielectric constant of a single sphere is increased. The photonic gap closes when the second sphere in the two sphere basis reaches approximately $\epsilon_{a2} = 3.4$.

Figure 5.7: The photonic band gap width as a function of the dielectric constant of a single sphere of the two-sphere basis of the the three-dimensional diamond lattice of low-dielectric spheres. The dielectric constant of the first sphere ($\epsilon_{a1} = 1$), the dielectric constant of the background ($\epsilon_b = 13$), and the packing fraction ($P_f = 0.34$) are fixed.

Chapter 6

Conclusions

Using a plane-wave expansion of the photonic crystal master equation, (equation 2.25), and by the use of a periodic dielectric constant, $\epsilon(\mathbf{r})$, the problem of the propagation of electromagnetic waves in several two-dimensional and three-dimensional photonic crystals has been solved. The problem was solved numerically using a frequency-domain computational method that took the vector nature of the electromagnetic field into account. The computational approach is based on the use of a periodic, position dependent dielectric constant $\epsilon(\mathbf{r})$ and an expansion of the electromagnetic field components in plane waves. The photonic band structure for a given photonic crystal then results from the solution of a standard Hermitian eigenvalue problem.

6.1 Summary of Results

In two dimensions, photonic band structures were calculated for electromagnetic waves of both transverse magnetic (TM) and transverse electric (TE) polarized modes. The modes were assumed to propagate in the plane perpendicular to a periodic array of identical, non-overlapping dielectric columns, of dielectric constant ϵ_a . The columns had a circular cross section and were embedded in a dielectric background whose dielectric constant ϵ_b differed from that of the columns. The intersection of the columns with a perpendicular plane formed either a square or triangular lattice.

For the two-dimensional square lattice of high-dielectric columns in an air background TM polarized modes do exhibit a photonic band gap, however, the TE polarized modes do not exhibit a photonic band gap in their photonic band structure. For the case of a square lattice of air columns in a high dielectric background, neither TM nor TE polarized modes exhibit photonic band gaps in their photonic band structures.

The triangular lattice of high-dielectric columns in an air background did not possess a complete photonic band gap for either TM or TE polarized modes. However, the triangular lattice of air columns in a high-dielectric background did in fact possess a complete photonic band gap for both TM and TE modes. This confirmed Joannopoulos' rule for photonic crystals [2] that TM band gaps are favored in a lattice of isolated high-dielectric regions, and that TE band gaps are favored in a connected lattice. The frequencies of this two-dimensional photonic band gap fall

into a reasonable experimental range. For example, when $a = 2 \text{ cm}$, and $R = 0.48a$, the width of the photonic band gap depicted in Figure 4.4 is approximately 1.20 GHz, and is centered at a frequency of about 7.35 GHz.

In three dimensions, a periodic lattices of dielectric spheres of dielectric constant ϵ_a embedded in a dielectric background of dielectric constant ϵ_b were investigated. Neither the three-dimensional fcc lattice of high-dielectric spheres in an air background nor the fcc lattice of air spheres in a high-dielectric background exhibit a photonic band gap in their photonic band structures.

The diamond lattice of high-dielectric spheres in an air background and the diamond lattice of air spheres in high-dielectric background both possess photonic band gaps in their photonic band structures. The frequencies of the three-dimensional photonic band gap for the diamond lattice of air spheres in a high-dielectric background fall into a reasonable experimental range. For example, when $a = 2 \text{ cm}$, and $R = 0.34a$, the width of the photonic band gap depicted in Figure 5.4 is approximately 0.38 GHz, and is centered at a frequency of about 5.44 GHz.

Figures 5.5 and 5.6 show the effect of the variation of background dielectric, ϵ_b , and packing fraction, P_f , on the photonic band gap width. These are useful photonic crystal design parameters, but would be difficult to dynamically tune in a practical photonic crystal design.

Figure 5.7 shows the effect of the variation of the photonic band gap width as a function of the dielectric constant of only a single dielectric sphere in the two-

sphere basis of the diamond lattice structure. The results presented in Figure 5.7 are important because they illustrate a novel means of controlling the photonic band gap width, and they indicate the degree to which the photonic band gap might be tuned to suit a photonic crystal designer's needs.

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Appendix A

MATLAB Code.

A.1 2D Photonic Band Structure Code

```
%=====
% Name:          pbs2D.m - 2D Photonic Band Structure Code.
% Author:        Aaron Morton.
% Date:          08/26/01  A.Morton - Orignal pbs2D.m code.
%
% Description:    Calculates photonic band structure for either
%                a square or triangular lattice of
%                dielectric columns of dielectric constant
%                epsilon_a in a dielectric background of
%                dielectric constant epsilon_b.
%=====
clear; clc; tic;

%=====
% Define real lattice vectors.
%=====
SQUARE      = 0;
TRIANGULAR  = 1;

if (SQUARE)
```

```

a = 1; % Lattice constant.
a1 = a*[1 0 0]; % Real square lattice vectors.
a2 = a*[0 1 0];
a3 = a*[0 0 1];
elseif (TRIANGULAR)
a = 1; % Lattice constant.
a1 = a*[ sqrt(3)/2 1/2 0]; % Real triangular lattice vectors.
a2 = a*[-sqrt(3)/2 1/2 0];
a3 = a*[0 0 1];
end;

%=====
% Dielectric lattice parameters.
%=====
epsa = 1; % Dielectric constant of column.
epsb = 13; % Dielectric constant of background.
Pf = 0.836; % Pf = Ac/Au is the packing fraction.
Au = norm(cross(a1,a2)); % Area of the primitive unit cell.
Rc = (Pf*Au/pi)^(1/2); % Radius of each dielectric column.
Ac = pi*(Rc)^2; % Area of column cross-section.

%=====
% Generate reciprocal lattice.
%=====
ra1 = (2*pi/a)*cross(a2,a3)/dot(a1,cross(a2,a3));
ra2 = (2*pi/a)*cross(a3,a1)/dot(a1,cross(a2,a3));
ra1 = ra1(1:2);
ra2 = ra2(1:2);

%=====
% Determine reciprocal vectors to use.
% (Circular region in k-space bounded by Gmax).
%=====
NrSquare = 20; % Cube size in k-space.
Gmax = 0.55*NrSquare*norm(ra1); % Max |G| to use.
G = zeros((2*NrSquare+1)^2,2); % Max number possible G's.
i = 1;

for l = -NrSquare:NrSquare
for m = -NrSquare:NrSquare

```

```

    G1m = l*ra1 + m*ra2;

    if (norm(G1m) < Gmax)                % Check |G1m|.
        G(i,:) = G1m;
        i      = i + 1;
    end;

end;
end;

NG = i - 1                               % Actual number G's used.
G  = G(1:NG,:);

%=====
% Generate k-space f(Gi-Gj) values for every i,j = 1 to NG.
%=====
f = zeros(NG,NG);

for i = 1:NG
    for j = 1:NG

        Gij = norm(G(i,:)-G(j,:));

        if (Gij == 0)
            f(i,j) = (1/epsa)*Pf + (1/epsb)*(1-Pf);
        else
            f(i,j) = (1/epsa - 1/epsb)*Pf*2*besselj(1,Gij*Rc)/(Gij*Rc);
        end;

    end;

end;
end;

%=====
% Define reciprocal lattice vectors which k-space trajectory.
% The k-space trajectory follows the irreducible portion
% of the Brillouin zone.
%=====
if (SQUARE)
    T = (2*pi/a)*[1e-4  0];
    M = (2*pi/a)*[1/2  1/2];
    X = (2*pi/a)*[1/2  0];

```



```

elseif(TRIANGULAR)
    T = (2*pi/a)*[1e-4      0];
    M = (2*pi/a)*[sqrt(3)/3  0];
    K = (2*pi/a)*[sqrt(3)/3  1/3];
end;

%=====
% Get eigenfreqs for each k-space point on the trajectory.
%=====
THETA_TM = zeros(NG,NG);      % TM matrix to solve.
THETA_TE = zeros(NG,NG);      % TE matrix to solve.
Nkpoints = 10;                % Number steps each k-space traj.
stepsize = 0:1/(Nkpoints-1):1; % Trajectory step size in k-space.

if (SQUARE)
    TX_TM_eig = zeros(Nkpoints,NG); % TM eig-freqs along TX traj.
    TX_TE_eig = zeros(Nkpoints,NG); % TE eig-freqs along TX traj.
    XM_TM_eig = zeros(Nkpoints,NG); % TM eig-freqs along XM traj.
    XM_TE_eig = zeros(Nkpoints,NG); % TE eig-freqs along XM traj.
    MT_TM_eig = zeros(Nkpoints,NG); % TM eig-freqs along MT traj.
    MT_TE_eig = zeros(Nkpoints,NG); % TE eig-freqs along MT traj.
elseif(TRIANGULAR)
    TM_TM_eig = zeros(Nkpoints,NG); % TM eig-freqs along TX traj.
    TM_TE_eig = zeros(Nkpoints,NG); % TE eig-freqs along TX traj.
    MK_TM_eig = zeros(Nkpoints,NG); % TM eig-freqs along MK traj.
    MK_TE_eig = zeros(Nkpoints,NG); % TE eig-freqs along MK traj.
    KT_TM_eig = zeros(Nkpoints,NG); % TM eig-freqs along KT traj.
    KT_TE_eig = zeros(Nkpoints,NG); % TE eig-freqs along KT traj.
end;

for n = 1:Nkpoints

    fprintf(['\n k-point:',int2str(n),'of',int2str(Nkpoints),'\n']);

    %=====
    % Calculate eigenfrequencies for the k-space step along the
    % TX (square) or TM (triangular) trajectory.
    %=====
    if (SQUARE)
        TX_step = stepsize(n)*(X-T) + T;
    elseif(TRIANGULAR)

```

```

    TM_step = stepsize(n)*(M-T) + T;
end;

for i = 1:(NG-1) for j = (i+1):NG

    if (SQUARE)
        kGi = TX_step + G(i,:);
        kGj = TX_step + G(j,:);
    elseif(TRIANGULAR)
        kGi = TM_step + G(i,:);
        kGj = TM_step + G(j,:);
    end;

    THETA_TM(i,j) = f(i,j)*norm(kGi)*norm(kGj); % Off-diag elements.
    THETA_TM(j,i) = THETA_TM(i,j);             % THETA_TM symmetric.
    THETA_TE(i,j) = f(i,j)*dot(kGi,kGj);       % Off-diag elements.
    THETA_TE(j,i) = THETA_TE(i,j);             % THETA_TM symmetric.

end; end;

for i = 1:NG

    if (SQUARE)
        kGi = TX_step + G(i,:);
    elseif(TRIANGULAR)
        kGi = TM_step + G(i,:);
    end;

    THETA_TM(i,i) = f(i,i)*norm(kGi)*norm(kGi); % Diag elements.
    THETA_TE(i,i) = f(i,i)*norm(kGi)*norm(kGi); % Diag elements.

end;

if (SQUARE)
    TX_TM_eig(n,:) = sort(sqrt(eig(THETA_TM))).';
    TX_TE_eig(n,:) = sort(sqrt(eig(THETA_TE))).';
elseif(TRIANGULAR)
    TM_TM_eig(n,:) = sort(sqrt(eig(THETA_TM))).';
    TM_TE_eig(n,:) = sort(sqrt(eig(THETA_TE))).';
end;

```

```

%=====
% Calculate eigenfrequencies for the k-space step along the
% XM (square) or MK (triangular) trajectory.
%=====
if (SQUARE)
    XM_step = stepsize(n)*(M-X) + X;
elseif(TRIANGULAR)
    MK_step = stepsize(n)*(K-M) + M;
end;

for i = 1:(NG-1)
    for j = (i+1):NG

        if (SQUARE)
            kGi = XM_step + G(i,:);
            kGj = XM_step + G(j,:);
        elseif(TRIANGULAR)
            kGi = MK_step + G(i,:);
            kGj = MK_step + G(j,:);
        end;

        THETA_TM(i,j) = f(i,j)*norm(kGi)*norm(kGj); % Off-diag elements.
        THETA_TM(j,i) = THETA_TM(i,j); % THETA_TM symmetric.
        THETA_TE(i,j) = f(i,j)*dot(kGi,kGj); % Off-diag elements.
        THETA_TE(j,i) = THETA_TE(i,j); % THETA_TE symmetric.

    end;
end;

for i = 1:NG

    if (SQUARE)
        kGi = XM_step + G(i,:);
    elseif(TRIANGULAR)
        kGi = MK_step + G(i,:);
    end;

    THETA_TM(i,i) = f(i,i)*norm(kGi)*norm(kGi); % Diag elements.
    THETA_TE(i,i) = f(i,i)*norm(kGi)*norm(kGi); % Diag elements.

end;

```

```

if (SQUARE)
    XM_TM_eig(n,:) = sort(sqrt(eig(THETA_TM))).';
    XM_TE_eig(n,:) = sort(sqrt(eig(THETA_TE))).';
elseif (TRIANGULAR)
    MK_TM_eig(n,:) = sort(sqrt(eig(THETA_TM))).';
    MK_TE_eig(n,:) = sort(sqrt(eig(THETA_TE))).';
end;

%=====
% Calculate eigenfrequencies for the k-space step along the
% MT (square) or KT (triangular) trajectory.
%=====
if (SQUARE)
    MT_step = stepsize(n)*(T-M) + M;
elseif (TRIANGULAR)
    KT_step = stepsize(n)*(T-K) + K;
end;

for i = 1:(NG-1)
    for j = (i+1):NG

        if (SQUARE)
            kGi = MT_step + G(i,:);
            kGj = MT_step + G(j,:);
        elseif (TRIANGULAR)
            kGi = KT_step + G(i,:);
            kGj = KT_step + G(j,:);
        end;

        THETA_TM(i,j) = f(i,j)*norm(kGi)*norm(kGj); % Off-diag elements.
        THETA_TM(j,i) = THETA_TM(i,j);              % THETA_TM symmetric.
        THETA_TE(i,j) = f(i,j)*dot(kGi,kGj);         % Off-diag elements.
        THETA_TE(j,i) = THETA_TE(i,j);              % THETA_TE symmetric.

    end;
end;

for i = 1:NG

    if (SQUARE)

```

```

    kGi = MT_step + G(i,:);
elseif(TRIANGULAR)
    kGi = KT_step + G(i,:);
end;

THETA_TM(i,i) = f(i,i)*norm(kGi)*norm(kGi); % Diag elements.
THETA_TE(i,i) = f(i,i)*norm(kGi)*norm(kGi); % Diag elements.

end;

if (SQUARE)
    MT_TM_eig(n,:) = sort(sqrt(eig(THETA_TM))).';
    MT_TE_eig(n,:) = sort(sqrt(eig(THETA_TE))).';
elseif(TRIANGULAR)
    KT_TM_eig(n,:) = sort(sqrt(eig(THETA_TM))).';
    KT_TE_eig(n,:) = sort(sqrt(eig(THETA_TE))).';
end;

end % for n = 1:Nkpoints

fprintf('\n Calculation time: %d sec.', toc);
save pbs2Ddata;

%=====
% Trajectory lengths different, account for this when plotting.
%=====
if (SQUARE)
    kaxis = 0; % Relative k-space axis offset used for plotting.
    TXaxis = kaxis:norm(T-X)/(Nkpoints-1):(kaxis + norm(T-X));
    kaxis = kaxis + norm(T-X);
    XMaxis = kaxis:norm(X-M)/(Nkpoints-1):(kaxis + norm(X-M));
    kaxis = kaxis + norm(X-M);
    MTaxis = kaxis:norm(M-T)/(Nkpoints-1):(kaxis + norm(M-T));
    kaxis = kaxis + norm(M-T);
elseif(TRIANGULAR)
    kaxis = 0; % Relative k-space axis offset used for plotting.
    TMaxis = kaxis:norm(T-M)/(Nkpoints-1):(kaxis + norm(T-M));
    kaxis = kaxis + norm(T-M);
    MKaxis = kaxis:norm(M-K)/(Nkpoints-1):(kaxis + norm(M-K));
    kaxis = kaxis + norm(M-K);
    KTaxis = kaxis:norm(K-T)/(Nkpoints-1):(kaxis + norm(K-T));

```

```

    kaxis = kaxis + norm(K-T);
end;

%=====
% Plot 2D Photonic Band Structure (PBS).
%=====
Ntraject = 3;           % Number of k-space trajectories to plot.
EigFreq_TM = zeros(Ntraject*Nkpoints,1);
EigFreq_TE = zeros(Ntraject*Nkpoints,1);

figure(1);
hold on;

Nk = Nkpoints;

for k = 1:NG
for i = 1:Nkpoints

    if (SQUARE)
        EigFreq_TM(i + 0*Nk) = TX_TM_eig(i,k)/(2*pi/a);
        EigFreq_TM(i + 1*Nk) = XM_TM_eig(i,k)/(2*pi/a);
        EigFreq_TM(i + 2*Nk) = MT_TM_eig(i,k)/(2*pi/a);
        EigFreq_TE(i + 0*Nk) = TX_TE_eig(i,k)/(2*pi/a);
        EigFreq_TE(i + 1*Nk) = XM_TE_eig(i,k)/(2*pi/a);
        EigFreq_TE(i + 2*Nk) = MT_TE_eig(i,k)/(2*pi/a);
    elseif (TRIANGULAR)
        EigFreq_TM(i + 0*Nk) = TM_TM_eig(i,k)/(2*pi/a);
        EigFreq_TM(i + 1*Nk) = MK_TM_eig(i,k)/(2*pi/a);
        EigFreq_TM(i + 2*Nk) = KT_TM_eig(i,k)/(2*pi/a);
        EigFreq_TE(i + 0*Nk) = TM_TE_eig(i,k)/(2*pi/a);
        EigFreq_TE(i + 1*Nk) = MK_TE_eig(i,k)/(2*pi/a);
        EigFreq_TE(i + 2*Nk) = KT_TE_eig(i,k)/(2*pi/a);
    end;

end; % for i = 1:Nkpoints

if (SQUARE)
    plot( TXaxis(1:Nk),EigFreq_TM(1+0*Nk:1*Nk),'b', ...
          XMaxis(1:Nk),EigFreq_TM(1+1*Nk:2*Nk),'b', ...
          MTaxis(1:Nk),EigFreq_TM(1+2*Nk:3*Nk),'b' );
    plot( TXaxis(1:Nk),EigFreq_TE(1+0*Nk:1*Nk),'r', ...

```

```

        XMaxis(1:Nk),EigFreq_TE(1+1*Nk:2*Nk),'r', ...
        MMaxis(1:Nk),EigFreq_TE(1+2*Nk:3*Nk),'r' );
elseif (TRIANGULAR)
    plot( TMaxis(1:Nk),EigFreq_TM(1+0*Nk:1*Nk),'b', ...
          MMaxis(1:Nk),EigFreq_TM(1+1*Nk:2*Nk),'b', ...
          KMaxis(1:Nk),EigFreq_TM(1+2*Nk:3*Nk),'b' );
    plot( TMaxis(1:Nk),EigFreq_TE(1+0*Nk:1*Nk),'r', ...
          MMaxis(1:Nk),EigFreq_TE(1+1*Nk:2*Nk),'r', ...
          KMaxis(1:Nk),EigFreq_TE(1+2*Nk:3*Nk),'r' );
end;

end; % for k = 1:NG

grid on;
hold off;

titlestr = ['2D Photonic band structure for'];
if (SQUARE)
    titlestr = [titlestr 'square '];
elseif (TRIANGULAR)
    titlestr = [titlestr 'triangular '];
end;
titlestr = [titlestr 'lattice of dielectric columns. '];
titlestr = [titlestr '(epsa = ',num2str(epsa),', ...
            epsb = ',num2str(epsb),')'];
title (titlestr);

xlabel ('k-Space');
ylabel ('Frequency (wa/c2pi)');

if(SQUARE)
    axis ([0 MMaxis(Nkpoints) 0 1]);
    set (gca,'XTick', [TMaxis(1) ...
                      TMaxis(Nkpoints) ...
                      XMaxis(Nkpoints) ...
                      MMaxis(Nkpoints)]);
    xtixlabel = strvcats('T', 'X', 'M', 'T');
elseif(TRIANGULAR)
    axis ([0 KMaxis(Nkpoints) 0 1]);
    set (gca,'XTick', [TMaxis(1) ...
                      TMaxis(Nkpoints) ...

```

```

            MKaxis(Nkpoints) ...
            KTaxis(Nkpoints) ]);
    xtixlabel = strvcat('T', 'M', 'K', 'T');
end;
set(gca,'XTickLabel',xtixlabel);

```

A.2 3D Photonic Band Structure Code

```

%=====
% Name:          pbs3D.m - 3D Photonic Band Structure Code.
% Author:        Aaron Morton.
% Date:          08/26/01  A.Morton - Orignal pbs3D.m code.
%
% Description:    Calculates photonic band structure for either
%                an fcc or diamond lattice of dielectric
%                spheres of dielectric constant
%                epsilon_a in a dielectric background of
%                dielectric constant epsilon_b.
%=====
clear; clc; tic;

%=====
% Define real lattice vectors.
%=====
FCC      = 0;
DIAMOND  = 1;

a  = 1;                % Lattice constant.
a1 = a*[0.50 0.50 0.00]; % Real fcc/diamond lattice vectors.
a2 = a*[0.00 0.50 0.50];
a3 = a*[0.50 0.00 0.50];

%=====
% Dielectric lattice parameters.
%=====
epsa  = 1;                % Dielectric constant sphere.
epsb  = 13;               % Dielectric constant background.

```



```

epsa1 = 1;           % Dielectric constant sphere 1 in basis.
epsa2 = 1;           % Dielectric constant sphere 2 in basis.

if (FCC)
    Pf = (pi/6)*sqrt(2); % Packing fraction for fcc.
elseif (DIAMOND)
    Pf = (pi/16)*sqrt(3) % Packing fraction for diamond.
end;

Vu = dot(a1,cross(a2,a3)); % Volume of primitive unit cell.

if (FCC)
    Rs = (3*Pf*Vu/(4*pi))^(1/3); % Radius of each sphere.
else %(DIAMOND)
    Rs = (3*Pf*Vu/(8*pi))^(1/3) % Radius of each sphere.
end;

%=====
% Generate reciprocal lattice.
%=====
ra1 = (2*pi/a)*cross(a2,a3)/dot(a1,cross(a2,a3));
ra2 = (2*pi/a)*cross(a3,a1)/dot(a1,cross(a2,a3));
ra3 = (2*pi/a)*cross(a1,a2)/dot(a1,cross(a2,a3));

%=====
% Determine reciprocal vectors to use.
% (Spherical region in k-space bounded by Gmax.)
%=====
Nrcube = 20;           % Cube size in k-space.
Gmax    = 0.183*Nrcube*norm(ra1); % Max |G| to use.
G       = zeros((2*Nrcube+1)^3,3); % Max number possible G's.
i       = 1;

for l = -Nrcube:Nrcube
for m = -Nrcube:Nrcube
for n = -Nrcube:Nrcube

    Glmn = l*ra1 + m*ra2 + n*ra3;

    if (norm(Glmn) < Gmax)           % Check |Glmn|.
        G(i,:) = Glmn;
    end
end
end
end

```

```

        i      = i + 1;
    end;

end;
end;
end;

NG = i - 1;                                % Actual number G's used.
G  = G(1:NG,:);

%=====
%  Generate k-space f(Gi-Gj) values for every i,j = 1 to NG.
%=====
f = zeros(NG,NG);

for i=1:NG
for j=1:NG

    Gij = norm(G(i,:)-G(j,:));

    if (Gij == 0)      % Diagonal element of dielectric matrix.

        f(i,j) = (1/epsb) + Pf*(1/(2*epsa1) + 1/(2*epsa2) - 1/epsb);

    else % (Gij ~= 0) % Off-diagonal element of dielectric matrix.

        if (FCC)
            f(i,j) = 3*Pf*(1/epsb - 1/epsa)*( Gij*Rs*cos(Gij*Rs) ...
                - sin(Gij*Rs) )/((Gij*Rs)^3);
        else %(DIAMOND)
            tau    = a*[1/8 1/8 1/8];
            f(i,j) = 3*Pf*( cos(dot(G(i,:)-G(j,:),tau))/epsb ...
                - exp(-sqrt(-1)*dot(G(i,:)-G(j,:),tau))/(2*epsa1) ...
                - exp(sqrt(-1)*dot(G(i,:)-G(j,:),tau))/(2*epsa2)) ...
                * (Gij*Rs*cos(Gij*Rs)-sin(Gij*Rs))/((Gij*Rs)^3);
        end;

    end;

end;

end;
end;

```

```

%=====
% Define reciprocal lattice vectors which k-space trajectory.
% The k-space trajectory follows the irreducible portion
% of the Brillouin zone.
%=====
X = (2*pi/a)*[1.00 0.00 0.00];
U = (2*pi/a)*[1.00 0.25 0.25];
L = (2*pi/a)*[0.50 0.50 0.50];
T = (2*pi/a)*[1e-4 0.00 0.00];
W = (2*pi/a)*[1.00 0.50 0.00];
K = (2*pi/a)*[0.75 0.75 0.00];

%=====
% Get eigenfreqs for each k-space point on the trajectory.
%=====
THETA = zeros(2*NG,2*NG); % Matrix to solve.
Nkpoints = 10; % Numb steps each k-space traj.
stepsize = 0:1/(Nkpoints-1):1; % Traj. step size in k-space.
XU_eig = zeros(Nkpoints,2*Neig); % THETA eig-freqs on XU traj.
UL_eig = zeros(Nkpoints,2*Neig); % THETA eig-freqs on UL traj.
LT_eig = zeros(Nkpoints,2*Neig); % THETA eig-freqs on LT traj.
TX_eig = zeros(Nkpoints,2*Neig); % THETA eig-freqs on TX traj.
XW_eig = zeros(Nkpoints,2*Neig); % THETA eig-freqs on XW traj.
WK_eig = zeros(Nkpoints,2*Neig); % THETA eig-freqs on WK traj.
ei = zeros(1,3); % Polarization vectors.
ej = zeros(1,3); % Polarization vectors.

for n = 1:Nkpoints

fprintf(['\n k-point:',int2str(n),'of',int2str(Nkpoints),'\n']);

%=====
% Calculate eigenfrequencies for the k-space step along the
% XU trajectory.
%=====
XU_step = stepsize(n)*(U-X) + X;

%=====
% Get the polarization vectors for the NG plane waves for
% the current step along the XU trajectory.

```

```

%=====
for i = 1:NG

    Ki = XU_step + G(i,:);
    [e1, e2] = get_polarization_vectors(Ki);
    e_polar_vec(1,i,:) = e1;
    e_polar_vec(2,i,:) = e2;

end;

%=====
% Determine the off-diag elements of THETA matrix for XU_step.
%=====
for i = 1:(2*NG-1)
    for j = (i+1):(2*NG)

        iG = ceil(i/2);
        jG = ceil(j/2);
        ie = mod(i,2) + mod(mod(i,2)+2,3);
        je = mod(j,2) + mod(mod(j,2)+2,3);

        ei(1:3) = e_polar_vec(ie,iG,:);
        ej(1:3) = e_polar_vec(je,jG,:);
        Ki      = XU_step + G(iG,:);
        Kj      = XU_step + G(jG,:);

        THETA(i,j) = f(iG,jG)*dot(cross(Ki,ei),cross(Kj,ej));
        THETA(j,i) = conj(THETA(i,j)); % THETA is symmetric.

    end;
end;

%=====
% Determine the diagonal elements of THETA matrix for XU_step.
%=====
for i = 1:(2*NG)

    iG = ceil(i/2);
    ie = mod(i,2) + mod(mod(i,2)+2,3);

    ei(1:3) = e_polar_vec(ie,iG,:);

```

```

    Ki      = XU_step + G(iG,:);

    THETA(i,i) = f(iG,iG)*norm(cross(Ki,ei))^2;

end;

XU_eig(n,:) = sort(sqrt(eig(THETA))).';

%=====
% Calculate eigenfrequencies for the k-space step along the
% UL trajectory.
%=====
UL_step = stepsize(n)*(L-U) + U;

%=====
% Get the polarization vectors for the NG plane waves for
% the current step along the UL trajectory.
%=====
for i = 1:NG

    Ki = UL_step + G(i,:);
    [e1, e2] = get_polarization_vectors(Ki);
    e_polar_vec(1,i,:) = e1;
    e_polar_vec(2,i,:) = e2;

end;

%=====
% Determine the off-diag elements of THETA matrix for UL_step.
%=====
for i = 1:(2*NG-1)
    for j = (i+1):(2*NG)

        iG = ceil(i/2);
        jG = ceil(j/2);
        ie = mod(i,2) + mod(mod(i,2)+2,3);
        je = mod(j,2) + mod(mod(j,2)+2,3);

        ei(1:3) = e_polar_vec(ie,iG,:);
        ej(1:3) = e_polar_vec(je,jG,:);
        Ki      = UL_step + G(iG,:);

```

```

    Kj      = UL_step + G(jG,:);

    THETA(i,j) = f(iG,jG)*dot(cross(Ki,ei),cross(Kj,ej));
    THETA(j,i) = conj(THETA(i,j)); % THETA is symmetric.

end;
end;

%=====
% Determine the diagonal elements of THETA matrix for XU_step.
%=====
for i = 1:(2*NG)

    iG = ceil(i/2);
    ie = mod(i,2) + mod(mod(i,2)+2,3);

    ei(1:3) = e_polar_vec(ie,iG,:);
    Ki      = UL_step + G(iG,:);

    THETA(i,i) = f(iG,iG)*norm(cross(Ki,ei))^2;

end;

UL_eig(n,:) = sort(sqrt(eig(THETA))).';

%=====
% Calculate eigenfrequencies for the k-space step along the
% LT trajectory.
%=====
LT_step = stepsize(n)*(T-L) + L;

%=====
% Get the polarization vectors for the NG plane waves for
% the current step along the LT trajectory.
%=====
for i = 1:NG

    Ki = LT_step + G(i,:);
    [e1, e2] = get_polarization_vectors(Ki);
    e_polar_vec(1,i,:) = e1;
    e_polar_vec(2,i,:) = e2;

```

```

end;

%=====
% Determine the off-diag elements of THETA matrix for LT_step.
%=====
for i = 1:(2*NG-1)
for j = (i+1):(2*NG)

    iG = ceil(i/2);
    jG = ceil(j/2);
    ie = mod(i,2) + mod(mod(i,2)+2,3);
    je = mod(j,2) + mod(mod(j,2)+2,3);

    ei(1:3) = e_polar_vec(ie,iG,:);
    ej(1:3) = e_polar_vec(je,jG,:);
    Ki      = LT_step + G(iG,:);
    Kj      = LT_step + G(jG,:);

    THETA(i,j) = f(iG,jG)*dot(cross(Ki,ei),cross(Kj,ej));
    THETA(j,i) = conj(THETA(i,j)); % THETA is symmetric.

end;
end;

%=====
% Determine the diagonal elements of THETA matrix for XU_step.
%=====
for i = 1:(2*NG)

    iG = ceil(i/2);
    ie = mod(i,2) + mod(mod(i,2)+2,3);

    ei(1:3) = e_polar_vec(ie,iG,:);
    Ki      = LT_step + G(iG,:);

    THETA(i,i) = f(iG,iG)*norm(cross(Ki,ei))^2;

end;

LT_eig(n,:) = sort(sqrt(eig(THETA))).';

```

```

%=====
% Calculate eigenfrequencies for the k-space step along the
% TX trajectory.
%=====
TX_step = stepsize(n)*(X-T) + T;

%=====
% Get the polarization vectors for the NG plane waves for
% the current step along the TX trajectory.
%=====
for i = 1:NG

    Ki = TX_step + G(i,:);
    [e1, e2] = get_polarization_vectors(Ki);
    e_polar_vec(1,i,:) = e1;
    e_polar_vec(2,i,:) = e2;

end;

%=====
% Determine the off-diag elements of THETA matrix for TX_step.
%=====
for i = 1:(2*NG-1)
    for j = (i+1):(2*NG)

        iG = ceil(i/2);
        jG = ceil(j/2);
        ie = mod(i,2) + mod(mod(i,2)+2,3);
        je = mod(j,2) + mod(mod(j,2)+2,3);

        ei(1:3) = e_polar_vec(ie,iG,:);
        ej(1:3) = e_polar_vec(je,jG,:);
        Ki      = TX_step + G(iG,:);
        Kj      = TX_step + G(jG,:);

        THETA(i,j) = f(iG,jG)*dot(cross(Ki,ei),cross(Kj,ej));
        THETA(j,i) = conj(THETA(i,j)); % THETA is symmetric.

    end;
end;

```



```

%=====
% Determine the diagonal elements of THETA matrix for TX_step.
%=====
for i = 1:(2*NG)

    iG = ceil(i/2);
    ie = mod(i,2) + mod(mod(i,2)+2,3);

    ei(1:3) = e_polar_vec(ie,iG,:);
    Ki      = TX_step + G(iG,:);

    THETA(i,i) = f(iG,iG)*norm(cross(Ki,ei))^2;

end;

TX_eig(n,:) = sort(sqrt(eig(THETA))).';

%=====
% Calculate eigenfrequencies for the k-space step along the
% XW trajectory.
%=====
XW_step = stepsize(n)*(W-X) + X;

%=====
% Get the polarization vectors for the NG plane waves for
% the current step along the XW trajectory.
%=====
for i = 1:NG

    Ki = XW_step + G(i,:);
    [e1, e2] = get_polarization_vectors(Ki);
    e_polar_vec(1,i,:) = e1;
    e_polar_vec(2,i,:) = e2;

end;

%=====
% Determine the off-diag elements of THETA matrix for XW_step.
%=====
for i = 1:(2*NG-1)

```

```

for j = (i+1):(2*NG)

    iG = ceil(i/2);
    jG = ceil(j/2);
    ie = mod(i,2) + mod(mod(i,2)+2,3);
    je = mod(j,2) + mod(mod(j,2)+2,3);

    ei(1:3) = e_polar_vec(ie,iG,:);
    ej(1:3) = e_polar_vec(je,jG,:);
    Ki      = XW_step + G(iG,:);
    Kj      = XW_step + G(jG,:);

    THETA(i,j) = f(iG,jG)*dot(cross(Ki,ei),cross(Kj,ej));
    THETA(j,i) = conj(THETA(i,j)); % THETA is symmetric.

end;
end;

%=====
% Determine the diagonal elements of THETA matrix for XW_step.
%=====
for i = 1:(2*NG)

    iG = ceil(i/2);
    ie = mod(i,2) + mod(mod(i,2)+2,3);

    ei(1:3) = e_polar_vec(ie,iG,:);
    Ki      = XW_step + G(iG,:);

    THETA(i,i) = f(iG,iG)*norm(cross(Ki,ei))^2;

end;

XW_eig(n,:) = sort(sqrt(eig(THETA))).';

%=====
% Calculate eigenfrequencies for the k-space step along the
% WK trajectory.
%=====
WK_step = stepsize(n)*(K-W) + W;

```

```

%=====
% Get the polarization vectors for the NG plane waves for
% the current step along the WK trajectory.
%=====
for i = 1:NG

    Ki = WK_step + G(i,:);
    [e1, e2] = get_polarization_vectors(Ki);
    e_polar_vec(1,i,:) = e1;
    e_polar_vec(2,i,:) = e2;

end;

%=====
% Determine the off-diag elements of THETA matrix for WK_step.
%=====
for i = 1:(2*NG-1)
    for j = (i+1):(2*NG)

        iG = ceil(i/2);
        jG = ceil(j/2);
        ie = mod(i,2) + mod(mod(i,2)+2,3);
        je = mod(j,2) + mod(mod(j,2)+2,3);

        ei(1:3) = e_polar_vec(ie,iG,:);
        ej(1:3) = e_polar_vec(je,jG,:);
        Ki      = WK_step + G(iG,:);
        Kj      = WK_step + G(jG,:);

        THETA(i,j) = f(iG,jG)*dot(cross(Ki,ei),cross(Kj,ej));
        THETA(j,i) = conj(THETA(i,j)); % THETA is symmetric.

    end;
end;

%=====
% Determine the diagonal elements of THETA matrix for WK_step.
%=====
for i = 1:(2*NG)

    iG = ceil(i/2);

```

```

    ie = mod(i,2) + mod(mod(i,2)+2,3);

    ei(1:3) = e_polar_vec(iG,ie,:);
    Ki      = WK_step + G(iG,:);

    THETA(i,i) = f(iG,iG)*norm(cross(Ki,ei))^2;

end;

WK_eig(n,:) = sort(sqrt(eig(THETA))).';

end; % for n = 1:Nkpoints

fprintf('\n  Total calculation time: %d sec.\n', toc);
save pbs3Ddata071201;

%=====
% Trajectory lengths different, account for this when plotting.
%=====
kaxis = 0; % Relative k-space axis offset used for plotting.
XUaxis = kaxis:norm(X-U)/(Nkpoints-1):(kaxis + norm(X-U));
kaxis = kaxis + norm(X-U);
ULaxis = kaxis:norm(U-L)/(Nkpoints-1):(kaxis + norm(U-L));
kaxis = kaxis + norm(U-L);
LTaxis = kaxis:norm(L-T)/(Nkpoints-1):(kaxis + norm(L-T));
kaxis = kaxis + norm(L-T);
TXaxis = kaxis:norm(T-X)/(Nkpoints-1):(kaxis + norm(T-X));
kaxis = kaxis + norm(T-X);
XWaxis = kaxis:norm(X-W)/(Nkpoints-1):(kaxis + norm(X-W));
kaxis = kaxis + norm(X-W);
WKaxis = kaxis:norm(W-K)/(Nkpoints-1):(kaxis + norm(W-K));

%=====
% Plot 3D Photonic Band Structure (PBS).
%=====
Ntraject = 6; % Number of k-space trajectories to plot.
EigFreq = zeros(Ntraject*Nkpoints,1);

figure(1); hold on;

Nk = Nkpoints;

```

```

for k = 1:Neig

    for i = 1:Nkpoints
        EigFreq(i + 0*Nk) = (XU_eig(i,k))/(2*pi/a);
        EigFreq(i + 1*Nk) = (UL_eig(i,k))/(2*pi/a);
        EigFreq(i + 2*Nk) = (LT_eig(i,k))/(2*pi/a);
        EigFreq(i + 3*Nk) = (TX_eig(i,k))/(2*pi/a);
        EigFreq(i + 4*Nk) = (XW_eig(i,k))/(2*pi/a);
        EigFreq(i + 5*Nk) = (WK_eig(i,k))/(2*pi/a);
    end;

    plot ( XUaxis(1:Nk), EigFreq(1 + 0*Nk:1*Nk), 'b', ...
           ULaxis(1:Nk), EigFreq(1 + 1*Nk:2*Nk), 'b', ...
           LTaxis(1:Nk), EigFreq(1 + 2*Nk:3*Nk), 'b', ...
           TXaxis(1:Nk), EigFreq(1 + 3*Nk:4*Nk), 'b', ...
           XWaxis(1:Nk), EigFreq(1 + 4*Nk:5*Nk), 'b', ...
           WKaxis(1:Nk), EigFreq(1 + 5*Nk:6*Nk), 'b' );

    plot ( XUaxis(1:Nk), EigFreq(1 + 0*Nk:1*Nk), 'r.', ...
           ULaxis(1:Nk), EigFreq(1 + 1*Nk:2*Nk), 'r.', ...
           LTaxis(1:Nk), EigFreq(1 + 2*Nk:3*Nk), 'r.', ...
           TXaxis(1:Nk), EigFreq(1 + 3*Nk:4*Nk), 'r.', ...
           XWaxis(1:Nk), EigFreq(1 + 4*Nk:5*Nk), 'r.', ...
           WKaxis(1:Nk), EigFreq(1 + 5*Nk:6*Nk), 'r.' );

end

grid on;
hold off;

if (FCC) titlestr = ['PBS for FCC '];
elseif (DIAMOND) titlestr = ['PBS for Diamond '];
end;
titlestr = [titlestr '(NG = ',int2str(NG), ...
            ', Pf = ',num2str(Pf), ...
            'epsa = ',num2str(epsa), ...
            ', epsb = ',num2str(epsb),')' ];

title(titlestr);
xlabel ('k-Space');
ylabel ('Frequency (wa/c2pi)');
axis ([0 WKaxis(Nkpoints) 0 1]);

```

```

set      (gca,'XTick', [XUaxis(1) ...
                        XUaxis(Nk) ...
                        ULaxis(Nk) ...
                        LTaxis(Nk) ...
                        TXaxis(Nk) ...
                        XWaxis(Nk) ...
                        WKaxis(Nk)]);
xtixlabel = strvcat('X', 'U', 'L', 'T', 'X', 'W', 'K');
set(gca,'XTickLabel',xtixlabel);

%=====
% Name:          get_polarization_vectors.m
% Author:        Aaron Morton.
% Date:          08/26/01  A.Morton - Original function code.
%
% Description:    Calculates polarization vectors e1 and e2 for
%                 a given k-space vector, k.
%=====
function [e1, e2] = get_polarization_vectors(k)

er = [randn randn randn];

%=====
% Loop until a vector is found which is not parallel to k.
%=====
if (er == k)
    while (er == k)
        er = [randn randn randn];
    end;
end;

e1 = cross(k,er);          % Set e1 to the cross of k and er.
e1 = e1./sqrt(dot(e1,e1)); % Normalize e1.
e2 = cross(k,e1);          % Set e2 to the cross of k and e1.
e2 = e2./sqrt(dot(e2,e2)); % Normalize e2.

if (dot(cross(e1,e2),k) < 0) % Check right-hand character e1xe2.
    e2 = -e2;
end;

```