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A Theoretical Investigation of a Dual Beam Holographic Lithography Method for the Fabrication of Omnidirectional Photonic Crystals

by

KHALED MNAYMNEH, P. ENG.

B.Sc., Electrical Engineering, University of Windsor. (1997)

A thesis submitted to the Faculty of Graduate Studies and
Research in partial fulfillment of the requirements for the
degree of

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DEPARTMENT OF ELECTRONICS

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Abstract

Photonic crystals have, and will continue to revolutionize optical systems. Their ability to control and manipulate light stems from principles similar to those that establish the electronic band structures of semiconductors. The intricate and translational spatial symmetries required to achieve an omnidirectional photonic band gap dictate complex fabrication technologies. The similarity between photonic crystals and volume holograms suggests that a holographic lithography process may simplify the fabrication process. This thesis investigates a dual-beam multiple-exposure holographic lithography approach for producing photonic crystal template structures. The use of a frequency-domain numerical analysis determines if such structures exhibit omnidirectional photonic band gaps. The thesis presents design examples by using the engineering parameters extracted from the proposed fabrication process.

Thesis Supervisor: Robert C. Gauthier
Title: Professor of Electronics

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Chapter 1

1 Introduction

1.1 A Brief History of Photonic Crystals

1.1.1 The Wings of Butterflies

In 1887, Lord Rayleigh [i] made a significant discovery while studying the peculiar reflective properties of crystalline minerals. He discovered that they had a narrow band gap prohibiting light propagation in a particular direction. The iridescent colours of butterfly wings and abalone shells also exhibit this effect [ii]. These beautiful materials comprise of alternating layers of two substances that are periodic in one direction. Because the natural dielectric contrast between the layers is weak, the frequency stopgap formed is small, resulting in only a specific wavelength (i.e. colour) being reflected. As the incidence angle of the light changes, the periodicity of the alternating layers in that direction alters and the associated frequency stopgap surrounds a different wavelength, resulting in a different colour reflected. The iridescent colours admired, therefore, are a result of different colours reflected at different incident angles. Figure 1-1 shows a close-up image of the periodic structure within the wings of butterflies.

This effect resembles a wavelength-dependent mirror and in 1971, Kogelnik and Shank [iii] utilized this feature and suggested that a periodic structure in the gain

medium of a laser's resonator cavity could replace the end mirrors. This back scattering effect

(or feedback effect) improved the coherence of the laser light and reduced the overall size of the laser.

The modification of the gain medium led to the design of the distributed feedback laser (DFB). By introducing defects within the periodic gain medium [iv], more control over emitted laser light became available. These and other effects correspond to one-dimensional photonic crystals (PhCs).

1.1.2 What exactly are Photonic Crystals?

Photonic crystals are structures having a spatially periodic modulation of the index of refraction that opens up a forbidden gap, or photonic band gap (PBG) in the electromagnetic dispersion relation. Figure 1-2 illustrates conceptual periodicity in one, two, and three dimensions.

The PBG identifies a range, or band, of wave frequencies forbidden to propagate in a particular direction. Wave frequencies outside this band can propagate in that direction. Based on whether the direction is in one, two or three dimensions determines whether this is a PhC which has a one, two or three-dimensional PBG. An omnidirectional PhC is a PhC with a 3D PBG.

The dispersion relation looks very similar to the electronic energy-momentum relations found in semiconductors. The periodicity and ionic potential contrasts lift

electron wavefunction degeneracy, and ultimately leads to the formation of electronic band gaps, giving semiconductors their lucrative properties.

Figure 1-1: Close-up images of butterfly wings reveal the periodic structure that is responsible for the beautiful shimmering of colours [Dr. Pete Vukusic, Exeter University].

Figure 1-2: One, two, and three-dimensional periodicity.

1.1.3 Pre-1987 Problems

The physical principles that lead to electronic bandstructure are the same principles that lead to photonic band gaps in one dimension. Actually, the characteristic equation used in solid-state physics to describe band gap formation [v] is also used to describe photonic band gap formation in one-dimensional photonic crystals [vi]. However, arriving at an omnidirectional photonic band gap proved to be a difficult task. The principles behind one-dimensional photonic crystals appeared to have set up a severe condition for three-dimensional Bragg scattering [v]. In addition, the quantum nature of light complicates things further by introducing helicity issues, a non-conservation law, and an ill-defined position operator [vii].

1.1.4 Light at the end of the Omnidirectional PhC Tunnel

In 1987, exactly one hundred years after Lord Rayleigh made his observations, two areas of research suggested the existence of omnidirectional photonic band gaps:

inhibited spontaneous emission [viii] and Anderson localization [ix]. As a result, two seminal papers emerged. One of them [x] introduced the notion of photonic band gaps by extending the effects that periodic structures have on the electromagnetic dispersion relations to three dimensions. It was the second paper [xi], which presented mathematical evidence for the existence of photonic band gaps.

It took three years to build a structure that showed an omnidirectional PBG. The reason for this delay had to do with the theory itself. When searching for possible structures that exhibit omnidirectional photonic band gaps [xii], band gap theorists noticed quickly that the familiar band theory of electron wavefunctions was in disagreement with experiments on photons. Due to the vector nature of photons [xiii], wave degeneracy occurred in unexpected regions of the Brillouin zone. This degeneracy was not present for electron wavefunctions. By realizing that the nature of photons truly is different from the nature of electrons, Ho, Chan and Soukoulis [xiv] were the first to overcome this problem, introducing the first omnidirectional photonic band gap material.

The missing link between theory and application was finally found, and the literature soon swelled with other possible photonic band gap structures [xv, xvi, xvii]. In order to realize such structures, fabrication processes [xviii, xix] and computational methods [xx, xxi] became important areas of research.

1.2 Fabrication Techniques

1.2.1 Fabrication Difficulties

Having a periodic modulation of the index of refraction in three dimensions is not the only requirement for building omnidirectional photonic crystals. As Chapter 2 will indicate, other problems need solving in order to open a full three-dimensional PBG. One such problem is getting the dispersion relation stopgap of each orthogonal dimension in space to overlap. One way to achieve this is by having a large contrast of refractive index, or a related quantity known as the dielectric constant, in each direction. Practically, there is a limit on how large this contrast can be and unfortunately, these limits do not help in getting these stopgaps to overlap.

Another less intuitive means of attaining full PBGs is to fabricate a structure that has a spherical Brillouin zone. Having a spherical Brillouin zone allows for the Bragg scattered wave peaks to align in the same region, in different directions. Again, Chapter 2 illuminates the importance of these Bragg scattered wave peaks to the formation of PBGs.

A natural lattice configuration that has a near spherical Brillouin zone is the face centered cubic (FCC) lattice. However, from the previous section, the photon wavefunction degeneracy is different from electron wavefunction degeneracy. Figure 1-3 shows the dispersion relation of an FCC structure. A full PBG is starting to open, but due to these degenerate states, the band closes at some regions of the Brillouin zone [xxii].

Opening a full PBG requires a deeper understanding of how the structure fabrication relates to the equations that describe band gap formation. This is why selecting a fabrication method is very important when building photonic crystals.

Figure 1-3: The dispersion relation for the lowest-frequency electromagnetic modes of a face-centered cubic lattice of dielectric ($\epsilon=13$) spheres in air. The wave vector varies across the Brillouin zone.

1.2.2 Current Techniques in PhC Fabrication Research

The following is a list of fabrication techniques currently researched by various groups around the world.

- a) **Semiconductor Microfabrication:** This well known fabrication process [xviii] is efficient and effective in building structure where the vertical direction is constant. Hence, one and two-dimensional photonic crystals are easily fabricated. However, because 3D photonic crystals require index modulation in the vertical direction, angle etching or regrowth is more difficult to realize. This is a nontrivial process for high spatial frequencies. Furthermore, the incorporation of specific and well-defined defects, which are crucial for many proposed applications, is extremely difficult. However, a recently suggested method known as glancing angle deposition (GLAD) allows periodicity to grow in the third dimension. By controlling the deposition angle, intricate three-dimensional periodic structures are possible. Figure 1-4 shows helix structures [xxiii] created from GLAD techniques.
- b) **Colloidal Crystallization (Self-Assembly):** Colloidal crystallization is the process of building three-dimensional periodic structures from small particles suspended in solution. Three-dimensional photonic band gaps are more likely to occur in FCC structures and this is the preferred natural structure of colloidal crystallization. However, parameters such as sedimentation rates and volume fraction on epitaxial structures are difficult to determine. Figure 1-5 shows cross sections of a colloidal crystallization structure, which clearly shows the different domains and defects that may effect PBG formation.

- c) Tightly Focused Laser Beam Scanning: The usual semiconductor fabrications processes are subtractive, while this process is additive. An additive process greatly facilitates the fabrication of defects and complex structures into underlying periodic structures [xxiv]. Figure 1-6 shows a structure fabricated by the tightly focused laser beam scanning method. However, the number of unit cells, limited by the size of the deposition chamber, restricts the flexibility of this process. In addition, similar to the semiconductor fabrication processes, deposition is a complicated process and requires sophisticated machinery.

Figure 1-4: Helix structure fabricated using GLAD [Courtesy Dr. T. Smy and Dr. M. Brett, Carleton University and University of Alberta].

- d) Two-Photon Polymerization: This fabrication method provides the means of activating chemical processes with high spatial resolution in three dimensions. The fundamental concept behind this method is the two-photon absorption probability which depends quadratically on intensity, so under tight-focusing conditions, the absorption is confined at the focus to a volume of the order of the laser wavelength [xxv]. Figure 1-7 shows a structure fabricated by the two-photon polymerization technique. However, this process requires high laser power and its widespread use remains impractical.

Figure 1-5: SEM image of a cleft edge of a colloidal structure [Courtesy Dr. Cefe López, Instituto de Ciencia de Materiales de Madrid].

Holographic lithography is yet another fabrication technique for photonic crystals. However, when compared to the above-mentioned techniques, it seems more suited for PhC fabrication. This is primarily due to the structural similarity PhCs have with volume holograms. Hologram fabrication has been around for quite some time, which means that the techniques involved in hologram formation are easily adaptable to the fabrication of PhCs. Instead of the silver halide emulsion, typically used for hologram fabrication, photosensitive polymers are used. In addition, the laboratory setup for

holographic lithography is relatively simpler and cheaper than other fabrication techniques.

Figure 1-6: Three-dimensional PBG structure fabricated by laser rapid prototyping [xxiv].

1.2.3 Dual Beam Holographic Lithography

Many papers have been published on using holographic lithography as a fabrication methodology for PhCs [xix, xlii, xliii]. However, these holographic lithography techniques utilized either lithography masks or more than two laser beams for recording 3D periodic patterns. If a lithography-mask is not required and only two laser beams are used, this would further simplify laboratory setup. In addition, two laser

beams do not have polarization problems seen when more than two non-coplanar beams interfere [xliii].

Figure 1-7: Periodic microstructure built by two-photon polymerization [xxv].

However, these simplifications must not limit or make the holographic lithography ineffective. Conventional semiconductor fabrication techniques are quite capable of building 1D and 2D PBG structures because of the uniformity of at least one dimension. The real benefit, however, in using a holographic lithography process is the ease in fabricating three-dimensional translationally symmetric microstructures.

1.3 Numerical Analysis

1.3.1 Determining the Domain

Theoretical analysis takes place in two domains, known as direct and inverse domains. Direct domains represent quantities human beings are very familiar with, such as distances and time. Inverse domains represent quantities that are less intuitive, namely reciprocal space and frequency.

Determining in which domain to perform numerical analysis rests on the answers to two questions:

1. Which domain gives the appropriate information based upon the questions posed?
2. Which domain is less “expensive” to work in?

The answer to the first question depends upon the analytical setting and problem characterization. For example, if transport issues such as energy flow and diffusion are of concern, space and time domains are appropriate. If spectral information, such as energy content and aliasing issues, need to be obtained, then spatial and temporal frequency domains are appropriate.

The second question is more practical. Less expensive takes the form of three issues:

1. Analytical Preprocessing
2. Linear Algebra Programming
3. Computational Complexity

Although the model is fashioned in one domain, perhaps it may be easier to compute it in the inverse domain. For example, if our electromagnetic modes were time harmonic, perhaps expressing them in a planewave expansion using definite frequency values would be more appropriate instead of performing an analysis in the time domain.

What would be the computational cost in getting results? How many operations need to be in the algorithm? How much time does the CPU require for each operation? Even though there may be more operations in one algorithm, does preconditioning elevate and provide an advantage over an algorithm with a smaller amount of operations and less preconditioning?

1.3.2 Generic Algorithm Description

An important parameter in algorithm descriptions is the *degrees of freedom* represented by N . The degrees of freedom represent the grid points in a discretized domain or the number of function bases in some expansion. If the computational process requires memory storage, this parameter helps determine the size of memory. Resolution is related to N , so as N increases and discretization units decrease, the result becomes more accurate.

Another important computational parameter is *computational complexity*, represented by the notation, $O(N)$, where N represents the degree of freedom. This parameter indicates the number of operations in a particular algorithm. CPU access times can be affected by this parameter. However, an algorithm with small computational complexity

is not necessarily an efficient algorithm. The Maxwellian operator, defined in Chapter 2, has a large computational complexity, however, after numerically preconditioning; it leads to a substantial speedup in iterative methods used to solve for the support electromagnetic modes.

1.3.3 Planewave Expansion Numerical Analysis

The main theme of this paper is not PhCs but the feasibility study of a possible fabrication method to build them. Therefore, an efficient numerical analysis is required to determine whether structures fabricated by DBHL do indeed exhibit one, two, or three-dimensional PBGs. At the end of Chapter 2, a method known as Planewave Expansion is introduced as the method of choice for identifying whether certain PhCs configurations sustain an omnidirectional PBG. The software is freely available on the Web [xxvi].

1.4 Thesis Outline

1.4.1 Thesis History: The Optical Gyroscope

The original thesis topic dealt with the characterization of a photonic crystal waveguide actuated by microelectromechanical (MEM) machines. By bringing together two slabs that supported a hexagonal array of dielectric rods, the overlapped region of rods would constitute a path of uniform dielectric. Then some coupled optical mode, with its fundamental frequency within the 2D PBG region, could propagate down this

dielectric path. Transverse containment would be by the PBG action while longitudinal containment would be by traditional index guiding.

The next step was to shape a Mach-Zehnder path for the overlap region. If the path lengths were unbalanced by $\lambda/2$, the beams in each path would join destructively. Due to the destructive interference, no coherent light would emerge at the other end. The beam would have no other choice but to return the way it came. If, however, the system spun suddenly, the optical path lengths in the arms would change accordingly, temporarily lifting the destructive interference, resulting in light emission at the output. The strength of the emitted light would be proportional to the strength of the system's rotary motion.

The characteristics of the above-mentioned system describe a possible application as an optical gyroscope. However, the longitudinal direction, which uses index guiding, would not be enough to contain the optical energy at the point where the beams merge. Instead of light returning the way it came, it would just diffuse in the direction of index guiding. The set back illuminated the demand for a 3D PBG that would sandwich this 2D photonic crystal unbalanced Mach-Zehnder waveguide.

Before realizing that light would escape longitudinally, DBHL was going to be the fabrication process of building 2D PhC structures. However, it became apparent, due to the leakage of optical energy, that a 3D omnidirectional containment was necessary. This leakage of optical energy raised the question of whether DBHL could fabricate PhCs with a 3D PBG. This is where the theme of the thesis changed from the

explanation of building a PhC device to the feasibility study of a fabrication methodology for omnidirectional PhC template structures.

1.4.2 Thesis Layout

The main theme of this thesis, therefore, is a feasibility study of a dual-beam holographic lithography methodology for the fabrication of omnidirectional photonic crystal template structures. These template structures will be the seed for suggested future work concerning the actual fabrication process that includes microfabrication process steps. Chapter 2 describes the origins of photonic band gaps, and provides the equations used to find them. Chapter 3 discusses holographic interferometry, and Chapter 4 presents the information required to proceed towards the DBHL fabrication process. Chapter 5 presents systematic design simulation examples of optimized PhC template structures, and finally, Chapter 6 presents the conclusion along with future work suggestions.

Chapter 2

2 The Origin of the Photonic Band Gap

2.1 Fundamental Equations

2.1.1 Maxwell's Equations in Photonic Crystals

Photonic crystals mold the flow of electromagnetic radiation. As a result, the analysis of photonic crystals must begin with Maxwell's equations [xxviii], presented here in cgs units,

$$\begin{aligned}\bar{\nabla} \cdot \mathbf{E}(\mathbf{r}, t) &= \rho(\mathbf{r}, t) & \bar{\nabla} \times \mathbf{B}(\mathbf{r}, t) - \frac{\partial \mathbf{E}(\mathbf{r}, t)}{c \partial t} &= \frac{4\pi}{c} \mathbf{J}(\mathbf{r}, t) \\ \bar{\nabla} \cdot \mathbf{B}(\mathbf{r}, t) &= 0 & \bar{\nabla} \times \mathbf{E}(\mathbf{r}, t) + \frac{\partial \mathbf{B}(\mathbf{r}, t)}{c \partial t} &= 0\end{aligned}\tag{2.1}$$

where $\mathbf{E}(\mathbf{r}, t)$ is the electric field vector, $\mathbf{B}(\mathbf{r}, t)$ is the magnetic flux density vector, $\rho(\mathbf{r}, t)$ is the source charge, and $\mathbf{J}(\mathbf{r}, t)$ is the current density. The equations in (2.1) describe electromagnetic radiation flowing through vacuum. If the medium is a photonic crystal, additional terms are required to represent such media analytically.

One way to represent the medium is to use the *constitutive relations*. These are approximate relations derived from the complex interactions [xxviii, xxix] between the original field and the induced fields produced by constitutive particles of the medium.

The approximations come from assuming low field strengths and linear responses of the particles that make up the medium. The constitutive relations are,

$$\begin{aligned}\mathbf{D}(\mathbf{r},t) &= \varepsilon(\mathbf{r},\omega)\mathbf{E}(\mathbf{r},t) \\ \mathbf{B}(\mathbf{r},t) &= \mu(\mathbf{r},\omega)\mathbf{H}(\mathbf{r},t)\end{aligned}\tag{2.2}$$

where $\mathbf{D}(\mathbf{r},t)$ is the electric flux density, and $\mathbf{H}(\mathbf{r},t)$ is the magnetic field vector. The term $\varepsilon(\mathbf{r},\omega)$ is the electric permittivity or dielectric function, and $\mu(\mathbf{r},\omega)$ is the magnetic permeability. The functions $\varepsilon(\mathbf{r},\omega)$ and $\mu(\mathbf{r},\omega)$ are precisely the terms required to represent the structural and material information of the propagation medium. Nevertheless, further approximations are required to represent photonic crystals. It was suggested [x] that dielectric materials are appropriate for the construction of photonic crystals because of their low loss features. Such suggestions begin to impose assumptions upon the terms representing the medium.

The first suggestion, mentioned above, is that the medium contains dielectric material for reducing losses. Imposing a purely real dielectric function represents lossless materials. A second suggestion is to construct photonic crystals from non-magnetic materials. This makes the magnetic permeability a value of one. A third suggestion is to ignore any explicit frequency dependence of the dielectric function. The dielectric function of the selected material varies slowly with radiation frequency. Instead, the dielectric value at any spatial coordinate is a constant based upon the appropriate frequency range of study.

Electromagnetic vector fields are complicated functions of space and time. Nonetheless, the vector fields are solutions to Maxwell's equations, and any solution can be constructed by an appropriate combination of frequency-definite (or time harmonic) solutions. This superposition property of solutions to Maxwell's equations facilitates the analytical focus on harmonic modes without taking away from any general solutions. Using complex notation,

$$\begin{aligned}\mathbf{E}(\mathbf{r}, t) &= \text{Re}\{\mathbf{E}(\mathbf{r})e^{i\omega t}\} \\ \mathbf{H}(\mathbf{r}, t) &= \text{Re}\{\mathbf{H}(\mathbf{r})e^{i\omega t}\}\end{aligned}\tag{2.3}$$

Replacing the vector fields in (2.1) with (2.3) and assuming a source-free and non-magnetic material,

$$\begin{aligned}\bar{\nabla} \cdot \epsilon(\mathbf{r})\mathbf{E}(\mathbf{r}) &= 0 & \bar{\nabla} \times \mathbf{H}(\mathbf{r}) - \frac{i\omega}{c}\epsilon(\mathbf{r})\mathbf{E}(\mathbf{r}) &= 0 \\ \bar{\nabla} \cdot \mathbf{H}(\mathbf{r}) &= 0 & \bar{\nabla} \times \mathbf{E}(\mathbf{r}) + \frac{i\omega}{c}\mathbf{H}(\mathbf{r}) &= 0\end{aligned}\tag{2.4}$$

The equations of (2.4) are the results of the assumptions given in this section.

The following list summarizes those assumptions:

1. low field strengths (linear regime)
2. source free
3. non-magnetic
4. purely real dielectric function
5. explicit frequency dependence of dielectric function ignored for a specified range of frequencies

The coupled equations in (2.4) are Maxwell's equations in a PhC. If the electric and magnetic field vector components of some mode satisfy the equations in (2.4), then that mode is self-sustaining within the photonic crystal described by the dielectric function in (2.4). However, when using the equations in (2.4) to characterize photonic crystals, it is not the sustainable modes, but rather the band of forbidden modes appearing in between the sustainable modes of the photonic crystal that are sought.

In order to characterize PhCs properly, the decoupling of the vector fields in (2.4) is important. This yields two “master” equations that are in an optimized form for numerical analysis.

2.1.2 The Master Equation[†]

The equations in (2.4) can be decoupled to give one equation in terms of either the electric field vector or the magnetic field vector. When choosing to isolate the electric field vector and using the constitutive relations, the decoupled equation is,

$$\nabla \times \nabla \times \frac{1}{\epsilon(\mathbf{r})} \mathbf{D}(\mathbf{r}) = \frac{\omega^2}{c^2} \mathbf{D}(\mathbf{r}) \quad (2.5)$$

[†] This is a fanciful name for what is commonly known as the wave equation. However, in the literature for photonic crystals, it has been renamed the master equation because of certain mathematical techniques used to solve it.

This equation yields possible modes that may exist in some structure defined by the dielectric function, $\epsilon(\mathbf{r})$. It is important to note that solutions of (2.5) must conform to the *transversality* conditions in (2.4) in order to be a supported mode. If the mode conforms to this condition and is a solution of (2.5), then this mode is a characteristic mode of the structure.

2.1.3 Cross Roads

After obtaining equation (2.5), a method is now required to solve it. However, the methodology of solving this equation hinges upon the reasons for solving it. There are two basic reasons for solving this equation. One reason is to obtain a spectral analysis for a given structure. This spectral analysis answers the questions of whether or not this structure supports a photonic band gap.

The other reason for solving this equation is to obtain its transmission characteristics, such as optical mode reactions to defects and bends along with input/output coupling and any real-time issue.

The main objective of the thesis, as stated in section 1.4.2, is to investigate the feasibility of the DBHL process in producing omnidirectional PhC templates. Frequency domain analysis, therefore, would be able to answer the question of whether a 3D PBG is present in structures produced by a DBHL process.

In order to prepare equation (2.5) for spectral analysis, the theory now focuses on the representation of the structure.

2.2 Media Descriptions

2.2.1 Structure Representation

The dielectric function can be resolved into 2 quantities, an average term, and a fluctuating term [xi],

$$\epsilon(\mathbf{r}) = \epsilon_0 + \epsilon_{fluct}(\mathbf{r}) \quad (2.6)$$

where ϵ_0 is the average dielectric constant (different from electric permittivity of vacuum in SI unit), and $\epsilon_{fluct}(\mathbf{r})$ is the fluctuating dielectric function of the medium.

This fluctuating term is composed of two more terms,

$$\epsilon_{fluct}(\mathbf{r}) = \sum_{\mathbf{G}} \epsilon_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} + V(\mathbf{r}) \quad (2.7)$$

where the first term on the right hand side is the reciprocal lattice representation of the periodic photonic crystal. The summation is over all inverse lattice vectors, $\mathbf{G}$.

The second term, $V(\mathbf{r})$, describes random fluctuations and satisfies the statistics $\langle V(\mathbf{r}) \rangle_{ens} = 0$ and $\langle V(x)V(y) \rangle \equiv B(x-y)$. The theoretical analysis which involves this term is quite involved and beyond the scope of this paper. However, before leaving this point, it is important to state the value of this term and its contribution to post-1987 photonics.

Without randomness, ideal conditions may lead to desired results. In this case, if the periodicity is perfect with no grain boundaries, no point or line defects, etc, then three-dimensional gaps may occur in the dispersion relations of periodic structures. Practically, randomness will always occur and this results in complicating the effort in achieving omnidirectional photonic crystals. Nevertheless, it was in studying this randomness term and using an effective Schrödinger equation in wave-vector space, that John [xi] put forward his postulate, which states,

“...photons near the band-edge frequency retain certain general features of the dispersion relation and that the phase space available for propagation is accordingly restricted.”

This postulate explains the fundamental reason why omnidirectional photonic crystals should exist regardless of fabrication defects.

Securing the validity of omnidirectional photonic crystals theoretically via the random variable, the focus now shifts to the first term on the right hand side of (2.7). This term represents periodicity, and periodicity is the fundamental reason for the formation of gaps in dispersion relations. As electromagnetic waves propagate through periodic material, one would expect scattering to occur at boundary interfaces. This, however, is not the case.

2.2.2 Bloch Theorem

In 1928, Felix Bloch [xxx] studied the propagation of electrons through periodic media and noticed that scattering was due to defects but not periodicity. He showed that the presence of the periodic media modulated the electron wavefunction with a periodic envelope function. Extending this result to any wave phenomena, including electromagnetic waves, the electric field intensity vector in a periodic media is,

$$\mathbf{E}_k(\mathbf{r}) = u_k(\mathbf{r})e^{j\mathbf{k} \cdot \mathbf{r}} \quad (2.8)$$

where $u_k(\mathbf{r})$ is the periodic envelope function satisfying,

$$u_k(\mathbf{r}) = u_k(\mathbf{r} + \mathbf{R}) \quad (2.9)$$

and where $\mathbf{R}$ is the direct lattice vector.

A *Bloch wave* would be an appropriate name for a wave with its electric field vector component resembling (2.8). The electric field intensity vector subscripted with the wavevector indicates how modes with wavevectors behave with the reciprocal lattice vector of a particular structure [xxii]. Bragg scattering is the principle reason for the formation of gaps in dispersion relations, and in the case of electromagnetic waves, the wavevector is the independent variable in these relations.

2.3 Dispersion Relation

2.3.1 Importance of Dispersion Relations: Density of States (DOS)

An important description that comes from the dispersion relation is the photonic density of states, (DOS). This plays a fundamental role in understanding the optical properties of photonic crystals. The photonic DOS $N(\omega)$ is defined by “counting” all allowed states with a given frequency ω . This “counting” is carried out by summing up all the bands of the integral over the Brillouin zone of a Dirac delta function,

$$N(\omega) = \sum_n \int_{BZ} d^3k \delta(\omega - \omega_n(\mathbf{k})) \quad (2.10)$$

For applications in quantum optics, it is necessary to investigate the local coupling between an excited atom that may possibly emit a photon of frequency ω , and the electromagnetic environment provided by the photonic crystal at that location.

2.3.2 The Bragg Condition

The relationship between the frequency, ω , and the wavevector, k , of light is,

$$\omega = ck \quad (2.11)$$

where c is the speed of light in vacuum. This relation, known as the dispersion relation, represents wave propagation in free space. Within a homogenous material, (2.11) is divided by the dielectric constant of that material.

If the material is now periodic in its dielectric constant, reflections will occur at the dielectric interfaces. If the difference of the incident and reflected wavevectors is equal to the reciprocal lattice's vector, $\mathbf{G}$, then constructive interference of the reflected waves will occur. This condition, known as the Bragg or Laue condition, is,

$$\Delta \mathbf{k} = \mathbf{G} \quad (2.12)$$

In addition, due to the periodicity of the reciprocal lattice, condition (2.12) also specifies a region within the reciprocal lattice that eliminates redundancy.

2.3.3 The Brillouin Zone

If scattering is elastic,

$$|\mathbf{k}| = |\mathbf{k}'| \quad (2.13)$$

where $\mathbf{k}'$ is the wavevector of the scattered wave. Rearranging (2.13) and using (2.12),

$$\mathbf{k} \cdot \frac{1}{2}\mathbf{G} = \left(\frac{1}{2}G\right)^2 \quad (2.14)$$

Equation (2.14) can then be used to describe a repeatable zone in reciprocal space, where the boundaries of that zone are the inverse lattice points that represent constructive interference of some wave with a wavevector $\mathbf{k}$. The description of this zone is similar to the definition of a Wigner-Seitz primitive cell but in reciprocal space. This zone, named after its discoverer, Léon Brillouin [xxxii] is illustrated in figure 2-1. The direct lattice that figure 2-1 represents is the face-centered cubic. The gamma-point, not shown, resides in the middle of the zone.

Figure 2-1: Brillouin zone of an FCC lattice [xii].

2.3.4 One Dimensional Scattering

One way to find the dispersion relation of a periodic structure is to go back and re-examine equation (2.5). By representing the field vector with a Fourier integral and the dielectric function with (2.6), the basis in which equation (2.5) exists transforms from direct space to inverse space. Hence, equation (2.5) becomes [vi],

$$\mathbf{k} \times [\mathbf{k} \times \mathbf{A}(\mathbf{k})] + \frac{\omega^2}{c^2} \sum_{\mathbf{G}} \epsilon_{\mathbf{G}} \mathbf{A}(\mathbf{k} - \mathbf{G}) = 0 \quad (2.15)$$

for all $\mathbf{k}$. The vector function $\mathbf{A}(\mathbf{k})$ is the function in k -space that represents $\mathbf{D}(\mathbf{r})$ in direct space. It is interesting to note that the argument of $\mathbf{A}(\mathbf{k})$ in the second term of (2.15) on the left hand side is the wavevector of Bragg scattered wave. In one-dimension, (2.15) becomes,

$$k^2 A(k) - \frac{\omega^2}{c^2} \sum_l \epsilon_l A(k - lg) = 0 \quad (2.16)$$

where $\mathbf{G} \rightarrow lg$. Because (2.15) and (2.16) is for all $\mathbf{k}$, the $\mathbf{k}$ of a particular Bloch wave is chosen. Expanding (2.16) for $A(k)$, $A(k - g)$ and $A(k + g)$,

$$\begin{aligned} A(k) &= \frac{\omega^2/c^2}{(k^2 - \omega^2/c^2)} [\epsilon_1 A(k - g) + \epsilon_{-1} A(k + g) + \dots] \\ A(k - g) &= \frac{\omega^2/c^2}{(k - g)^2 - \omega^2/c^2} [\epsilon_1 A(k - 2g) + \epsilon_{-1} A(k) + \dots] \\ A(k + g) &= \frac{\omega^2/c^2}{(k + g)^2 - \omega^2/c^2} [\epsilon_1 A(k) + \epsilon_{-1} A(k + 2g) + \dots] \end{aligned} \quad (2.17)$$

Assuming that the condition in (2.13) holds, and equation (2.11) is approximate in a periodic material, then $A(k)$ and $A(k - g)$ will be the dominant terms in (2.17). Taking only the first few terms in the expansion, the two algebraic coupled equations are,

$$\begin{aligned} \left(k^2 - \frac{\omega^2}{c^2} \epsilon_0\right) A(k) - \frac{\omega^2}{c^2} \epsilon_1 A(k-g) &= 0 \\ -\frac{\omega^2}{c^2} \epsilon_{-1} A(k) + \left[(k-g)^2 - \frac{\omega^2}{c^2} \epsilon_0\right] A(k-g) &= 0 \end{aligned} \quad (2.18)$$

When solving two coupled equations, a quick method to determine if a nontrivial solution does exist is to determine whether the determinant vanishes:

$$\begin{vmatrix} k^2 - \frac{\omega^2}{c^2} \epsilon_0 & -\frac{\omega^2}{c^2} \epsilon_1 \\ -\frac{\omega^2}{c^2} \epsilon_{-1} & (k-g)^2 - \frac{\omega^2}{c^2} \epsilon_0 \end{vmatrix} = 0 \quad (2.19)$$

or

$$\left(k^2 - (\omega^2/c^2) \epsilon_0\right) \left[(k-g)^2 - (\omega^2/c^2) \epsilon_0\right] - \left[(\omega^2/c^2) \epsilon_1\right]^2 = 0 \quad (2.20)$$

This equation becomes the new dispersion relation of a Bloch wave traversing through material with periodically modulated dielectric.

2.3.5 Gap Formation

From the elasticity condition, a point in the inverse lattice, which is a Bragg scattering point, is $k = \frac{1}{2}g = \pi/\Lambda$ where Λ the spatial period. Substituting this condition into (2.20) gives,

$$\omega^2 = \frac{c^2 k^2}{(\epsilon_0 \pm |\epsilon_1|)} \quad (2.21)$$

This looks like a modified version of (2.11) and indeed, it is. The presence of the square, however, gives the frequency two roots and at frequencies between these roots gives complex k values. Complex wavevectors imply evanescence. Bloch waves with frequencies related to these k will not propagate but become evanescent. This is the origin of the band gap. From (2.20), the wavevector at the center of the band gap is,

$$k = \frac{1}{2}g \left(1 \pm i \frac{|\epsilon_1|}{2\epsilon_0} \right) \quad (2.22)$$

which corresponds to the frequency interval,

$$\Delta\omega_{gap} = \omega \frac{|\epsilon_1|}{\epsilon_0} \quad (2.23)$$

This yields a mathematical expression for the band gap. Note that the size of the gap is proportional to the Fourier expansion coefficients of the dielectric constant. This means that a larger dielectric contrast between periodic layers gives a larger gap size.

To expand the one dimensional band gap to two or three dimensions requires a dispersion relation for each dimension. The periodicity in each dimension must open a band gap in the dispersion relation associated with a particular direction. All the band gaps that open for all the directions must overlap in the same frequency range. This condition is severe [v] and is still only a classical problem. Quantum mechanical problems complicate the creation of these band gaps, especially for three dimensions.

Perhaps another mathematical formulation of photonic crystal equations would assist in obtaining two and three dimensional photonic crystal structures, and provide a starting point for efficient computational methods to find band gaps. One such formulation is found in quantum mechanics: eigenvalue problems.

2.4 An Eigen-Explanation of Photonic Crystals

2.4.1 Eigenvalues Problems

Eigenvalues and their corresponding eigenvectors are a special set of scalars and vectors, respectively, which are associated with matrices. Originally, they were tools only used in pure mathematics up until 1925. Born made the connection of Heisenberg's non-commutative product to matrix multiplication. Schrödinger realized that the Sommerfeld-Wilson conditions, including DeBroglie's matter waves, resembled an

eigenvalue problem. Hence, eigenvalues problems became critical in the foundations of quantum mechanics [xxxii].

2.4.2 Matrices, Operators and Commutation

An important result from quantum mechanics was that mathematical operators could be associated with matrices. The eigenvalues and eigenvectors of these matrices represent observable values and wavefunction configurations that are particular to the operators represented by these matrices.

If this is the case, then equation (2.5) appears to have the form of an eigenvalue problem,

$$\Omega \mathbf{D}(r) = \zeta \mathbf{D}(r) \quad (2.24)$$

where the operator Ω is

$$\Omega \equiv \nabla \times \nabla \times \frac{1}{\epsilon(\mathbf{r})} \quad (2.25)$$

and ζ is the eigenvalue of that operator and $\mathbf{D}(\mathbf{r})$ would now be considered as the eigenvector or eigenmode of the operator Ω .

This approach seems to be very beneficial for the study of photonic crystals, especially for band gap hunting, regardless of dimensions. The structure is included into the operator, which has eigenmodes associated with it. The interpretation of these

eigenmodes is the electromagnetic modes sustained within this structure. The eigenvalues are the values associated with the eigenmodes.

Another beneficial characteristic of eigenvalue problems is operator commutation, defined as,

$$[A, B] = AB - BA \quad (2.26)$$

where A and B are some operators. Two operators are said to commute if (2.26) vanishes. Whenever two operators commute, their eigenmodes are the same. This is very convenient, since eigenvalues and eigenmodes of simple symmetry operators are easily determined, whereas those of Ω are not. In addition, if Ω commutes with a symmetry operator, the eigenmodes of Ω can be cataloged using the properties of the symmetry operator.

Solving (2.24) as an eigenvalue problem, gives the eigenvalue spectrum. If there was a photonic band gap, it would be immediately apparent. However, there are a few constraints. The eigenvalues of (2.24) need to be positive and real. Remember that these eigenvalues represent the frequency of the mode and *observable* frequencies [xxxiii, xxxiv] need to be real. In addition, the eigenmodes associated with the operator must be orthogonal in order to build other possible modes via the superposition principle stated earlier in this chapter. Operators of eigenvalue problems generally do not guarantee these constraints. However, there are particular classes of operators that do and they are known as Hermitian operators.

2.4.3 Hermitian Operators

A proper description of Hermitian operators requires the definition of two mathematical concepts: the inner product, and adjoints. The inner product of two vector fields is,

$$\langle \mathbf{F}(\mathbf{r}) | \mathbf{G}(\mathbf{r}) \rangle = \int d\mathbf{r} \mathbf{F}^*(\mathbf{r}) \cdot \mathbf{G}(\mathbf{r}) \quad (2.27)$$

The Dirac notation, elaborated further in Appendix A, is used. The adjoint of an operator is,

$$\langle \mathbf{F}(\mathbf{r}) | \Theta \mathbf{G}(\mathbf{r}) \rangle = \langle \Theta^\dagger \mathbf{F}(\mathbf{r}) | \mathbf{G}(\mathbf{r}) \rangle \quad (2.28)$$

where Θ is an operator, and $\Theta^\dagger$ is its adjoint. Hermitian operators are operators that are their own adjoints and are therefore, mathematically guaranteed to have real eigenvalues and, when their eigenvalues are distinct, have orthogonal eigenmodes.

It turns out that the operator in (2.24) is not Hermitian. If the master equation, however, is formulated using the magnetic field vector, the operator in that equation is Hermitian [xxii]. The new master equation is,

$$\nabla \times \left[\frac{1}{\epsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) \right] = \left(\frac{\omega}{c} \right)^2 \mathbf{H}(\mathbf{r}) \quad (2.29)$$

where the new operator is,

$$\Theta = \nabla \times \left[\frac{1}{\epsilon(\mathbf{r})} \nabla \times \right] \quad (2.30)$$

Now that an eigenvalue problem has been setup and the operator is Hermitian, a method is required to solve this problem. A certain principle, borrowed from quantum mechanics, seems like a possible candidate as a solution method. Not only will this principle help present a more proper understanding of the formation of photonic band gaps, but it will also be of great benefit as the mathematical description of the problem that can be used as the starting point in some computational analysis.

2.5 Electromagnetic Variational Principle

2.5.1 Variational Principles

From the work of D'Alembert and Hamilton [xxxv], it was observed that if certain functionals, which represent physical systems, were minimized, the values which minimize these functionals tend to be the observable values found in the physical system.

From the discussion in the previous sections, observable variables are the eigenvalues of some Hermitian operators. If an expression were set up to average all possible eigenvalues of that operator, and that expression became the functional to

minimize, the eigenvalue that minimizes that functional would be associated with the lowest order eigenmode. Minimizing the functional again, but this time excluding the first eigenvalue, would yield the next lowest order orthogonal eigenmode.

There is a functional in quantum mechanics known as the expectation value. It is an averaging expression for the eigenvalues of some Hermitian operators. In the case of photonic crystals, that operator is (2.30), also called the Maxwellian operator.

2.5.2 Eigenvalue Expectation Value

The expectation value expression is,

$$\langle \Theta \rangle = \frac{\langle \mathbf{H} | \Theta | \mathbf{H} \rangle}{\langle \mathbf{H} | \mathbf{H} \rangle} \quad (2.31)$$

where $\langle \Theta \rangle$ is the average eigenvalue of the Maxwellian operator. In addition, $\langle \mathbf{H} | \Theta | \mathbf{H} \rangle$ is another way of representing $\langle \mathbf{H} | \Theta \mathbf{H} \rangle$. Expanding (2.26) with the proper definitions,

$$\begin{aligned} \langle \mathbf{H} | \Theta | \mathbf{H} \rangle &\equiv \int \epsilon^{-1} |\nabla \times \mathbf{H}|^2 d\mathbf{r} = \left(\frac{\omega}{c} \right)^2 \int \frac{1}{\epsilon} |\mathbf{D}|^2 d\mathbf{r} \\ \langle \mathbf{H} | \mathbf{H} \rangle &\equiv \int \mathbf{H}^* \cdot \mathbf{H} d\mathbf{r} = \int |\mathbf{H}|^2 d\mathbf{r} \end{aligned} \quad (2.32)$$

The numerator of (2.31) is the energy of an electric field multiplied by the squared frequency term. The denominator is the energy in the magnetic field. It is important to

note that the magnetic and electric field energies are equal if the fields are time harmonic [xxii].

The variational principle not only presents an efficient method for finding eigenmodes, but it also explains the mechanism of how band gaps emerge.

2.6 The Origin of Photonic Band Gaps

2.6.1 Two Principles

There are two principles at work that cause the formation of photonic band gaps, and they are very similar to the formation of electronic band gaps. This is the reason why many papers found in the literature draw the reader's attention to the similitude of PhCs to semiconductors. The first principle is the same for both the photonic and electronic band gaps because it does not depend upon the particles, but on their associated wavefunctions. This first principle is Bragg diffraction. The incident and reflected planewave at a Bragg plane will begin to add up into two standing waves. Part (a) in figure 2-2 shows this degenerate behavior of some mode due to the Bragg reflection. When the periodic media is present, the second principle, the variational principle, goes into effect.

The operator in the eigenvalue problem represents the structure while the eigenmodes and eigenvalues represent the supported modes and their associated frequencies. The lowest mode supported by the structure will minimize (2.31) the most because, after all, is the lowest order mode. The second mode, also supported by the

structure, will tend to minimize (2.31). However, because the operator is Hermitian, i.e. distinct eigenvalues have orthogonal eigenmodes; the second mode must be orthogonal to the first mode. In order to accomplish this, the second mode must be concentrated in the lower dielectric and/or have a sign oscillation inside the high dielectric to make the orthogonality integral zero. Both of these possibilities will incur a large increase in frequency resulting in a band gap, as shown in part (b) of figure 2-2.

2.6.2 Nomenclatures

Modes below the band gap, known as 'dielectric band' modes, concentrate their energies into regions of high dielectric constant. Modes above the gap are known as 'air band' modes. These nomenclatures are similar to valence and conduction bands for electrons.

After describing how photonic band gaps originate, a method to quantify them can be useful for the extraction of application parameters.

Figure 2-2: The figure in (a) represents the first principle that degenerates modes, while figure (b) shows the action of the second principle which lifts this degeneracy.

2.7 Photonic Band Gap Structure

2.7.1 Bloch Modification

In order to quantify photonic band gaps, a good place to start is to find an expression that relates the eigenmodes to a dispersion relation, which contains the bandstructure of the material. From the Bloch theorem,

$$\mathbf{H}_{\mathbf{k}}(\mathbf{r}) = \mathbf{u}_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (2.33)$$

inserting the Bloch states into equation (2.29) gives,

$$\Theta_{\mathbf{k}}\mathbf{u}_{\mathbf{k}}(\mathbf{r}) = [\omega/c]^2\mathbf{u}_{\mathbf{k}}(\mathbf{r}) \quad (2.34)$$

where $\Theta_{\mathbf{k}}$ is the Bloch operator and is given by,

$$\Theta_{\mathbf{k}} \equiv (i\mathbf{k} + \nabla) \times \left(\frac{1}{\varepsilon(\mathbf{r})} i\mathbf{k} + \nabla \times \right) \quad (2.35)$$

This new Maxwellian operator now depends upon $\mathbf{k}$. Equation (2.34) is an eigenvalue problem, and solving it will give all the mode profiles of a particular $\mathbf{k}$. It is important to note that equation (2.34) is subject to the condition (2.9). Restricting an eigenvalue problem to a finite volume leads to a discrete spectrum of eigenvalues, similar

to the quantum well of electrons. As such, for each value of $\mathbf{k}$, an infinite set of modes with discretely spaced frequencies, labeled with a band index n , can be found.

2.7.2 Eigenvalue Dispersion Relation

Since $\mathbf{k}$ enters only as a parameter in (2.34), the frequency of each band for a given $\mathbf{k}$ varies continuously with $\mathbf{k}$. This gives a description of the modes in a photonic crystal similar to a dispersion relation. In fact, this is a dispersion relation because the frequency, $\omega_n(\mathbf{k})$, indexed in order of increasing frequency, is a function of $\mathbf{k}$. Equation (2.34) rewritten so that the dispersion relation is visibly apparent,

$$\Theta_{\mathbf{k}} \mathbf{u}_{\mathbf{k}}(\mathbf{r}) = [\omega_n(\mathbf{k})/c]^2 \mathbf{u}_{\mathbf{k}}(\mathbf{r}) \quad (2.36)$$

Studying the bandstructure of a crystal supplies the information needed to predict its optical properties, as indicated in section 2.3.1.

Equation (2.36) is a generic equation regardless of dimensions. The chapters on holographic lithography and numerical analysis utilize (2.36) but in two different ways. Holographic lithography provides the structure and material information found in $\Theta_{\mathbf{k}}$ while numerical analysis transforms (2.36) into matrix form and provides $\omega_n(\mathbf{k})$.

2.8 Two and Three Dimensional Photonic Band Gaps

2.8.1 Mirror Symmetry

If the dielectric structure is symmetric in a given plane, incoming modes can separate into transverse electric (TE) and transverse magnetic (TM) modes. The reason for this separation is due to the induced commutation of the Maxwellian operator and some mirror operator O_M , defined as,

$$O_M \mathbf{f}(\mathbf{r}) = M \mathbf{f}(M\mathbf{r}) \quad (2.37)$$

where M changes the sign of a point reflected in a plane associated with M . Operating on some Bloch wave with the mirror operator give,

$$O_M \mathbf{H}_{\mathbf{k}}(\mathbf{r}) = e^{i\phi} \mathbf{H}_{M\mathbf{k}}(M\mathbf{r}) \quad (2.38)$$

where ϕ is some arbitrary phase due to the reflection. The induced commutation occurs when $M\mathbf{k} = \mathbf{k}$ and $M\mathbf{r} = \mathbf{r}$. When this is true, (2.38) becomes an eigenvalue problem. Using (2.37) in (2.38), $\mathbf{H}_{\mathbf{k}}(\mathbf{r})$ must obey,

$$O_M \mathbf{H}_{\mathbf{k}}(\mathbf{r}) = M \mathbf{H}_{\mathbf{k}}(M\mathbf{r}) = \pm \mathbf{H}_{\mathbf{k}}(\mathbf{r}) \quad (2.39)$$

The electric field vector obeys a similar equation, so that both the electric and magnetic fields must be either even or odd under mirror operations. At $M\mathbf{r} = \mathbf{r}$, the only nonzero field components of an even mirror operation must be H_x , E_y , and E_z (TM). The odd modes are described by the components, E_x , H_y , and H_z (TE).

It appears that the separation of polarizations holds under restricted conditions and is not useful for three-dimensional photonic crystal analysis. However, this is not the case for two-dimensional PhCs. If the $\hat{\mathbf{z}}$ -axis is the perpendicular axis to the plane of symmetry, it follows that $M_z \mathbf{k}_{||} = \mathbf{k}_{||}$ for all wavevectors $\mathbf{k}_{||}$ in the two-dimensional Brillouin zone. Thus, the major classifications of modes for every two-dimensional photonic crystal are two: TM or TE modes.

Mirror symmetry is important to the description of two-dimensional photonic crystals. The reason is if a PBG exists for one polarization, it will not necessarily exist for the other polarization. This is due primarily to how the energy in that polarization distributes itself based on the particular two-dimensional spatial periodicity. An example is that a square lattice of dielectric columns will exhibit a PBG for TM modes but not for TE modes. Figure 2-3 shows such an arrangement and figure 2-4 shows the dispersion relation. Notice in the dispersion relation that the TM mode has a PBG while the TE does not.

Figure 2-3: Dielectric columns in a square lattice.

Figure 2-4: Dispersion relation of dielectric columns in a square lattice. Only TM modes have a PBG.

The reason for this that the electric flux density in the homogenous direction of the TM modes localize within the rods due to the variational principle, but the continuous field lines of the TE modes are compelled to penetrate the air regions to connect neighboring rods. As a result, consecutive TE modes cannot exhibit markedly different fill factors, and band gaps do not appear. For a square lattice of dielectric veins, the opposite effects occur, leading to a PBG for TE modes but not for TM modes [xxii]. Figure 2-5 and figure 2-6 show TM and TE mode arrangements in a square lattice of dielectric columns.

A triangular lattice of air columns has a PBG for polarizations. This configuration, shown in figure 2-7, compromises between the two structure arrangements discussed above. If the radius of the air columns is set properly, the region between three columns will look like dielectric columns that satisfy TM modes and the region between two air columns will look like dielectric veins that satisfy TE modes. These combined effects will yield a PBG for all polarizations, as shown in figure 2-8.

Figure 2-5: Containment nature of TM modes in dielectric rods.

Figure 2-6: Distributive nature of TE modes in dielectric rods.

Figure 2-7: Air columns in a triangular lattice arrangement in some dielectric. The TM mode “sees” the region surrounded by three columns as a rod, while the TE mode “sees” the region between two columns as a vein.

Figure 2-8: Dispersion relation showing PBG for both polarizations.

2.8.2 Rounding Off

Mirror symmetry may explain effects in two-dimensional photonic crystals, but is not much use for three-dimensional photonic crystals [xxii]. The key concept for obtaining three-dimensional photonic crystals is the shape of the Brillouin zone. The more spherical it is the better chance a 3D PBG might occur. Of course, the basis distribution is an important factor in opening a PBG. The direct lattice that has the most spherical Brillouin zone is the FCC lattice. However, if the basis distribution is not

properly calculated, a 3D PBG will not form, regardless of how spherical the Brillouin zone is.

2.8.3 Rule of Thumb

To obtain two and three-dimensional PBGs, only rules of thumb are available [xxxvii], such as the column/vein hybrid for 2D PBGs and round Brillouin zones with a trial and error basis distribution. This is due to the lack of rigorous design criteria that have yet to be determined. Perhaps the rigorous criteria may lie in complex quantum electrodynamic (QED) calculations that incorporate the photon wavefunction and degenerate perturbation theory incorporating helicity issues. Until then, rules of thumb with trial and error are the current method of finding two and three-dimensional PBGs.

2.9 Numerical Methods for PhC Analysis

2.9.1 Déjà Vu

Expanding (2.5) by incorporating the expression for the dielectric constant (2.6) gives,

$$-\nabla(\nabla \cdot \mathbf{E}) + \nabla^2 \mathbf{E} + \frac{\omega^2}{c^2} [\bar{\epsilon} - \epsilon(\mathbf{r})] \mathbf{E} = \frac{\omega^2}{c^2} \bar{\epsilon} \mathbf{E} \quad (2.40)$$

which resembles the stationary Schrödinger equation [xxxviii] with a few changes. These changes represent the inherent difference between electrons and photons. For example, the wavefunction is not scalar but vectorial. The ‘periodic potential’ term depends on the ‘energy eigenvalue’, and an added ‘kinetic term’ other than the Laplacian is present.

These differences greatly affect the search for photonic band gaps. However, that does not mean that computational methods for photonic crystals must start from scratch. By incorporating these differences into the computational methods of electronic bandstructure calculations, the reinvention of the wheel can be avoided.

The next few subsections discuss electronic bandstructure methods that are possible candidates for photonic bandstructure methods.

2.9.2 Planewave Methods

A straightforward way of solving eigenvalues and eigenmodes is to expand the dielectric constant as well as the periodic part of the Bloch function into a Fourier series on the reciprocal lattice. This would transform equation (2.5) into an eigenvalue

problem for an infinite matrix. This would then be suitable to truncate at a desired point for resolution purposes that would then be accessible to approximate numerical solutions. The divergence-free nature of the magnetic field allows for a further simplification by limiting the number of expansion coefficients to only two transverse polarizations for any given plane wave. For a total of N planewaves, this leads to a $2N \times 2N$ matrix problem instead of the $3N \times 3N$ matrix problem. Another simplification is the continuity of the magnetic field reduces the number of planewaves necessary for results to converge.

An issue with this method is that structures that have step-like discontinuities have convergence problems [xxxviii]. Step-like discontinuities are essential to have a photonic band gap. A solution to this problem is important if the planewave method is going to simulate photonic crystals appropriately.

2.9.3 KKR Method

Another method that may be adopted into photonic bandstructure computations is the famous electronic bandstructure method known as the Kohn, Korringa, and Rostocher (KKR) method [xxxix]. This method requires that the wave function expand into a series of vector spherical harmonic functions centered on individual lattice sites.

The electromagnetic radiation emanating from all but the central scatter matches to the electromagnetic field expanded around this central scatterer using the Graf addition theorem for Bessel functions. This method, similar to the planewave method

described above, transforms (2.36) into an infinite matrix system which can be truncated anywhere for numerical computation and accuracy. For systems with spherical symmetry, the KKR method is superior to the planewave method.

The difference between the two methods is converse. The KKR method relies on the eigenmodes of an individual scatterer and therefore represents discontinuities in the dielectric function very accurately. The planewave method bases its approach on the accurate representation of the underlying lattice structure via the expansion into an appropriate set of planewaves. It incorporates the discontinuities in the dielectric constant through the corresponding Fourier coefficients.

A major issue for the KKR method is that, for non-spherical scatterers, it loses its attractive feature of accurately incorporating the discontinuities of the dielectric constant. In view of the numerous structures with non-spherical structures that exhibit complete photonic band gaps, the KKR method is unable to replace the planewave method as the preferred choice of photonic bandstructure calculation methods.

2.9.4 Real Space Methods

Convergence issues with the planewave method and limitation to spherical scatterers for the KKR method has prompted researches of photonic crystals to look elsewhere for bandstructure calculations rather than solid-state methods.

Even though the transfer matrix method (TMM) [xl] is not a solid-state method for solving electronic bandstructure, it can be quite useful when studying photonic

crystals [xli]. At a fixed frequency, field amplitudes at one end of a unit cell relate to the field amplitudes at the other end via a transfer matrix. This matrix is similar to a transfer function found in electronics. The creation of this matrix comes about by finite difference, analytical or other possible methods. Obtaining this matrix yields the transmission spectrum directly.

A good practical utilization of this method is the calculation of transmission and reflection coefficients for finite slab photonic crystal materials. In addition, this method would work well if the dielectric function requires the explicit dependence upon frequency.

The issues with this method are the differencing or analytical preprocessing required in obtaining the matrix, the work involved in changing the matrix if the configuration of the structure changes (non-generic nature), and considerable computational resources that are required.

The computational method chosen for the band gap analysis of structures fabricated by holographic lithography is the planewave method. The next section explains why this particular method would be suitable for this task.

2.10 The Planewave Basis

2.10.1 Task Orientation

Since the focus is not on photonic crystals per se, but the fabrication of them, the chosen computational method should be generic. This method should be free from

constantly modifying some transfer matrix, which would depend upon structure configuration, and should not be specific to certain lattice types, such as the spherical basis of lattices.

Planewave basis methods would be the selection for this objective because its underlying equations do not need modification every time the structure changes. In addition, the handling of spherical and non-spherical configurations is available.

However, the main reason for the selection of the planewave basis is how well it works in the frequency domain.

2.10.2 The Frequency Case for Photonic Crystals

Frequency domain analysis provides spectral information about some systems. When the concern is whether a fabrication method is appropriate for the fabrication of photonic crystals, the general characterization of such a fabricated structure is important. The planewave basis method provides exactly this. By turning the Maxwellian operator, which contains the structural information of the fabricated edifice, into an eigenvalue matrix problem, all sustainable modes (i.e. the eigenmodes) become available.

Of course, time domain methods, such as finite difference time domain (FDTD), can characterize a given structure, but the basis change may mask hidden modes. In order to use time domain tools to characterize a structure, the transformation of the impulse response of the system to the frequency domain is required. The resulting peaks in the frequency spectrum correspond to the eigenfrequencies. However, two

closely spaced peaks may appear as one, which will mask out that particular eigenfrequency along with its eigenmode. In addition, the source must not be near orthogonal to any eigenmode. This would be another source of masking out important information in the characterization of these fabricated structures. One final note about using time domain tools as a characterization tool, is the problem of having to perform (at least one) more calculations. The initial transformation from time to frequency domains only yields the eigenfrequencies. At least one more calculation would be required to give one eigenmode. If more eigenmodes are required, then more calculations are required. It is a one-to-one relationship which may be computational expensive.

The TMM method is a hybrid of time and frequency domain methods, but as outlined in the previous section, requires preprocessing each time the structure changes. Again, this would be a costly approach.

The planewave-basis expansion method does have its hindrances. As explained previously, there is a convergence problem, especially with discontinuities. However, a computational tool [xxvi], freely available on the Web, is the implementation of possible solutions to the convergence problem, and other computational problems [xx].

Chapter 3

3 PBG Engineering: Holographic Interferometry

3.1 Theoretical Considerations

3.1.1 Photonic Crystals and Holograms

Photonic crystals and holograms share the same structural principles: spatially periodic dielectric functions. The application of PhCs and holograms is different. PhC design is for spatially selective optical isolation, while holograms perform the complete reconstruction of some electromagnetic field. Nonetheless, from a structural point of view, PhCs are a particular class of holograms.

The reciprocal lattice vector characterizes the intersecting families of planes that give holograms and PhCs their periodic structure. Given a particular structure with a particular reciprocal lattice, the constructive interference of the reflected wavevectors depends upon the Bragg condition. If Bragg's condition describes the reflected wavevector, can Bragg's condition also describe the structure doing the reflecting? It is this principle that establishes holographic design. The difference of wavevectors gives the reciprocal lattice vectors of the lattice, hence defining the periodicity.

Berger, Gauthier-Lafaye and Costard [xlii], were the first to notice the similarity between photonic crystals and holograms, and proposed a possible fabrication method.

Later, other researchers understood the importance of this fabrication method and proposed further suggestions concerning holographic lithography fabrication of PhCs [xix, xliii].

Before discussing the lithography part of DBHL however, the interference pattern used to expose recording media requires some discussion. Feature lengths, along with dielectric contrast, are what forms PBGs. DBHL controls feature lengths by the interference patterns generated from the beams and imprinting it into the recording material. Hence, the control of interference patterns requires detailed analysis, which is the topic of this chapter.

3.1.2 Interference Patterns

Holographic interferometry [xliv] techniques are critical to the understanding of how beams interfere and how their interference pattern can be manipulated.

Another name for dual beam interferometry is the Lippman or Denisyuk configuration [xlv]; two beams traveling in opposite directions. The lithography of this fabrication process does not depend upon a mask to shape the desired patterns. The shaping of these patterns arises from the projected interference pattern of two or more lasers upon a given volume of photosensitive material. Therefore, the interference parameters are of prime importance in designing a photonic crystal structure for some specific application.

The theoretical description of laser beam interference begins by studying its electric field vector component. The electric field vector of any radiation describes any polarization effects. Polarization is certainly an important factor in interference and no theory of interference would be complete without including it. In addition, the squared modulus of the electric field vector component of the interference beam describes its intensity. This intensity renders certain resins within the exposed material to be soluble or insoluble, depending upon its polymer composition.

The general expression of the electric field vector of the incoming laser beam, p or exposure step i is,

$$\mathbf{E}_{ip} = E_{ip} e^{j(\mathbf{k}_{ip} \cdot \mathbf{r}_{ip} + \varphi_{0ip})} \mathbf{e}_{ip} \quad (3.1)$$

where E_{ip} is the electric field amplitude, $\mathbf{k}_{ip}$ is the propagation wavevector normal to the plane surface, φ_{0ip} is the initial phase, and $\mathbf{e}_{ip}$ is the unit vector of the plane wave's polarization direction. Since the laser beam is coherent, the wavevector can have its wavelength factored out.

$$\mathbf{k}_{ip} = (k_{xip}, k_{yip}, k_{zip}) = \frac{2\pi}{\lambda} (l_{xip}, m_{yip}, n_{zip}) \quad (3.2)$$

where l_{ip} , m_{ip} and n_{ip} are the direction cosines of the wavevector.

When two incoming waves of the type represented in (3.1) interfere, the result is,

$$\mathbf{E}_{res} = E_{res} e^{j\phi_{res}} \mathbf{e}_{res} = E_1 e^{j(\mathbf{k}_1 \cdot \mathbf{r} + \phi_{01})} \mathbf{e}_1 + E_2 e^{j(\mathbf{k}_2 \cdot \mathbf{r} + \phi_{02})} \mathbf{e}_2. \quad (3.3)$$

The resultant intensity proportional to the magnitude of the electric field vector squared is,

$$I_{res} = |\mathbf{E}_{res}|^2 = \mathbf{E}_{res} \cdot \mathbf{E}_{res}^* \quad (3.4)$$

this gives an interference relation,

$$I_{res} = E_1^2 + E_2^2 + 2E_1 E_2 \cos([\mathbf{k}_1 - \mathbf{k}_2] \cdot \mathbf{r} + \phi_{01} - \phi_{02}) \cos \theta_{12}. \quad (3.5)$$

An advantage with dual beam interference results from the fact that polarization directions can be parallel [xlv]. This allows θ_{12} to be set to 0° . The initial phases depend upon the laboratory setup. Theoretically, the initial phases are set to zero and corresponds experimentally to adjusting the plane of one beam relative to the other. These simplifications result in the intensity represented as,

$$I_{res} = E_1^2 + E_2^2 + 2E_1 E_2 \cos([\mathbf{k}_1 - \mathbf{k}_2] \cdot \mathbf{r}). \quad (3.6)$$

The intensity is greatest when the interference phase is

$$[\mathbf{k}_1 - \mathbf{k}_2] \cdot \mathbf{r} = 2\pi w_i \quad (3.7)$$

where w_i an integer. Expanding equation (3.7) further,

$$A_i x + B_i y + C_i z + D_i = 0 \quad (3.8)$$

where $A_i = (l_{i1} - l_{i2})$, $B_i = (m_{i1} - m_{i2})$, $C_i = (n_{i1} - n_{i2})$ and $D_i = -\lambda w_i$. The greatest intensity condition yields a family of planes represented by equation (3.8). Figure 3-1 shows such a family of planes.

Families of periodically spaced planes fabricated from one exposure by the dual beams interferometry provide feature-lengths that are critical to forming a PBG. Using the famous relation in crystal physics, the distance between planes is,

$$d_{hkl} = \frac{2\pi}{|\mathbf{G}(h,k,l)|} \equiv d_i = \frac{\lambda}{\sqrt{A_i^2 + B_i^2 + C_i^2}} \quad (3.9)$$

Figure 3-1: Family of planes waves fabricated from one exposure by the dual beams.

This parameter is one of the important parameters elaborated on at the beginning of this subsection. This parameter describes the Bragg condition required for band gap formation, and relates to the dielectric function in a complicated way. From Chapter 2, the structure of the dielectric function determines the size and location of the photonic band gap. Therefore, *by induction*, there is an intimate relationship between the wavevectors of the interfering beams and the formation of PBGs. Representing this mathematically,

$$d_i \propto \varepsilon(\mathbf{r}) \quad (3.10)$$

Rather than having more than two interference beams which requires polarization adjustments [xliii], a *rotatable* sample stage with two beams and exposures at each sample

orientation could relax the polarization considerations and other background effects which complicates multiple beam exposures [34].

3.1.3 Sample Orientation

Sample rotations are included in the mathematical expressions by a matrix that represents the Euler angles. Figure 3-2 shows the Euler angles.

Figure 3-2: Euler angles and their associated rotations.

The matrix representing Euler angle rotations, known as the Euler matrix is,

$$\mathbf{R} = \begin{bmatrix} \cos\psi\cos\phi - \cos\theta\cos\phi\sin\psi & \cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi & \sin\psi\sin\theta \\ -\sin\psi\cos\phi - \cos\theta\sin\phi\cos\psi & -\sin\psi\sin\phi + \cos\theta\cos\phi\cos\psi & \cos\psi\sin\theta \\ \sin\theta\sin\phi & -\sin\theta\cos\phi & \cos\theta \end{bmatrix} \quad (3.11)$$

Applying this rotation matrix will give the exposure position for the sample of the next exposure.

Having established a connection between the dielectric function, feature lengths and structure orientation, the next section presents suggestions of fabricating structures using holographic lithography along with a photonic band gap analysis to determine whether the fabricated structure actually has a photonic band gap.

3.2 Practical Implementation

3.2.1 One-Dimensional Photonic Crystals

With only one exposure, perhaps holographic lithography could be the most efficient method for building Bragg gratings. Other fabrications are proficient in building Bragg gratings but the real benefit of holographic lithography is the easy building of omnidirectional periodic structures quickly relative to other fabrication methods [xliii].

3.2.2 Two-Dimensional Photonic Crystals

Two dimensional photonic band gap structures require translational symmetry in two dimensions, while the third is homogenous in the dielectric.

If one exposure in holographic lithography gives a family of planes that is *translationally* symmetric in one direction, then two exposures will yield a family of lines translationally symmetric in two directions, because the intersection of planes yields lines. Two exposures yields two families of planes,

$$\begin{aligned} A_1x + B_1y + C_1z + D_1 &= 0 \\ A_2x + B_2y + C_2z + D_2 &= 0 \end{aligned} \quad (3.12)$$

A parametric relation of the intersection of these planes is obtainable. Figure 3-3 shows this intersection of the exposure plane families at right angles to each other resulting from two exposures. The first exposure would yield a family of planes in the direction of the yz-plane, as shown in figure 3-1. The sample is then rotated 90° using the Euler angles and the second exposure is then applied. Figure 3-3 represents the exposure dosages (intensity interference pattern) that a photopolymer would receive in some photoresist.

Parameterizing the x-direction and performing simple linear algebra, yields,

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{C_1(B_1D_2 - B_2D_1)}{B_1(B_1C_2 - B_2C_1)} - \frac{D_1}{B_1} \\ \frac{(B_1D_2 - B_2D_1)}{(B_1C_2 - B_2C_1)} \end{bmatrix} + t \begin{bmatrix} 1 \\ \frac{C_1(A_2B_1 - A_1B_2)}{B_1(B_1C_2 - B_2C_1)} - \frac{A_1}{B_1} \\ \frac{(A_1B_2 - A_2B_1)}{(B_1C_2 - B_2C_1)} \end{bmatrix} \quad (3.13)$$

If $(B_1C_2 - B_2C_1)$ is zero, then it is simply a matter of changing the orientations of the incoming radiation so that this term does not become zero.

Figure 3-3: Intersection of two families of planes at right angles.

3.2.3 Rod Structures: Building Pillars

One of the earlier structures in the hunt for photonic band gaps greater than one dimension was the rod structure [xlvii].

A two-exposure process is required to fabricate such a structure. Initially, the sample orientation is at $(0,0,0)$. If the two beams are orthogonal with respect to each other, the distance between the planes is a minimum [xlv].

The two orthogonal wavevectors are,

$$\begin{aligned} \mathbf{k}_{1i} &= \frac{2\pi}{\lambda} \left(\frac{1}{\sqrt{2}}, 0, \frac{-1}{\sqrt{2}} \right) \\ \mathbf{k}_{2i} &= \frac{2\pi}{\lambda} \left(\frac{-1}{\sqrt{2}}, 0, \frac{-1}{\sqrt{2}} \right) \end{aligned} \quad (3.14)$$

The plane equation would be,

$$\begin{aligned} [\mathbf{k}_{1i} - \mathbf{k}_{2i}] \cdot \mathbf{r} - 2\pi w_i &= \left[\left(\frac{1}{\sqrt{2}} - \frac{-1}{\sqrt{2}}, 0, \frac{-1}{\sqrt{2}} - \frac{-1}{\sqrt{2}} \right) \right] \cdot \mathbf{r} - \lambda w_i \\ &= \sqrt{2}x - \lambda w_i = 0 \end{aligned} \quad (3.15)$$

and the distance between planes in each exposure would be,

$$d_i = \frac{\lambda}{\sqrt{A_i^2 + B_i^2 + C_i^2}} = \frac{\lambda}{\sqrt{(\sqrt{2})^2}} = \frac{\lambda}{\sqrt{2}} \quad (3.16)$$

In the first exposure, since the sample is orientated at $(0,0,0)$, the plane families would be parallel to the (y, z) plane. A sample rotation of 90° followed by the second exposure would have planes parallel in the (x, z) plane.

These steps would then yield rods in the z -direction. This structure gives a square lattice of rods translationally symmetric along the z axis. Figure 3-4 shows the structure configuration.

Figure 3-4: Isometric view of the rectangular arrangement of rods.

After running a computational band gap analysis on such a structure, this configuration gives a 35% photonic band gap between the second and third eigenmodes for TM modes, as shown in figure 3-5.

Figure 3-5: Dispersion relation of rectangular arrangement of rods. The largest PBG is 35%.

3.2.4 Triangular Lattice Arrangements

A triangular lattice may also be designed which increases the size of the photonic band gap [xliv]. This structure can be obtained by having the first exposure similar to the square lattice structure, and the second exposure would be upon a sample rotated only 30° , rather than 90° . This would give the y-direction a spacing of,

$$y = \frac{1}{B_2} \left(D_2 - \frac{A_2}{A_1} D_1 \right) \quad (3.17)$$

Figure 3-6 shows the intersection of these planes to yield the triangular lattice arrangement of rods.

Figure 3-6: Plane intersections that yield hexagonal arrangement of rods.

This structure yields PBGs for the TM modes only, similar to the square lattice formation in the last section. Figure 3-7 show the top view of the triangular lattice of rods. The rods are not round because of angle of the plane interference. This makes the PBG smaller. The PBG, shown in figure 3-8, of this arrangement is 28% compared to the 35% of the square lattice arrangement of rods in section 3.2.3.

Figure 3-7: Top view of hexagonal arrangement of rods.

Figure 3-8: Dispersion relation for ellipse shaped rods in a triangular lattice. The largest PBG is 28%.

A circular array of hexagonal rods can be obtained using the following Euler planes,

$$\begin{pmatrix} 1 \\ \text{step : } 2 \\ 3 \end{pmatrix} = \begin{pmatrix} (0, 0, 0) \\ \text{sample orientation : } (90, 0, 60) \\ (90, 0, 120) \end{pmatrix} \quad (3.18)$$

Using an exposure dose of 8 mJ/cm^2 , the resultant PBG is 41.2%, which results in a difference of 6.1% when compared to the square array of rods. The dispersion relation is shown in figure 3-9.

Figure 3-9: Dispersion relation for circular rods in a triangular lattice. The PBG is 41.2%.

3.2.5 Three Exposures: Building 3D PBGs

As explained in section 1.4.1, DBHL was a suggested fabrication method to build 2D photonic band gaps for an optical waveguide. However, the suggested operation of this waveguide would have had a lot of leakage due to the index guiding in the vertical direction. The work shifted towards using DBHL to build 3D photonic band gaps in order to contain this leakage problem [xlviii].

As established in Chapter 2, a 3D PBG is associated with a structure having a three-dimensional spatial periodicity. In order for DBHL to give structures with that kind of periodicity, three exposures are required. If two exposures yield a 2D periodic array of lines, then three exposures should yield a 3D periodic array of points. These points can be determined from,

$$\begin{bmatrix} A_1 & B_1 & C_1 \\ A_2 & B_2 & C_2 \\ A_3 & B_3 & C_3 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} D_1 \\ D_2 \\ D_3 \end{bmatrix} \quad (3.19)$$

which would leave translational symmetry in all three dimensions. To obtain a cubic lattice of dielectric spheres, the sample orientation in between exposures steps is,

$$\begin{pmatrix} 1 \\ \text{step : } 2 \\ 3 \end{pmatrix} = \begin{pmatrix} (0,0,0) \\ \text{sample orientation : } (90,0,0) \\ (90,90,0) \end{pmatrix} \quad (3.20)$$

which give the following intercept relations,

$$\begin{aligned}x &= D_1/A_1 \\y &= D_2/A_2 \\z &= D_3/A_3\end{aligned}\tag{3.21}$$

The intersections of these families of planes at right angles to each other yield cubic lattice structures of spheres. Figure 3-10 shows this intersection of three families of exposure planes. This figure is similar to figure 3-3 but with an additional exposure perpendicular to the last two. Overall, the sample is rotated three times with one rotation in between each exposure. The radius of these spheres is directly proportional to the exposure times. Figure 3-11 and figure 3-12 show the difference in sphere sizes, controlled by exposure dosage. A larger dose would leave smaller, unconnected spheres. A smaller dose would leave larger, possibly connected spheres.

Figure 3-10: Three families of intersecting exposure planes.

A PBG analysis of all the possible sphere sizes produced by the three exposures showed that no PBG could open with such a configuration. Figure 3-13 shows the dispersion relation of the cubic arrangement of spheres. It shows a gap is opening but degeneracy is occurring at the X point of the Brillouin zone. The Brillouin zone of a cubic lattice is cubic. If it were more spherical, perhaps the degeneracy at the X point would lift. A spherical Brillouin zone corresponds to direct lattice that is face-centered cubic (FCC).

Figure 3-11: Cubic arrangement of dielectric spheres created by three exposures at a large dose.

Figure 3-12: Cubic arrangement of interconnected dielectric spheres created by three exposures at a medium dose.

3.2.6 Face Centered Cubic (FCC)

Dielectric spheres arrangement in an FCC lattice proved that PBG could not form, as indicated in section 1.2.1 of the introduction. Degeneracy is actually greater than the cubic lattice of spheres in the above section. The dispersion relation, figure

3-14, of the inverse situation, air spheres in a dielectric media looks similar to figure 3-13. The degeneracy point however moved from the X point to the W point.

Figure 3-13: Dispersion relation of cubic arrangement of dielectric spheres.

Figure 3-14: Dispersion relation of FCC arrangement of air spheres in some dielectric medium.

The FCC structure with a spherical dielectric basis analyzed in [xliv] presented the same findings. A subsequent paper, [xv] showed that the degeneracy at the W point was lifted using a nonspherical basis. It suggested that in order to make an FCC structure with a nonspherical basis, an array of three angled drill actions at specific points on a slab of isotropic homogenous dielectric material were required. The three drill angles would be at 35° with respect to the vertical axis of the material, and 120° with respect to each other. Figure 3-15 shows the structure with the associated positions of the drills.

The structure yielded a 21% PBG with the structure being 78% empty. The nonspherical basis helped a great deal in lifting the W-point degeneracy. The structure was named Yablonovite after one of the authors of the paper [xii].

Figure 3-15: Mechanical method of building structure with an FCC lattice and nonspherical basis [xii].

3.2.7 The Yablonovite Structure

Could DBHL fabricate Yablonovite, or a structure similar to it? The answer to this question depends on whether DBHL can produce structures that have an underlying FCC lattice. In order for DBHL to produce an FCC lattice of points, three non-coplanar exposures are required. In the DBHL process, the exposure sample is rotated according to the Euler angles in order to obtain planes in the desired direction. In order to obtain the Euler angles it is necessary to obtain the normals of the exposure

planes then compute the Euler angles from (3.11). Figure 3-16 shows the intersect points of the three planes and the associated angles between them.

After selecting the three points for an exposure plane, obtaining the normal of that plane and using the Euler matrix, the Euler angles for the first exposure are, (60.7°, 202.3°, 58.8°). To complete the FCC, two more exposures are required with ϕ being increased by 120° in-between exposures.

The resultant photonic crystal designed in this fashion will have an FCC lattice. The basis will be nonspherical because of angle of interference between the three planes. Nonetheless, having a spherical basis will not yield a PBG anyway [xii].

Proceeding with all three exposures, the required Euler angles are,

$$\begin{pmatrix} 1 \\ \text{step} : 2 \\ 3 \end{pmatrix} = \begin{pmatrix} (60.693, 202.268, 58.76) \\ \text{sample orientation} : (60.693, 202.268, 178.76) \\ (60.693, 202.268, 298.76) \end{pmatrix} \quad (3.22)$$

Figure 3-17 shows the exposure plane intersections and figure 3-18 shows the resultant structure after the cumulative effect of the entire family of planes expose a photoresist.

Figure 3-16: Isometric view of plane interference for FCC lattice.

The primitive cell of this structure is required for the numerical analysis tool in order to determine whether it has a PBG. Figure 3-19 shows the associated primitive cell.

Figure 3-17: Three families of exposure planes at the appropriate angles to yield an FCC lattice with a nonspherical basis.

The dispersion relation, shown in figure 3-20 yielded a 5% gap for this structure, not the 21% found for the similar structure in [xii]. This is due to the same problem that gave rise to a smaller PBG in section 3.2.4. The angles of intersection distort the exposed area. In order to remove this distortion, six exposures are required, with development done every two exposures. Since the intersection of two planes is a line, the exposed line would be similar to the drill bits used in figure 3-15. The initial two exposures would give the first drill bit line. Then, development removes the exposed

photoresist along the line. With the sample still tilted 35° from the vertical, a rotation of 120° for the next two exposures yield the next drill bit line, followed by a second development. Finally, another sample rotation of 120° provides the last two exposures that give the final drill bit line. The last development should reveal a Yablonovite structure found in figure 3-15.

Figure 3-18: Resultant FCC structure with a nonspherical basis similar to Yablonovite.

The main result of this chapter is the engineering of a PBG by controlling the appropriate interference parameters (or degrees of freedom). Before proceeding to a design example, it is important to discuss exposure doses, exposure times, and development of photosensitive materials. These are also important parameters when designing PhC using DBHL.

Figure 3-19: The nonspherical basis found in the primitive cell of the FCC fabricated by DBHL.

Figure 3-20: Dispersion relation of FCC structure with nonspherical basis fabricated by a three exposure DBHL process. The PBG is 5%.

Chapter 4

4 Dual Beam Holographic Lithography Fabrication

4.1 Holographic Lithography

4.1.1 Interference Parameters

Holographic lithography is a fabrication process used to shape a volume out of photosensitive material with one or more exposures by the interference pattern of two or more coherent laser beams.

The lasers interference pattern, rather than a 3D mask, exposes parts of the material. After or in between exposures, the undesired material may be washed away in a chemical bath. The result is a periodic structure in one, two, or three dimensions.

Photonic crystals require precisely designed feature sizes and proper dielectric contrasts. This means that if holographic lithography is the fabrication method chosen, the laser characteristics, exposure durations, and material properties are parameters all requiring precise control. Table 4-1 presents the parameters that are available in the holographic lithography process.

System Parameter	Symbol	Influence
Beam Polarization	$\mathbf{e}_n$	Fringe contrast
Beam Propagation Vector	$\mathbf{k}_n$	Plane spacing, orientation.
Phase Factor	φ_n	Relative plane offset in sample.
Beam Amplitude	E_n	Intensity and fringe contrast.
Wavelength	λ	Interference plane spacing.
Sample Orientation Angles	(ψ, θ, ϕ)	Orientation of planes in sample.
Exposure Dose	N	Exposure dose in sample.
Exposure Number	$t_{,N}$	Structure complexity.

Table 4-1: Dual Beam Holographic Lithography Parameters

4.1.2 Irradiance and Optical Density

The frequency of light is in the visible range of 400 THz to 750 THz. Photosensitive media, including the human eye, cannot respond to these extremely rapid variations. What they respond to, however, is a cumulative effect, known as irradiance. Irradiance is the time-averaged energy flux of light and is represented mathematically as,

$$I = \epsilon v \langle \mathbf{E}^2 \rangle \quad (4.1)$$

where I is the irradiance, ϵ is the dielectric constant of the medium, v is the velocity of light in that medium and $\langle \mathbf{E}^2 \rangle$ is the time-averaged electromagnetic energy density in terms of the electric field vector.

The irradiance upon some photosensitive material causes a chemical reaction, rendering the illuminated portions to be either soluble or insoluble when the material is a photoresist. Irradiance alters the optical transmittance (T) of a photosensitive material. The inverse of transmittance is opacity. Opacity is logarithmically proportional to the material chemistry, and this relationship is known as the optical density (D). Mathematically,

$$D = \log[1/T] \quad (4.2)$$

where T is the optical transmittance.

4.1.3 Exposure Dose

Exposure dose (H) is a measure of the amount of light used to perform a chemical reaction in a given application time. Stated mathematically,

$$H = It \quad (4.3)$$

where I is the irradiance, and t is the exposure time. Exposure and optical density are related quantities and their relationship is known as the responsivity (R) of the material. Characteristic curves show the relationship between the optical density (D) and the logarithm of the exposure (H). Typical examples of such curves are shown in figure 4-1 and figure 4-2.

These curves are important because the sensitivity (γ) of the material can be found from the slope of these curves. Sensitivity is related to the optical density of material that has been chemically altered. The chemical reaction depends upon the radiation absorption. In addition, sensitivity is related to exposure, and exposure is related to exposure time and the wavelength of the irradiance. Figure 4-3 shows the absorbance spectrum of SU-8, which is the negative-tone photoresist used in this thesis as the suggested recoding material for PhCs.

Figure 4-1: Characteristic curve [Courtesy Kodak].

Figure 4-2: Characteristic curve of inverse material [Courtesy Kodak]

Figure 4-3: SU-8 absorption spectrum at different wavelengths.
[Courtesy MicroChem Corp.]

4.1.4 The Law of Reciprocity: Exposure Limits

The law of reciprocity [xiv] establishes that the photochemical reaction is determined by the total exposure, regardless of the range of values assumed by either the irradiance or time. A failure of this law implies that the material is becoming insensitive. This means that more exposure time is needed at extreme levels of irradiance to produce a given optical density.

This failure of the reciprocity law might not give multiple beam holographic lithography the benefits it claims over stability. In multiple beam holographic

lithography, Q-switched lasers and femtosecond pulses were utilized so that exposure times were too short for system vibrations to impart 'fuzziness' into the resultant pattern. Due to a failure in the reciprocity law, longer exposure times may be required, reducing the overall stability. A measure of reciprocity failure can be found when plotting the logarithm of exposure versus the logarithm of illuminance.

4.2 Photoresists and Photopolymers

4.2.1 Photoresists: Type and Application

Photoresists, known for their applications in fabricating electronic circuitry, have high diffraction efficiency and index modulation capabilities suitable for application in optical engineering [1].

There are two engineering categories of photoresists: type and application. Firstly, photoresists are available in two types, or polarities: negative or positive. A negative photoresist becomes insoluble when exposed to recording radiation wavelengths. A positive photoresist operates in the reverse manner; exposed regions become soluble.

Secondly, photoresists come in the form of resins suitable for application onto a clean surface. The procedure of deposition, exposure, and development vary, depending on the particular kind of photoresist and application. Spin-coating is the preferred method for depositing photoresist film. Photoresist thickness depends upon the angular speed of rotation. Fast rotations, i.e. 4000 to 7000 rpm, give thin films in the

range of 1 to 5 μm , while slower rotations, i.e. 1000 rpm, give thicker films. However, thicker films are generally non-uniform.

System tradeoffs and factors like sensitivity, linearity, film thickness, resolution capability, and ease of application and processing dictate the selection of a particular photoresist.

Nonetheless, the main job of the photoresist is to carry the photopolymer, which is the main ingredient that absorbs light and changes chemically to give the soluble or insoluble attributes of photoresists.

4.2.2 Photopolymers: Putting Light to Work

Photopolymers have two main ingredients related to the overall structure after development. As well, there are other ingredients not related to the overall structure, but they improve the photopolymerization process.

The two related ingredients are the polymerizable substance and photoinitiator. The polymerizable substance is the soluble or insoluble substance before exposures. The photoinitiator is the chemical that absorbs the photons and generates the active species, radicals, or ions capable of triggering polymerization. The polymerization is what changes the substance to insoluble or soluble when exposed.

The unrelated ingredients act on improving this process. There are two categories: sensitizers and binders. Sensitizers extend the spectral range of sensitivity, while binders increase the viscosity of photochemical diffusion during recording.

In [li], SU-8 has an absorption wavelength of 350 nm, while the datasheets available from MicroChem Corp. [lii] is advertised as having a range of absorption wavelengths.

Exposure shrinkage could potentially be a problem for PhCs. When two beams interfere and generate plane families, as presented in section 3.1.1, the distance between them dictates feature lengths critical to PBG formation. Shrinkage may push the PBG out of the intended frequency range, or destroy the PBG altogether. The material shrinkage factor would be required in the holographic interferometry process that generates the lithography patterns.

4.3 Physical Implantation

4.3.1 The Fabrication Laboratory: DBHL FAB LAB

Figure 4-4 shows the configuration of the proposed DBHL experimental setup. The sample resides on a three axis linear stage and a co-pivot point triple rotation stage unit. Euler angles, described in section 3.1.3, indicate the series of rotation performed for each exposure step. The two laser beams are directed towards the sample where they interfere, exposing the photosensitive material. Exposures of the sample consist of orienting the sample and beam two relative to beam one and then controlling the exposure time, t_p of the two beams.

After presenting the general outline of the fabrication arena, more detail about the individual components would be appropriate.

4.3.2 Component Descriptions

Placed in the path of the laser is a polarizer, which is one of the distinguishing features of DBHL. Because there are only two beams from the same polarized source, beam polarizations are in the same direction. This removes the complications of having to produce and manipulate several coherent beams directed onto a sample at specific angles. In addition, multiple non-coplanar beams have no common polarization direction. This has an effect on the overall contrast of the resultant pattern. Coplanar beams, i.e. two beams, do not have this problem. In addition, having more than one beam splitter is a problem. It complicates the experimental setup and suffers vibration problems. If exposure time lengths are not fast [liii], vibrations in the system result in fuzzy patterns. Fuzzy patterns introduce disorder terms into the dispersion relation of the structure that may ultimately lead to degenerative problems, closing any PBGs that may, otherwise remain open if the “fuzzy-ness” was not there in the first place. Stability problems are present in DBHL, however, the point is that having fewer components in a fabrication procedure helps to reduce the amount of variables that affect the result. Section 4.3.6 presents this and other problems with the DBHL procedure and suggests possible means of circumventing such issues.

Figure 4-4: Experimental setup of the DBHL process.

The first component to describe is the laser source. The choice of laser depends upon the absorbance of the recording material. The ultrathick SU-8 negative photoresist will be the choice of the material discussed here. The next sub-section will give the reasons as to why SU-8 is the particular choice.

The absorbance of SU-8 is in the range 350 nm to 400 nm. The nUVo™ laser, an all-solid-state continuous wave (CW) UV laser, from Light Age Corp., delivers fixed wavelengths between 360 nm and 400 nm. Next in the path of the laser would be the polarizer.

Using DBHL removes polarization problems inherent in multiple beam configurations. To make sure that the two beams do not have any polarization issues, the laser output passes through a polarizer before the main beam splits. The colorPol® UV-Polarizer has its peak transmittance at 370 nm, so that if the laser delivers only 360 nm or 380 nm, transmittance is still acceptable.

The beam must pass through a beamsplitter. The Polka-Dot Beamsplitter® from Edmund Industrial Optics® is suitable for this function because its spectral range is quite large (i.e. 200 nm to 2500 nm). After splitting the beam in two and traveling in directions orthogonal with respect to each other, there must be mirrors in their path to redirect them towards the recording medium.

Mirrors with good reflectance at 45° at the required wavelength and good thermal stability are ideal. Thermal expansion of mirrors is a problem that can affect image resolution. The 09 Enhanced Aluminum Diamond machined mirrors from Lincoln Laser® exhibit an extremely low thermal expansion of $\pm 0.10 \times 10^{-6}$ per °C as well as providing a broad spectral range of 300 nm to 10600 nm. Now that the beams are redirected towards the sample, the sample must be at the appropriate orientation so that the family of planes generated by the interfering beams will be oriented in the proper direction.

The sample sits on a rotatable stage. The stage may or may not be computerized. However, the advantage of having a computerized stage comes from software routines that quickly apply Euler angles calculated from nontrivial plane orientations. Linear motion is provided by using the X-Z Bracket®, a computer controlled linear movement stage from Edmund Industrial Optics®. Rotation is possible from a rotary stage, which may also be purchased from Edmund Industrial Optics®. The volume of SU-8 photoresist resides upon this stage.

4.3.3 SU-8 Properties and Process

SU-8 [li] is a negative type photoresist consisting of Epon-SU8 resin (Shell Chemical®) where its sensitizer is triaryl sulfonium salt (0.5 – 3.0 wt%) and its binder is a solution of γ -butyrolactate (50 – 60 wt%). This photoresist is available from MicroChem®.

The photoresist can then be spin-coated at about 1000 rpm. This is done so that the photoresist has a thickness of about 200 μm . Baking on a hot plate at 90-95°C for 15 minutes would then prepare it for the exposure stage.

The final step after all the exposures is an ultrasonic bath in propylene glycol methyl ether acetate. This entire process should deliver prepared microperiodic films with thicknesses in the range of 10 – 60 μm , corresponding to 14 – 80 closed-packed layers of the resultant structure.

4.3.4 Exposure Time Calculations of SU-8 Multiple Exposures

The exposure is dependent upon the irradiance (i.e. laser intensity) and time of exposure. DBHL is not a one shot recording process. For 3D PhCs, a minimum of three exposures are required. Assuming linear material response, the best way to handle this would be to underexpose, either by varying the irradiance or exposure time for all exposures, but work out such that after the three exposures, the cumulative effect would be one full exposure.

The total dose in [xix], to build three-dimensional PhCs was about 80 to 200 mJ/cm². In [xix], a 6 ns pulse delivered the dose once. Suppose the total dose is 200 mJ/cm². If in the DBHL three exposures are required to deliver the total dose, each exposure dose could be 66 mJ/cm². If the laser source delivers an irradiance of 0.62 mW/cm², the time for each exposure should be about, $t = 97s$, with an overall exposure process time of about 5 minutes.

Smaller exposures times are attainable by reducing the exposure area or increasing the irradiance of the laser, or both. However, extremely short exposure times or extremely large irradiance will cause the reciprocity law to fail. The failure of the reciprocity law means that the material is inadequately exposed which requires a longer exposure time.

4.3.5 Proof of Concept

Exposure thresholds in a multiples beam, single exposure process are not an issue. The only factor is that the delivered dose must be above the photoresist's exposure threshold. However, in a dual beam, multiple exposure process, the delivery of the overall exposure dose is in smaller doses. The concern was whether the photoresist could be underexposed enough during subsequent exposures, so that the final exposure would bring the recording material over its threshold and retain the final interference pattern. Figure 4-5 shows the results of such an exposure process. The two-dimensional periodicity is evident, and this is exactly what was expected. The recoding

material was NRP504 positive-tone resist with a wavelength absorbance of about 400 nm and spin-coated thickness of 3 – 4 μm .

Figure 4-5: Dual beam exposure producing dimples.
[Courtesy Chris Raum, Carleton University]

This experiment was critical to the validation of the concepts presented in this thesis. In the conclusion, suggestions to improve such exposures will be presented, but the main point here is that dual beam, dual exposure processes do indeed give periodic patterns that can be processed to become photonic crystals.

4.3.6 Stability of DBHL Fabrication

If exposure times are required to be relatively large, stability might become an issue. Vibrations from laboratory equipment will cause the exposed image to be fuzzy and perhaps introduce enough defects to cause degeneracy of the PBGs.

Other methods use ultra-fast exposure rates in order to circumvent these stability issues [xix, xliii, liv, lv]. However, these recommendations involve more than two beams. Having more than two beams leads to polarization issues that still need to be solved [xliii, xlvi]. In addition, the reciprocity law discussed in section 4.1.4, places a limit on how short the exposure times are. This means that stability may still be a factor with these multiple beam ultrafast exposure methods.

Two ways are suggested that might help in circumventing stability issues. The first is to take great care in choosing the laboratory setup. The optical bench used could possibly be situated on top a large heavy slab of concrete with a bed of inflatable tires in-between the bench and the slab. Another method for controlling stability – and this could be used in conjunction with the previous suggestion – is to monitor the dual exposure profile and adjust the relative phase on one beam with respect to the other using a phase modulator.

Chapter 5

5 Engineering a PBG: The Kielovite Structure

5.1 The Yablonovite Structure Revisited

5.1.1 Mode Analysis

Chapters 3 and 4 outline techniques required to obtain lattice configuration and dielectric basis distributions for opening a PBG. The techniques described in those chapters, therefore, establish the engineering link between DBHL and PBG formation.

Before proceeding to design examples using DBHL, it is worth noting another technique in designing PhCs using DBHL. This technique shows the strong correlation between electromagnetic computational methods and the DBHL fabrication process.

Figure 5-1 and figure 5-2 show the electromagnetic energy of two lower order modes of a structure having a cubic lattice with a spherical basis distribution. As indicated in section 3.2.5, this structure does not have a PBG. However, it is interesting to note that the first mode distributes itself in a fashion similar to the dielectric structure found in Yablonovite.

By studying the mode configurations in structures that may not have a PBG and utilizing the electromagnetic variational principle, engineering dielectric distributions along mode paths might help in opening a PBG. Due to the ability of the DBHL

process to expose patterns in any orientation, fabricating dielectric distributions tailored to mode arrangements may be possible. This is where computational analysis is important because it would provide the mode arrangements, and from this data, the DBHL fabrication parameters can be determined.

Figure 5-1: Lowest order mode energy distribution in a cubic lattice.

Figure 5-2: Second order mode energy distribution in a cubic lattice.

5.1.2 Intensity Threshold

An important issue not mentioned in chapter 3, is the intensity threshold. Assuming electric field vector amplitude of one, equation (3.6) gives the maximum intensity to be 4 mW/cm^2 . Each additional exposure adds 4 to the maximum, so that for three exposures, the maximum intensity would yield 12 mW/cm^2 . If 100% of the exposure time is used, then the maximum exposure dose of 12 mJ/cm^2 is delivered.

However, if the full exposure dose is used, the entire structure would be exposed and no pattern would emerge. Feature lengths, such as radii and 3D periodicity lengths, are directly dependent upon exposure dose. In the case for DBHL Yablonovite, a maximum exposure dose of 7 mJ/cm^2 was used to get a PBG of 5%. Other dosages were analyzed, but 7 mJ/cm^2 yielded the largest PBG.

When designing some structure, the intensity threshold is what determines the dielectric fill factor. The dielectric fill factor is critical because it shapes how the optical modes arrange themselves, which might, if the appropriate fill factor is available open a PBG.

5.1.3 Increasing the PBG

Due to the distortion caused by the intersection of planes, the basis of the DBHL Yablonovite structure does not have the same PBG size as the mechanical version. One way of increasing the PBG is to perform six exposures. The first three are the same as described in section 3.2.7. The last three have the same Euler angles but the recording wavelength is half the value of the previous three exposure wavelengths. Figure 5-3 shows the six interference planes. In addition, the last three exposures are 65% the exposure doses of the previous three exposures. The overall effect of the additional exposures helps to shape the basis further. Figure 5-4 shows the new dielectric basis associated with each lattice point and figure 5-5 shows the six-exposure DBHL

Yablonovite resultant structure. The PBG of this structure rises to 10.6%. Figure 5-6 shows the dispersion relation of this six-exposure DBHL Yablonovite structure.

Table 5-2 shows the iterations of different parameters and associated PBGs used to hunt for the largest PBG. However, this was a manual effort and in order to obtain an optimum analysis, a computer simulation linking the DBHL parameters with a PBG calculator would be the best combination to arrive at the largest possible PBG.

Figure 5-3: Exposure plane intersections of six exposures. The first three are same as the DBHL Yablonovite structure, while the last three are half the wavelength.

Figure 5-4: Basis associated with primitive cell of the six exposure DBHL Yablonovite structure.

Figure 5-5: DBHL Yablonoite structure using six exposures.

Figure 5-6: Dispersion relation of DBHL Yablonovite structure with six exposures. The PBG is 10.6%.

5.2 Design Example: The Kielovite Structure

5.2.1 Lattice and Basis Calculations

This section will present the systematic design of a three-exposure DBHL structure with a larger PBG than the three-exposure DBHL Yablonovite structure.

The first issue is determining the lattice of the new structure. From Chapter 3, the direct lattice that will give the most spherical Brillouin zone is the FCC lattice. An FCC lattice is obtained when the intersect lines of three planes are 35° from some

vertical, as shown in figure 3-16. Suppose this angle is changed to 29° . The required Euler angles for the three exposures become,

$$\begin{pmatrix} 1 \\ \text{step : } 2 \\ 3 \end{pmatrix} = \begin{pmatrix} (195.997, 75.726, 295.957) \\ \text{sample orientation : } (195.997, 75.726, 175.957) \\ (195.997, 75.726, 55.957) \end{pmatrix} \quad (5.1)$$

The calculation of the primitive vectors requires the solution of three sets of three equations. Figure 5-7 shows four lattice points and the three basis vectors required to move from one point to another.

By using equation (3.19) three times and replacing the D values with associated distances between the two points of the basis vector yields,

$$\begin{bmatrix} A_1 & B_1 & C_1 \\ A_2 & B_2 & C_2 \\ A_3 & B_3 & C_3 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} = \begin{bmatrix} \lambda \\ 0 \\ 0 \end{bmatrix} \quad (5.2)$$

$$\begin{bmatrix} A_1 & B_1 & C_1 \\ A_2 & B_2 & C_2 \\ A_3 & B_3 & C_3 \end{bmatrix} \begin{bmatrix} x_2 \\ y_2 \\ z_2 \end{bmatrix} = \begin{bmatrix} 0 \\ \lambda \\ 0 \end{bmatrix} \quad (5.3)$$

$$\begin{bmatrix} A_1 & B_1 & C_1 \\ A_2 & B_2 & C_2 \\ A_3 & B_3 & C_3 \end{bmatrix} \begin{bmatrix} x_3 \\ y_3 \\ z_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \lambda \end{bmatrix} \quad (5.4)$$

Using Kramer's rule for solving three equations that have three unknowns, gives the coordinates of the three points relative to (x_0, y_0, z_0) . Assuming the point (x_0, y_0, z_0) is the origin, the primitive vectors are,

$$\begin{aligned} \mathbf{a}_1 &= (x_1, y_1, z_1) \\ \mathbf{a}_2 &= (x_2, y_2, z_2) \\ \mathbf{a}_3 &= (x_3, y_3, z_3) \end{aligned} \quad (5.5)$$

Figure 5-7: Conceptual image showing how primitive basis vectors are calculated.

Using the dot product,

$$\theta_{ij} = \cos^{-1} \left(\frac{\mathbf{a}_i \cdot \mathbf{a}_j}{|\mathbf{a}_i| |\mathbf{a}_j|} \right) \quad (5.6)$$

where i, j can be 1, 2 or 3, but $i \neq j$. Equation (5.6) gives the angles between each primitive vector. It turns out that if the Euler angles are the ones shown in (5.1), then the angles between the primitive vectors is 50° . This is clearly not an FCC, since the angle between the primitive vectors of an FCC are 60° . Figure 5-8 shows the three exposure planes, figure 5-9 shows the associated basis of the primitive cell and figure 5-10 shows the resultant structure, known in the literature as Kielovite [lvi].

The reciprocal lattice basis vectors, found from,

$$\mathbf{b}_i = 2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k)} \quad (5.7)$$

where i, j, k range from 1, 2 and 3 but $i \neq j \neq k$. These reciprocal basis vectors gives the reciprocal lattice vector, $\mathbf{G}$, represented as,

$$\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3 \quad (5.8)$$

Comparing the PBG with the PBG of the Yablonovite structure, shows an increase from 5% to almost 7%.

Figure 5-8: Exposure planes of DBHL Kielovite.

Figure 5-9: Dielectric basis associated with the primitive cell of the DBHL Kielovite.

Figure 5-10: The DBHL Kielovite structure.

Figure 5-11: Dispersion relation of the DBHL Kielovite structure. The PBG is almost 7%.

5.2.2 Angle Variations

If the exposure plane line intersection angle of 29° with some vertical yield a larger PBG than an angle of 35° , could other angles yield yet larger PBGs? Three PBG calculations were performed, with each calculation having a different angle. The first was 20° , which is shallower than the 29° . A PBG analysis yielded no PBG at all for any exposure dose. An angle of 25° gave a PBG of 6.7% at an exposure dose of $7 \text{ mJ}/\text{cm}^2$. Finally, an angle of 41° gave a 2.33% PBG at the same exposure dose. A finer analysis, shown in table 5-1, was performed and shows that an angle of 28.7° yielded the largest PBG at 7.08%.

Angle From Vertical	PBG Size
29.1°	6.9713%
29.0°	6.9941%
28.9°	7.0337%
28.8°	7.05836%
28.7°	7.0828%
28.6°	7.0344%

Table 5-1: PBG variation with angle from vertical in DBHL Kielovite design.

5.2.3 Increasing the Kielovite PBG

Similar to the DBHL Yablonovite, the Kielovite PBG increases further with six exposures. The first three exposures remain the same, while the next three have the same Euler angles, but at half the wavelengths. In addition, the exposure doses of the last three exposures are 55% of the first three exposure times. This yielded a PBG of about 9.5%. By simulating post-processing wet etch that reduces the dielectric content from 25.3% to 22.6%, the PBG grows by about 0.2%.

Figure 5-12 shows the exposure planes, figure 5-13 shows the associated basis of the primitive cell, figure 5-14 shows the resultant DBHL Kielovite structure, and figure 5-15 shows the dispersion relation of the structure.

5.2.4 Design Results

Three-exposure DBHL Kielovite yields a larger PBG than the three-exposure DBHL Yablonovite, however, it does not respond to six exposures as well. The reason is the basis of DBHL Kielovite is more distorted than the DBHL Yablonovite basis. Adding more shape, via the six exposures, distorts the basis further, but only to a certain plateau. Any more shaping of the basis, via increasing or decreasing exposure doses of the last three exposures only decreases the size of the PBG.

Table 5-2 and table 5-3 present the manual iterations and parameter correlations performed in order to find the maximum PBG for both DBHL Yablonovite and Kielovite.

Figure 5-12: Six exposure planes of DBHL Kielovite.

Figure 5-13: Primitive cell basis for the six-exposure DBHL Kielovite.

Figure 5-14: DBHL Kielovite structure fabricated from six exposures.

Figure 5-15: Dispersion relation of DBHL Kielovite with a 9.7% PBG.

dosage [mJ/cm ²]	wet etching [+/-]	% dosage of last 3 of 6 exposures	dielectric fill factor [%]	PBG [%]
5	0	0	62.7	0.0
6	0	0	48.7	3.15
7	0	0	34.4	5.09
8	0	0	20.3	0.0
6	-	0	38.4	4.33
6	-	0	32.1	4.5
6	-	0	29.5	3.4
7	-	0	29.5	3.0
7	-	0	32.0	4.0
7	+	0	36.9	5.2
7	+	0	39.4	4.95
9	0	35	32.9	8.76
10	0	35	23.5	9.93
11	0	35	14.7	4.89
10	+	35	26.1	9.94
10	+	35	28.7	9.60
9	0	45	41.4	4.56
10	0	45	28.68	9.83
11	0	45	20.1	9.88
12	0	45	12.8	4.28
11	+	45	22.9	10.3
10	0	55	35.5	6.54
11	0	55	25.3	10.45
12	0	55	17.4	9.17
11	-	55	22.6	10.59
11	-	55	19.8	10.13
11	-	65	22.0	9.99
12	0	65	22.3	10.6
12	-	65	19.5	10.0
12	0	75	28.3	8.0
13	0	75	19.7	10.1
14	0	75	13.9	6.5
13	+	75	22.6	10.55
13	+	75	25.0	10.55
13	+	75	28.1	9.69
13	0	85	26.8	7.0
14	+	85	23.8	9.68
14	+	85	20.9	8.0

Table 5-2: Manual iteration and parameter correlation to PBG of DBHL Yablonovite structure. The bold entry has the largest PBG of the entire run. The dotted rows signify initial guesses.

dosage [mJ/cm ²]	wet etching [+/-]	% dosage of last 3 of 6 exposures	dielectric fill factor [%]	PBG [%]
5	0	0	62.7	0.0
6	0	0	48.7	4.87
7	0	0	34.4	6.92
8	0	0	20.3	0.0
6	-	0	35.3	7.3
6	-	0	32.8	6.86
7	+	0	36.9	7.0
7	+	0	39.4	6.7
10	0	45	28.68	9.11
11	0	45	20.1	9.41
12	0	45	12.8	3.97
11	+	45	22.7	9.0
10	0	55	35.5	5.73
11	0	55	25.3	9.51
12	0	55	17.4	8.35
13	0	55	11.4	2.45
11	-	55	22.6	9.7
11	0	65	31.6	6.29
12	0	65	22.3	9.58
12	-	65	19.4	9.0
12	+	75	25.0	9.4
11	0	75	41.7	0.0
12	0	75	28.3	6.69
13	0	75	19.73	8.77
14	0	75	13.97	5.0

Table 5-3: Manual iteration and parameter correlation of DBHL Kielovite. The bold entry is the largest PBG in the run. The dotted rows signify initial guesses.

Chapter 6

6 Conclusion

6.1 Thesis Objectives

6.1.1 Thesis Results

In this thesis, the potential for a DBHL process was investigated as a method of building template structures, which after appropriate fabrication processes yield omnidirectional PhCs. The investigation was carried out by performing computer simulations of the DBHL process that creates the template structures, followed by a numerical analysis of the resultant silicon-air PhC structures, assuming proper fabrication steps have been taken. It was shown that the formation of omnidirectional PBGs are dependent upon the delicate interplay between lattice arrangement and the dielectric distributions that form the crystal basis. However, lattice and basis configurations are directly controlled by DBHL parameters. In conclusion, this thesis establishes a conceptual link between omnidirectional PBG formation and the DBHL process.

6.1.2 Implications

The thesis results presented here can be used as a primer for an experimental study directed towards the physical building of PhCs. The logistics of the physical setup

is left to future work, but the guiding principles have been provided. DBHL offers many advantages over other PhC fabrication methodologies. Polarization issues are

inherently handled by the use of two beams, the experimental setup is obviously simple, and the associated cost is relatively low when compared to other fabrication methods.

6.2 Future Work

6.2.1 Experimental Implementation

The next step would be to build omnidirectional PhCs. This involves the logistics of the physical laboratory configurations, the purchasing of components to facilitate the fabrication and the physical testing of the product. Instead of the computer generated dispersion curves seen throughout this thesis, instrumentation is required to achieve physically measured dispersion relations.

6.2.2 Computational Analysis

This thesis demonstrates the link between fabrication parameters and PBG formation. To optimize the search technique the PBG numerical analysis needs to be intimately connected to the DBHL computer simulation. Then, through a series of permutations and combinations of the proposed fabrication parameters the largest PBG fabrication parameters are determined iteratively and user independent.

The computer simulation of DBHL could only provide the basis vectors of three exposures. New lattice structures with an optimized basis may result from a larger number of exposures. However, the basis vectors need to be known in order for a PBG numerical analysis to be run. Adding this feature adds yet another parameter for the hunt of larger PBGs.

Finally, once a PhC with an optimized PBG has been found, time domain analysis is then required to characterize transport issues, which are critical in using omnidirectional PhCs in real-world optical systems.

6.2.3 Defect Design and Analysis

The real benefit of PhCs with large omnidirectional PBGs comes in the form of defect design. Defects are analogous to doping in semiconductors. Creating a defect within a PBG allows only modes with frequencies inside the defects to propagate through the crystal with almost 100% optical containment, regardless of path. This allows optical waveguides to have small radius and shallow coupler/splitter angles, resulting in an overall size reduction. In addition, the optical circuitry will be more efficient, since less power leakage would occur.

DBHL could also be used to create the defects required for optically containing modes. In Chapter 3 it was shown that applying two exposures results in “rods”. These “rods” could be the embedded waveguides within the DBHL-fabricated PhCs.

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References

-
- [i] Rayleigh, Lord J. W. S. 1887. "On the maintenance of vibrations by forces of double frequency, and on the propagation of waves through a medium endowed with a periodic structure." *Philos. Mag* **24**, 145.
 - [ii] Tayeb, G., S. Enoch, and B. Gralak. 2003. "Structural Colors in Nature." *OSA Opt* **14**, 40.
 - [iii] Kogelnik H., and C. V. Shank. 1971. "Stimulated Emission in a periodic structure." *App. Phys. Lett.* **18**, 152.
 - [iv] Haus, H. A., and C. V. Shank. 1976. "Antisymmetric Taper of Distributed Feedback Lasers." *IEEE J. Quant. Elec* **12**, 532.
 - [v] Kittel, C. 1953. *Introduction to Solid State Physics*. Wiley.
 - [vi] Yariv A., and P. Yeh. 1984. *Optical Waves in Crystals: Propagation and Control of Laser Radiation*. Wiley.
 - [vii] Bialynicki-Birula, I. 1996. "Photon Wave Function." *Progress in Optics* **XXXVI**, 245.
 - [viii] Kleppner, D. 1981. "Inhibited Spontaneous Emission." *Phys. Rev. Lett.* **47**, 233.
 - [ix] Anderson, P. W. 1958. "Absence of Diffusion in Certain Random Lattices." *Phys. Rev.* **109**, 1492.
 - [x] Yablonovitch, E. 1987. "Inhibited spontaneous emission in solid-state physics and electronics." *Phys. Rev. Lett.* **58**, 2059.
 - [xi] John, S. 1987. "Strong localization of photons in certain disordered dielectric superlattices." *Phys. Rev. Lett.* **58**, 2486.
 - [xii] Yablonovitch, E., T. J. Gmitter, and K. M. Leung. 1991. "Photonic Band Structure: The Face-Centered-Cubic Case Employing Nonspherical Atoms." *Phys. Rev. Lett.* **67**, 2295.
 - [xiii] Arya, K., Z. B. Su, and J. L. Birman. 1986. "Anderson Localization of Electromagnetic Waves in a Dielectric Medium of Randomly Distributed Metal Particles." *Phys. Rev. Lett.* **57**, 2725.
 - [xiv] Ho, K. M., C. T. Chan, and C. M. Soukoulis. 1990. "Existence of a Photonic Gap in Periodic Dielectric Structures." *Phys. Rev. Lett.* **65**, 3152.
 - [xv] Yablonovitch, E. 1992. "Photonic band-gap structures." *J. Opt. Soc. Am B* **10**, 283.
 - [xvi] Blanco, A., E. Chomski, S. Grabtchak, M. Ibisate, S. John, S. W. Leonard, C. Lopez, F. Meseguer, H. Miguez, J. P. Mondia, G. A. Ozin, O. Toader, and H. M. van Driel. 2000. "Large-scale synthesis of a silicon photonic crystal with a complete three-dimensional bandgap near 1.5 micrometers." *Nature* **405**, 437.
 - [xvii] Johnson, S. G., and J. D. Joannopoulos. 2000. "Three-dimensionally periodic dielectric layered structure with omnidirectional photonic band gap." *App. Phys. Lett.* **77**, 3490.
 - [xviii] Cheng, C., A. Scherer, R. Tyan, Y. Fainman, G. Witzgall and E. Yablonovitch. 1997. "New Fabrication techniques for high quality photonic crystals." *J. Vac. Sci. Tech. B* **15**, 2764.

-
- [xix] Campbell, M., D. N. Sharp, M. T. Harrison, R. G. Denning, and A. J. Turberfield. 2000. "Fabrication of photonic crystals for the visible spectrum by holographic lithography." *Nature* **404**, 53.
 - [xx] Johnson, S. G., and J. D. Joannopoulos. 2001. "Block-iterative frequency-domain methods for Maxwell's equations in a planewave basis." *OE* **8**, 173.
 - [xxi] Busch, K. 2002. "Photonic band structure theory: assessment and perspectives." *C. R. Physique* **3**, 53.
 - [xxii] Joannopoulos, J. D., R. D. Meade, and Joshua N. Winn. 1995. *Photonic Crystals: Modeling the Flow of Light*. Princeton.
 - [xxiii] John, S., and O. Toader. 2001. "Proposed Square Spiral Microfabrication Architecture for Large Three-Dimensional Photonic Band Gap Crystals." *Science* **292**, 5519.
 - [xxiv] Wanke, M. C., O. Lehmann, K. Müller, Q. Z. Wen, and M. Stuke. 1997. "Laser rapid prototyping of photonic band-gap microstructures." *Science* **275**, 1284.
 - [xxv] Cumpston, B. H., S. P. Ananthavel, S. Barlow, D. L. Dyer, J. E. Enrlich, L. L. Erskine, A. A. Heikal, S. M. Kuebler, I. Y. Sandy Lee, D. McCord-Maughon, J. Qin, H. Röckel, M. Rumi, X. Wu, S. R. Marder, and J. W. Perry. 1999. "Two-photon polymerization initiators for three-dimensional optical data storage and microfabrication." *Nature* **398**, 51.
 - [xxvi] Johnson, S. G., and J. D. Joannopoulos. The MIT Photonic-Bands Package home page <http://ab-initio.mit.edu/mpb/>.
 - [xxvii] Maxwell, J. C. 1865. "A dynamical theory of the electromagnetic field." *Philos. Trans. Roy. Soc. Lond.* **155**, 459.
 - [xxviii] Bloembergen, N. 1965. *Nonlinear Optics*. W. A. Benjamin.
 - [xxix] Anderson, J. C. 1968. *Magnetism and magnetic materials*. Chapman & Hall.
 - [xxx] Bloch, F. 1928. "Über die quantenmechanik der electronen in kristallgittern", *Z. Physik* **52**, 555.
 - [xxxi] Ashcroft, N. W., and Mermin, N. D. 1976. *Solid State Physics*. Saunders College Publishing.
 - [xxxii] Jammer, M. 1966. *The Conceptual Development of Quantum Mechanics*. McGraw-Hill.
 - [xxxiii] Pankove, J. I. 1971. *Optical Processes in Semiconductors*. Dover Publication.
 - [xxxiv] Hawking, S. 1999. *A Brief History of Time*. Princeton.
 - [xxxv] Lanczos, C. 1970. *The Variational Principles of Mechanics*. Dover Publication.
 - [xxxvi] Johnson, S. G., and J. D. Joannopoulos. 2003. "Introduction to Photonic Crystals: Bloch's Theorem, Band Diagrams, and Gaps (But No Defects)." *Internet article*. <http://ab-initio.mit.edu/mpb/>.
 - [xxxvii] Schrödinger, E. 1928. "Quantisation as a Problem of Proper Values." *Annalen der Physik*. **79**, 361.
 - [xxxviii] Sözüer, H. S., J. W. Haus, and R. Inguva. 1992. "Photonic bands: Convergence problems with the plane-wave method." *Phys. Rev. B*. **45**, 13 962.
 - [xxxix] Kohn, W., and Rostoker, N. 1954. "Solution of the Schrodinger Equation in Periodic Lattices with an Application to Metallic Lithium." *Phys. Rev.* **94**, 1111.

-
- [xl] Yeh, P. 1988. *Optical Waves in Layered Media* John Wiley & Sons.
 - [xli] Khorasani, S., and B. Rashidian. 2002. "Analysis of Kronig-Penny photonic crystals by modified transfer matrices." *Proc SPIE* **4655**, 260.
 - [xlii] Berger, V., O. Gauthier-Lafaye, and E. Costard. 1997. "Photonic band gaps and holography." *J. Appl. Phys.* **82**, 60.
 - [xliii] Cai, L. Z., X. L. Yang, and Y. R. Wang. 2002. "Formation of three-dimensional periodic microstructures by interference of four noncoplanar beams." *J. Opt. Soc. Am. A.* **19**, 2238.
 - [xliv] Vest, C. M. 1979. *Holographic Interferometry*. Wiley.
 - [xlv] Calixto, S., and D. J. Lounnot. 2001. "Light-Sensitive Materials: Silver Halide Emulsions, Photoresists and Photopolymers." *Handbook Opt. Eng.* **73**, 879
 - [xlvi] Gauthier, R. C., and K. W. Mnaymneh. *Yet to be published*
 - [xlvii] Meade, R. D., K. D. Brommer, A. M. Rappe, and J. D. Joannopoulos. 1992. "Existence of a photonic band gap in two dimensions." *Appl. Phys. Lett.* **61**, 495.
 - [xlviii] Gauthier, R. C., and K. W. Mnaymneh. 2002. *Private communication*
 - [xlix] Yablonovitch, E., and T. J. Gmitter. 1989. "Photonic Band Structure: The Face-Centered Cubic Case." *Phys. Rev. Lett.* **63**, 1950.
 - [l] *Optical Engineering* (vol. **33**, pp. 3504-3669)
 - [li] Lee, K. Y., N. LaBianca, S. A. Rishton, S. Zolgharnain, J. D. Gelorme, J. Shaw, and T. H. P. Chang. 1995. "Micromachining applications of a high resolution ultrathick photoresist." *J. Vac. Sci. Technol. B* **13**, 3012.
 - [lii] MicroChem Corp. *NanoTM SU-8 Negative Tone Photoresist Formulations 2-25*. Datasheet.
 - [liii] Kondo, T., S. Matsuo, S. Juodkazis, and H. Misawa. 2001. "Femtosecond laser interference technique with diffractive beam splitter for fabrication of three-dimensional photonic crystals." *App. Phys. Lett.* **79**, 725.
 - [liv] Cai, L. Z., X. L. Yang, and Y. R. Wang. 2001. "All fourteen Bravais lattices can be formed by interference of four noncoplanar beams." *Opt. Lett.* **27**, 900.
 - [lv] Cai, L. Z., X. L. Yang, and Y. R. Wang. 2001. "Formation of a microfiber bundle by interference of three noncoplanar beams." *Opt. Lett.* **26**, 1858.
 - [lvi] Birner, A., R. B., Wehrspohn, U. Gösele, and K. Busch. 2001. "Reviews – silicon – based photonic crystals." *Adv. Materials*. **13**, 377.