Experimental Verification of a Three Dimensional Photonic Crystal Bandgap

by

Sri Abhishek Rao Jamalapur

A thesis submitted in conformity with the requirements for the degree of Master of Applied Science
Graduate Department of Electrical and Computer Engineering
University of Toronto

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Abstract

Photonic crystals (PC) are periodic structures that dictate the behavior of electromagnetic radiation and can be one-dimensional, two-dimensional or three-dimensional (3D). A 3DPC was modeled and fabricated based on a three-layer design resulting in a face centered cubic structure. Different simulation methods were used to show the existence of a complete 3D bandgap, and were verified experimentally by obtaining transmission measurements in several directions. A prototype of the structure was fabricated using ECCOSTOCK HiK high dielectric sheets (dielectric of 12) and machined using a computer and numerical controlled mill. Experiments to test this structure were performed in an anechoic chamber making use of a network analyzer, a pair of horn antennas, collimating lenses, and a track for alignment. Free-space Thru-Reflect-Line measurements were taken between 10GHz and 15GHz to obtain the transmission through the prototype. Finally, a defect layer was added to the structure at different locations and localized modes observed.
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1 Introduction

1.1 Photonic Crystals

Photonic Crystals (PC) are periodic structures that manipulate the behavior of electromagnetic (EM) radiation and are analogous to the behaviour of electrons in a crystal lattice [1]. They are designed for their photonic bandgap, a range of frequency where incident EM radiation is reflected and guided modes are not supported. PCs are fundamentally one of three types (see Figure 1.1), one-dimensional (1DPC), two-dimensional (2DPC), and three-dimensional (3DPC). As the name suggests, 1DPCs are periodic along one axis and the bandgap exists for propagation along that axis only. Similarly, 2DPCs and 3DPCs have periodicity and a bandgap in two and three dimensions respectively. The different colours in Figure 1.1 represent materials of different dielectric constants.

![Figure 1.1: Depiction of a (a) 1DPC, (b) 2DPC, (c) 3DPC](image)

The periodicity of these structures is analogous to the periodicity of a crystal lattice giving rise to many of the same concepts. Concepts such as the unit cell, reciprocal lattice, and Brillouin zone will be discussed here.
1.2 Crystal (Periodic) Structures

A periodic structure is one that can be constructed by the repetition of a group of points in space [2]. These points can be translated along vectors in certain directions to generate the lattice.

![Figure 1.2: Basis vectors and unit cells](image)

In Figure 1.2, $\mathbf{a}_1$ and $\mathbf{a}_2$ are one possible set of basis vectors that can be used to generate the triangular lattice shown. Another choice of basis vectors are $\mathbf{b}_1$ and $\mathbf{b}_2$, and both sets of vectors are primitive lattice vectors. The shaded areas are possible unit cells for the lattice. The repetition of the unit cell along the basis vectors generates the entire periodic structure.

For a three-dimensional lattice with primitive lattice vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$, we can define the primitive reciprocal lattice vectors $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$ to be the Fourier Transform of the spatial function of the original lattice. This space is known as the reciprocal space or $k$-space:

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}$$  \hspace{1cm} (1.2.1)

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}$$  \hspace{1cm} (1.2.2)
The reciprocal lattice allows us to define the Brillouin Zone. If a point in the reciprocal lattice is chosen, the Brillouin Zone is the region of space that is closest to our chosen point than any other point in the lattice. In Figure 1.3, the Brillouin Zone is the shaded area for a square lattice.

![Figure 1.3: The Brillouin Zone for a square lattice in reciprocal space.](image)

### 1.3 Maxwell’s Equations for Photonic Crystals

The equations describing the behaviour of PCs are derived from Maxwell’s Equations, listed below:

\[
\begin{align*}
\nabla \cdot \mathbf{B} &= 0 \\
\nabla \cdot \mathbf{D} &= \rho \\
\n\nabla \times \mathbf{H} &= \frac{\partial \mathbf{D}}{\partial t} \\
\n\nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t}
\end{align*}
\]

(1.2.4)

\(\mathbf{B}\) denotes the magnetic field flux density, \(\mathbf{E}\), the electric field intensity, \(\mathbf{D}\), the electric displacement field, \(\mathbf{H}\), the magnetic field intensity, \(\mathbf{J}\), the current density, and \(\rho\) is the charge density. From here on we restrict ourselves to lossless, linear materials. The constitutive relations connect \(\mathbf{B}\) and \(\mathbf{H}\), and \(\mathbf{E}\) and \(\mathbf{D}\) and are given by:
\[ \mathbf{D}(\mathbf{r}) = \varepsilon_0 \varepsilon(\mathbf{r}) \mathbf{E}(\mathbf{r}) \]
\[ \mathbf{B}(\mathbf{r}) = \mu_0 \mu(\mathbf{r}) \mathbf{H}(\mathbf{r}) \]  

(1.2.5)

We note that by definition PCs are inhomogenous, which is why the permittivity \((\varepsilon)\) and permeability \((\mu)\) are functions of space. The permittivity and permeability of free space are denoted by \(\varepsilon_0\) and \(\mu_0\) respectively (constants), while \(\varepsilon(\mathbf{r})\) and \(\mu(\mathbf{r})\) are the relative permittivity and permeability of the materials that make up the PC.

Eq. 1.2.4 is a function of both time and space, so we employ the technique of time harmonics to separate these variables.

\[ \mathbf{H}(\mathbf{r}, t) = \mathbf{H}(\mathbf{r}) e^{-j\omega t} \]
\[ \mathbf{E}(\mathbf{r}, t) = \mathbf{E}(\mathbf{r}) e^{-j\omega t} \]  

(1.2.6)

Here, \(\omega\) is the angular frequency and \(i\) is the complex number satisfying \(i^2 = -1\).

We can now write Eq. 1.2.4 entirely in terms of \(\mathbf{E}\) and \(\mathbf{H}\).

\[ \nabla \cdot \mathbf{H} = 0 \]
\[ \nabla \cdot \mathbf{E} = 0 \]
\[ \nabla \times \mathbf{E} = i \omega \mu_0 \mathbf{H} \]
\[ \nabla \times \mathbf{H} = -i \omega \varepsilon_0 \mathbf{E} \]  

(1.2.7)

We substitute Eq. 1.2.6 into Eq. 1.2.7, and solving the two curl equations for \(\mathbf{H}\), we obtain the following master equation [1]:

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

(1.2.8)

Here, \(c\) is the speed of light in vacuum and is given by

\[ c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \]  

(1.2.9)

Eq. 1.2.8 enables us to find \(\mathbf{H}\). We can then find \(\mathbf{E}\) using Eq. 1.2.10
\[ \mathbf{E}(\mathbf{r}) = \frac{i}{\omega \varepsilon_0 \varepsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) \]  \hspace{1cm} (1.2.10)

At this stage, we need only to define \( \varepsilon(\mathbf{r}) \). The periodic nature of PCs enables us to write

\[ \varepsilon(\mathbf{r}) = \varepsilon(\mathbf{r} + \mathbf{R}) \]  \hspace{1cm} (1.2.11)

\( \mathbf{R} \) is the translation vector, the vector along which the structure repeats. The distribution of the dielectric \( \varepsilon(\mathbf{r}) \) is usually known, enabling us to solve these equations using methods such as Transfer Matrix Method (TMM) [3], Plane Wave Expansion (PWE) [4, 5], Finite Element Method (FEM) [6, 7], and Finite Difference Time Domain (FDTD) [8]. The reader can learn more about these methods in detail in the references provided. In this work TMM was implemented using MATLAB, PWE was implemented using MIT Photonic Bands (MPB), and FEM was implemented using Ansoft HFSS.

### 1.4 Photonic Crystal Characterization

Photonic crystal bandgaps are most commonly characterized in one of two ways, transmission (or alternatively reflection) curves and photonic band (or dispersion) diagrams. Both characterizations are used in this text and are discussed in detail.

#### 1.4.1 Transmission

Transmission plots are obtained by sweeping through a frequency range and comparing the output to the input in a log scale. They are extremely useful in observing the behavior in a particular direction and are popular due to their ease in verifying through experimentation by measurement of S-Parameters, specifically \( S_{11} \) or \( S_{21} \). Information such as the bandgap (frequency range where there is little to no transmission), bandwidth (size of the bandgap) and percent bandwidth (width of the bandgap in relation to the center frequency of the gap) are easily discernable from transmission plots.

#### 1.4.2 Band Diagrams

Band diagrams are obtained by sweeping through the different k-vectors in reciprocal space along the principal directions of the Brillouin Zone, and ultimately for all directions of the crystal. They are able to completely calculate the frequency ranges where modes are forbidden.
thus showing the existence. Another advantage band diagrams possess is that they are normalized in frequency, so one band diagram is sufficient to characterize a photonic crystal regardless of scale. As long as relevant parameters are kept constant the photonic crystal can be scaled to any size.

1.5 Photonic Crystal Defects and Applications

Defects in a photonic crystal occur when the translational symmetry is intentionally broken. This break in periodicity allows for localized modes to exist within the bandgap, and defects can appear as a peak in the bandgap of a transmission plot. There are many applications of defects in photonic crystals. For example, a 2DPC such as the one described in Section 2.2 can have a line of cylinders that are removed, allowing for modes to exist in that line. This can be used as a waveguide as the energy is confined in the defect [1], [10-11]. Photonic crystals have also seen use in lasing applications [12-13] along with widespread use as antenna substrates and backgrounds [14-15] to improve antenna characteristics such as gain and directivity [16]. Recently, photonic crystal structures have also seen use in molecular biosensing applications [17].

1.6 Shape of the Field and Challenges

The first experimental demonstration of a three-dimensional photonic crystal was done in 1991 using an array of holes drilled into a high dielectric material and having a bandgap between 13-15 GHz [18]. Since then, most of the focus in photonic crystal fabrication and experimentation has been in the optical regime [19]. In this regime, techniques such as standard microelectronics fabrication [20], three-dimensional holographic lithography [21], photofabrication by multibeam laser interference [22], and electron beam lithography [23] have all been used to fabricate 3DPCs. As a result, not much work has been done at the centimeter scale and this work explores the fabrication of a 3DPC in that regime.

1.7 Scope and Organization

The main contribution of this work is to fabricate a 3DPC at the centimeter scale and verify the existence of a full 3D bandgap via $S_{21}$ measurements over several angles of incidence and orientations of the photonic crystal. This will be the first 3DPC to be fabricated at this scale for
which experimental verification is obtained, and can lead to its use in potential applications discussed later on in this thesis.

Chapter 1 provided a brief introduction to photonic crystals, the physics behind them, their characterization, and the importance of defects. Chapter 2 will discuss some of the more common photonic crystals and look at the possibility of amalgamating 1D and 2D photonic crystal structures to create a quasi-3DPC with a full 3D bandgap. Chapter 3 discusses the fabrication of a 3DPC structure, fabrication challenges, and solutions to those challenges. Chapter 4 documents the experimental procedure used to verify theoretical results, and discusses the results obtained. Chapter 5 concludes this thesis and looks at future work.
2 Background and Theory of Photonic Crystals

2.1 One-dimensional Photonic Crystal: Omni-directional Bragg Reflector

In [24], Winn et al., designed a one-dimensional photonic crystal (1DPC) that exhibited an omni-directional bandgap for a wide range of incident wave vectors. The two-material structure consisted of a series of quarter-wave thick dielectric slabs with alternating indices of refraction $n_1$ and $n_2$ with a necessary condition being $n_1/n_2 \geq 1.5$. The center frequency of the gap, $\omega_0$ and the gap – mid-gap ratio, $\Delta \omega/\omega_0$, were able to be controlled to an extent by systematic selection of $n_1$ and $n_2$. This structure exhibited a complete bandgap for angles of incidence between $0^\circ – 89^\circ$, for both $s$-polarization (perpendicular) and $p$-polarization (parallel). Figure 2.1 shows a schematic of the structure described in [24].

![Figure 2.1: The 1DPC proposed by Winn et. al. in [24]. The different colours represent different dielectrics.](image-url)
Figure 2.2: Verification of the existence of a bandgap exhibited by the 1DPC for normal incidence and perpendicular polarization

Figure 2.3: Verification of the existence of a bandgap exhibited by the 1DPC for normal incidence and parallel polarization
The results obtained by Winn *et al.*, were verified independently using both Ansoft HFSS and Matlab, making use of the Finite Element Method and Transfer Matrix Method respectively. The result for 0° incidence for both polarizations is shown above in Figure 2.2 and Figure 2.3 as an example. The two simulation methods agree well and match the results provided in [17], and reproduced here in Figure 2.4.

There are a few shortcomings of the photonic crystal that are discussed here. Although this 1DPC exhibits omni-directional reflection, it is important to note that it does *not* have a complete photonic bandgap as there are propagating states within the crystal. Additionally, if the angle of the incident wave is increased, the center frequency of the bandgap shifts. If this photonic crystal is used as an antenna substrate, it would be inferior to one with a full 3D bandgap [16] as a portion of the input power is lost into the dielectric stack.

### 2.2 Two-Dimensional Photonic Crystal: Triangular Lattice of Air Columns

In [1], Joannopoulos presents a two-dimensional photonic crystal (2DPC) that has an omni-directional bandgap for both Transverse Electric (TE) and Transverse Magnetic (TM) polarizations. The structure consists of a high dielectric background (\(\varepsilon_b\)) in which cylindrical holes of a low dielectric (\(\varepsilon\)) are drilled or etched in a triangular lattice pattern. The defining parameters of the bandgap are given by the radius of the cylinders, \(r\), and the lattice constant \(a\). The condition \(r/a = 0.48\) must be satisfied and the ratio \(\varepsilon_b : \varepsilon\) must be sufficiently large (13:1). The periodicity of this structure lies in the \(x\)-\(y\) plane while the axis of the cylinders is along the \(z\)
axis. The complete bandgap is for wave vectors in the $x$-$y$ plane. Figure 2.5 shows the structure described.

![Figure 2.5: The 2DPC presented by Joannopoulos in [1]. The red material has a dielectric of 12 while the cylindrical holes are are air. This structure was simulated in a software package called MIT Photonic-Bands (MPB) developed by S. Johnson at the Massachusetts Institute of Technology (MIT). The result was matched to the one obtained by Joannopoulos and is shown below in Figure 2.6.](image-url)
Figure 2.6: The band diagram for a triangular lattice of air columns drilled into a high dielectric background. (a) The result obtained in [1]. (b) Result independently verified by us.

2.3 Quasi-3DPC: A Proposed Structure

Unlike 1D and 2D photonic crystals, 3DPCs exhibit a complete bandgap for all possible wave vectors. However, they are very difficult to manufacture due to the complex nature of their
structure, and as a result they are not as prominent as their 1D or 2D counterparts. Attempting to mitigate the issue of fabrication led to the idea of a quasi-3DPC. The objective was to create an easily realizable structure that would yield a full 3D bandgap just as a typical 3DPC would.

The idea was to amalgamate the 1D Bragg Reflector and the 2D Triangular lattice of air columns to create a multilayer structure as seen in Figure. 2.7. Note that the “Bragg Reflector” is composed of the red and green layers, while the cylindrical air holes are as described in Section 2.2.

![Figure 2.7: Combining the 1DPC and 2DPC to create a quasi-3DPC](image)

The aim of this structure was to obtain a full 3D bandgap by overlapping the two bandgaps discussed in Section 2.1 and Section 2.2. However, this task was not simple as there were a multitude of factors to consider. First, the introduction of the holes in the Bragg reflector (1DPC) would change the behavior of the bandgap and may even result in the gap disappearing entirely. The introduction of the multiple layers of alternating dielectrics in the 2DPC could lead to the same problem. Furthermore, there are three different dielectrics that affect the gap, the two from the 1DPC (red and green in the figure) and the third being the cylindrical holes. The holes are air filled for now but can be a different dielectric altogether. The relationship between the thicknesses of the two layers and the radius of the cylinders to the triangular lattice constant also needs to be taken into consideration. With so many factors to consider, it would not be easy to come up with a solution to this problem, if at all one existed.
Simulations were performed with the aid of both MPB and HFSS to determine whether an omnidirectional bandgap existed or not. Given the structure is finite (and relatively short) along the z-direction, we needed to evaluate the transmission function for waves propagating along this direction in particular, and for angles subtended from the z-axis (propagation in the x-z or y-z planes) in order to determine whether or not a bandgap exists along these directions. For this, HFSS was used. Once this gap is found, MPB is used to find a gap in the x-y plane. Then these gaps are attempted to be matched by varying parameters including the thicknesses of the two layers ($d_1$ and $d_2$), the dielectric constants of the layers ($\varepsilon_1$ and $\varepsilon_2$), and the radius of the cylinders in relation to the lattice constant ($r/a$). Figure 2.8 and Figure 2.9 provide further details about the structure.

Figure 2.8: Side view of the quasi-3DPC
The HFSS simulations required a fair amount of setup due to the changing incident angles. $S_{21}$ simulations making use of waveports would yield the transmission for normal incidence but the other angles of incidence could not be simulated this way. A method outlined by Remski [25] making use of integration planes and the HFSS field calculator was used and the simulations performed for several incident angles. However, there was a limitation with using this method. As the angle of incidence increased, the edges of the integration planes got closer and closer to the perfectly matched layer (PML) boundaries. We cannot have these planes intersect the PML boundaries, nor can they come too close to them, thus limiting the angle of incidence to $45^\circ$ in our simulations. After systematically testing values for the parameters of interest, a combination of $\varepsilon_1 = 3$, $\varepsilon_2 = 12$, $d_1 = 6.4 \text{ mm}$, $d_2 = 3.2 \text{ mm}$, and $r/a = 0.20$ yielded a gap in transmission along the $z$-direction for angles of incidence up to $60^\circ$.

MPB simulations were needed to show the behaviour of our structure in the $x$-$y$ plane. The simulations in MPB assume that the structure is infinite in all directions. However, when
considering the challenges associated with fabricating the structure, we find that accommodating a large number of periods in the x-y plane is not an issue (we can easily fit upwards of 10 periods). This is not the case for the number of periods along the z-direction, where at most 3 or 4 periods can be fabricated. To overcome this issue, a *super-cell* was used to simulate the actual structure. In the case of the super-cell, a column of air is left above and below the unit cell in the z-direction. The idea here is that when this cell repeats itself in the z-direction, the gaps of air prevent the multi-layer in one unit cell from interacting with the multi-layer in the unit cell above and below it. Essentially, the structure behaves as if it were finite along z. The structure is assumed infinite in the x-y plane.

Many attempts were made in order to obtain a gap in the x-y plane but to no avail. The relevant parameters were varied systematically in order to obtain a gap but with no success. With a finite sized PC, there are two types of modes that can be found, those that are guided within the structure and those that radiate into the background above and below it. The distinction between these two modes can be made with the use of the *light cone* or *light line* in the band diagram [10]. Any bands below the light line are guided within our structure while bands above the light line are radiated modes. A second approach was to introduce a high dielectric capping layer above and below the multi-layer. Increasing the dielectric constant of this layer pushes the light line down to lower frequencies, and a high enough dielectric (*ε₇ = 12*) would ensure that there were no guided modes within the multi-layer. This capping layer needs to be sufficiently thick (25.4 mm) and is shown in yellow Figure 2.11.
Since the structure is now considered to be finite along the $z$-direction in our simulations, the characterization of the modes changes to even and odd, instead of TE and TM respectively. **A horizontal symmetry plane bisects the slab, and the modes are classified based on even or odd symmetry with respect to reflections through this plane.** The structure already has a gap in the $z$-direction as seen earlier, so a gap in the guided modes is essential for there to be a gap in the $x$-$y$ plane.

Figure 2.12 shows the band diagram for the quasi-3DPC structure with the capping layers. The red curves represent the first three even modes while the blue curves represent the odd modes. The light cone is defined by the bold line. There are no modes below the light line thus ensuring that no guided modes exist in the multi-layer structure. The points defined along the horizontal axis in the figure correspond to the points in the irreducible Brillouin zone of a triangular lattice. The center of the zone is Γ, the corner point, K, while M is a midpoint. This is the bottom face of the Brillouin Zone seen is Figure 2.13.
Figure 2.11: Band diagram for the Quasi-3DPC structure. The red curves are the even modes and the blue curves are the odd modes. The solid black line is the light line.

One of the motivations of trying to design a simple structure that possessed a full 3D bandgap was for its practical uses as an antenna substrate. However, there is a small drawback with using the structure as designed. It is true that no modes exist in the multi-layer as seen from the figure above. However, this does not mean that no energy is radiated above and below the multi-layer into the capping layer for propagations in the x-z or y-z planes (i.e. wave vectors in the aforementioned planes). In other words, an analysis based solely on the band diagram in 2D (x-y plane) and transmissions from angles subtended from the z-axis, is insufficient. To ensure that our quasi-3DPC structure has a true omni-directional bandgap, a full 3D band diagram is needed. Pavarini and Andreani have investigated a similar issue in [26] and have arrived at a similar conclusion.

Figure 2.14 shows the 3D band diagram for the quasi-3DPC for which the Brillouin zone is shown in Figure 2.13. The figure clearly shows a gap in the 2D plane (Γ-M-K-Γ), but it appears that the 1D gap (Γ-A) is closed off by a mode starting around a normalized frequency of 0.26. This mode, however, cannot be excited by a plane wave incident upon this structure because it is “symmetry uncoupled” [26]. Hence, a claim can be made that the 2D gap overlapped with the
1D gap along Γ-A. However, no full 3D bandgap exists for this structure as seen by the closing of the gap in the other directions (A-L and Γ-H). In short, the proposed quasi-3DPC structure is simply not capable of supporting a full 3D bandgap.

Figure 2.12: Brillouin Zone for the quasi-3DPC without the capping layers
Figure 2.13: Band diagram for the quasi-3DPC structure. The red arrow highlights the spurious mode that arises, while the yellow strip highlights the bandgap we were investigating.

2.4 Three Dimensional Photonic Crystal

Given the shortcomings of the quasi-3DPC structure discussed in detail in the previous section, it was necessary to investigate a structure that exhibited a full 3D bandgap. A layered structure was proposed by Johnson in [27] that met these requirements. Each period in the z-direction is comprised of three layers of the same thickness \((A, B, C)\) to form a face centered cubic (FCC) lattice. This is possible by close cubic packing (CCP) of the elements of the three layers. As such, there are two separate lattices that are in play, one is the FCC lattice \((a_{FCC})\), and the other is the triangular lattice \((a)\). As viewed from the top, each layer has 2 sets overlapping triangular lattices (as seen in Figure 2.15). Consider this to be layer \(A\) for example. The first lattice of holes (orange) is overlapped by the second lattice (yellow). The orange holes penetrate completely through the layer (as seen in Figure 2.16) while the holes in yellow penetrate only to a certain depth. The triangle outlined in purple at the center of the figure represents a third triangular lattice of holes centered at its vertices. Now, in layer \(B\) (directly below layer \(A\)), the holes that penetrate completely are the “purple” holes (that don’t appear in \(A\)), while the holes of partial depth align with the orange ones from above. Finally in layer \(C\), the yellow holes
penetrate completely and the purple holes penetrate partially. The unit cell of the structure is shown in Figure 2.17.

Figure 2.14: Overlapping triangular lattices in layer A
Figure 2.15: Side view schematic of the 3DPC structure showing the behaviour of the holes in the layers.

Figure 2.16: Unit cell of the 3DPC
Simulations showed that there is a complete bandgap when the dielectric contrast is 12:1. This result was independently verified using MPB and is shown below in Figure 2.18. The Brillouin Zone for the FCC lattice is shown in Figure 2.19.

Figure 2.17: Verification of the band diagram of the 3DPC proposed by Joannopoulos [27]. There is a full 3D gap in the structure highlighted in yellow.
Figure 2.18: FCC Brillouin Zone [1]
3 Design and Fabrication of the Three-Dimensional Photonic Crystal

This chapter deals with the fabrication of the three-dimensional photonic crystal (3DPC), the materials and equipments used, difficulties faced during this process, and how the issues were resolved.

3.1 Design

The most flexible parameter in the design of this structure is the triangular lattice constant, $a$ (see Figure 3.1), as this distance can be controlled precisely with the computer numerical control (CNC) milling machine. The more problematic parameters are the thickness of the layers and the sizes of tools available. The material used was ECCOSTOCK HiK line of low loss dielectrics with $\varepsilon = 12$ and this material is available in 12"×12" sheets having thicknesses of 1/4", 3/8", 1/2", and so on. Based on the thickness of a single layer, we are able to calculate the rest of the parameters needed to fabricate the PC [27].

![Figure 3.1: (a) Top view of a single layer showing the triangular lattice constant, $a$. (b) Side view of the same layer showing the thickness of the layer, $d$.](image)

We start with the thickness of the layer, $d$. 
\[ d = \frac{a_{\text{FCC}}}{\sqrt{3}} \]  

(3.1.1)

And for ECCOSTOCK HiK thickness of 0.25\" , we have:

\[ \frac{a_{\text{FCC}}}{\sqrt{3}} = 0.25\" \Rightarrow a_{\text{FCC}} = 0.433" \]  

(3.1.2)

The triangular lattice constant that we require for machining (\( a \)) is related to \( a_{\text{FCC}} \) by:

\[ a = \frac{a_{\text{FCC}}}{\sqrt{2}} = 0.3062" \]  

(3.1.3)

The hole radius, \( r \) is related to the FCC lattice constant by:

\[ \frac{r}{a_{\text{FCC}}} = 0.293 \Rightarrow r = 0.127" \]  

(3.1.4)

The depth of the holes, \( h \) can be calculated using:

\[ h = 0.93a_{\text{FCC}} \Rightarrow h = 0.402" \]  

(3.1.5)

Subtracting the thickness of the layer from this value, we calculate the depth of the hole into each layer to be 0.152" from the top surface.

We must add that that units used here are imperial and not metric, to correspond with the industry standard in machining. Tools are available in a much larger selection. Drill radii can be as small as 1/64" to as large as 1". The closest hole size that could be drilled with readily available tools had a radius of 0.125" (1/4" diameter) as compared to 0.127" required for our holes. This corresponds to a 1.57% difference in the two values and was used in the fabrication. The triangular lattice constant, \( a \) was found to be 0.3062" and the depth of the holes to be drilled partially into each layer was calculated to be 0.152" from the top surface. Note that the parameters \( a \) and \( h \) only depend on the value of \( a_{\text{FCC}} \) (and in turn the thickness, \( d \)) and are not affected by \( r \).
3.2 Fabrication

Each layer of this structure can be manufactured by drilling two sets of holes into the high dielectric sheet (see Figure 2.15). The first set of holes is drilled completely through the layer while the second set of holes is drilled to a depth of 0.152". A fully automated CNC milling machine is necessary as this level of accuracy cannot be reached by hand. A HAAS® CNC milling machine is used for this task and was kindly provided by the Casa Loma campus of George Brown College. The Mechanical Engineering Technology program coordinator John Camarda and student Riccardo De Rosa aided in the fabrication process and their assistance is greatly appreciated. Figure 3.2 shows the CNC mill used.

![CNC Mill](image)

Figure 3.2: (a): The HAAS Mill used for fabricating the structure. (b): Close-up of the control panel. The commands are displayed on screen with the current operation highlighted

The HiK material came in large 12"×12" sheets so they were cut into four smaller 6"×6" sheets for ease of fabrication and to allow for manufacturing more layers. Since the three layers are very similar in nature and differ only by a transposition of the lattice, the top left corner of each sheet was chosen to be the reference point. The three layers were designed in Mastercam®, a computer aided machining (CAM) software. This software is capable of keeping track of the
location of each hole, the tool needed for the drilling operation, and the depth to which the hole must be drilled. Figure 3.3 shows a screen capture of Mastercam with one of the layers designed. Once this design was completed in Mastercam, it was converted into a format called G-code that was transferred to the CNC milling machine. The tool used for this drilling operation was a 1/4" diameter high strength steel (HSS) end mill.

Figure 3.3: Screen capture of Mastercam showing the design of one of the layers

3.2.1 Fabrication of the 3DPC

The fabrication process proved to be much more difficult than expected. The biggest problem was the nature of the ECCOSTOCK HiK material. The material was very fragile and highly susceptible to fracturing and cracking. In machining, the standard method of securing the plate while drilling is by the use of a vice to clamp the top and bottom edges of the plate. In this case however, the force exerted by the clamp caused the plate to stress and ultimately crack during the course of drilling the holes. To rectify this issue, the tool used to drill was changed to a 90° carbide end mill as seen in Figure 3.4.
Furthermore, a fixture to hold the plate and clamp it in place from the top was made. The fixture was designed so that the top left corner of every plate was always at the same position since this was chosen as the reference point. Initially, the holding fixture was made of plastic but issues with the fixture deforming were encountered so the fixture was remade using aluminum. Figure 3.5 shows the fixture used.

**Figure 3.4: Carbide end mill with a 90° tip used to drill the 0.250” diameter holes**

**Figure 3.5:** (a) The base of the aluminum fixture used while drilling into the plates. The top left corner of every plate is located at the same position and is used as the reference point. (b): A white plastic frame is used to hold the dielectric sheet in place by clamping the sheet down from above with screws.
Figure 3.6 shows the fixture in use while the part was being machined. This use of the new tool along with the fixture yielded better results but the machining was still not successful as the plates still cracked.

Figure 3.6: Clamping fixture in use. A: The table-top vice. B: The aluminum fixture. C: The white plastic clamping frame.

Examples of the unsuccessful attempts are shown in Figure 3.7.

Figure 3.7: Unsuccessful attempts at manufacturing a layer of the 3DPC
Drilling the first set of holes (those that went all the way through the sheet, see Figure 2.15) did not cause any issues. Drilling the second set of holes (those of partial depth, also see Figure 2.15) was the cause of the cracking. The cracking could not be attributed to clamping but instead to the nature of drilling. When the second set of holes was being drilled, the center of the bit was always drilling into material while the outer edge of the bit was drilling into a combination of air (from the first set of holes) and dielectric material. As a result, all of the force exerted by the bit was concentrated onto a smaller area thus cracking the plate.

The only solution to this problem was to reduce the size of the second set of holes. A 1/8” diameter end mill (HSS with a flat tip) was used and the entire drilling process was completed without any problems. The effect of this geometry is discussed in detail in Section 3.3. In total nine plates were machined (3 of layer A, 3 of layer B, and 3 of layer C) providing three periods of the 3DPC. The unit cell of this structure is shown in Figure 3.8.

![Figure 3.8: Unit cell of the modified 3DPC structure. (a) Top view. (b) Oblique view. The hole of partial depth is smaller than the hole penetrating the layer.](image)
The final step was to make a fixture to hold all the layers together with precise alignment so that the experiments could be carried out. It was made out of plastic and can be seen in Figure 3.9. The large shoulder bolts seen in Figure 3.9c are used to align the top and left edges of the plates. When the experiments were performed, these bolts were removed and the structure was held together by the four screws in the corners. Figure 3.9 shows the fixture with the PC secured.

![Figure 3.9: Holder made for the 3DPC. (a) Oblique view showing the top and side of the fixture. (b) Front view of the fixture. (c) A different perspective of the fixture. The three large shoulder bolts align the layers.](image)

Figure 3.10 shows more clearly how the alignment of the layers was achieved. The layers are placed one at a time such that the top edge is pressed against the two shoulder bolts at the top while the left edge is firmly pressed against the shoulder bolt on the left. This ensures that the layers are aligned and unable to be rotated out of place.
Figure 3.10: Alignment of the layers occurs by having the edges pressed up against the two shoulder bolts at the top and one on the left.

3.3 Geometry Change and Effects

Prior to machining all the plates, the change in drill bit from 1/4" to 1/8" diameter was simulated and it was found that a full bandgap existed. The result of this simulation is seen in Figure 3.11. It is important to note that a change in drill bit size also introduces a change in the geometry of the unit cell as seen by comparing Figure 2.16 and Figure 3.8. A side by side comparison of the two geometries for a given layer can be seen in Figure 3.12.
Figure 3.11: Band diagram of the structure after the proposed geometry modification. A full bandgap still exists, although smaller.

Figure 3.12: This figure shows the effect of the change in geometry for a single layer. The left half is the original geometry while the right half is the modified geometry. The "stand-outs" no longer look like hexagons but more like a Y.
Close-up pictures of the actual structure can be seen in Figure 3.13. The new geometry is clearly visible.

![Close-up pictures of the actual structure](image)

**Figure 3.13**: Close up of the machined layer where the geometry modification is clearly visible. (a) Top view showing the layers below. The center of the large hole coincides with the center of the small hole in the layer below. (b) Oblique view of the Y stand-outs.

### 3.4 Details of Machining Process

Obtaining the correct machining settings was not a simple task and was another source of difficulty during the fabrication process. There were two important factors needed to be considered. The first was the spindle revolutions per minute (RPM), the speed at which the tool rotates to cut into the material. Speeds that are too slow or too fast cause cracking in the plate as the tool cannot drill effectively. The second factor is the *feed rate*, the rate at which the tool moves while drilling. It is specified as the number of inches the tool moves downward in a minute. Feeding too slowly causes the process to take an extremely long time to finish and feeding too quickly causes the plate to crack as the material cannot be removed fast enough.

For the first set of holes, the spindle was set to 1000 RPM and the feed rate was 1.0 with the 1/4" carbide end mill. For the second set of holes, the spindle RPM was kept the same while the feed rate was increased to 1.5. These settings provided the best results for machining the plates.
4 Experimental Procedure and Results

This chapter discusses the experimental setup and procedure used to test the fabricated three-dimensional photonic crystal (3DPC) and the results of these tests. To experimentally demonstrate the existence of a bandgap in the 3DPC, it would be easiest to demonstrate a gap in the transmission measurements ($S_{21}$) for several angles of incidence and orientations for our 3DPC.

Once the measurements on the 3DPC were finished, sheet defects were introduced into our structure and again the transmission characteristics were measured for varied orientations and angles of incidence. Details of the setup and procedure are provided next.

4.1 Experimental Setup and Procedure

The experimental setup included the use of two identical horn antennas, two collimating lenses, a rotating platform, network analyzer, cables, and a straight track. The antennas, lenses, and rotating platform were positioned on the track as shown in Figure 4.1.

Figure 4.1: Experimental setup used. 1 - Horn antenna, 2 - Collimating lens, 3 – 3DPC placed on top of a rotating platform, 4 - HP8722C Network Analyzer, 5 - Track.
The 3DPC was positioned on the rotating platform and was aligned to be centered with the lenses and antennas. The platform was marked to indicate this position, and all measurements were taken with the 3DPC located at that spot. Furthermore, the platform had markings on it for the different angles of rotation required for the experiments as seen in Figure 4.2.

![Figure 4.2: Figure showing the rotating platform. (a) The rotating platform showing the markings for different angles. The red circles are the corners of the fixture ensuring that the 3DPC is always located at the same spot. (b) The 3DPC positioned on the rotating platform.](image)

The PC was designed to have a gap in the 10 GHz – 15 GHz range. Thus, antennas operating between these frequencies were needed for our experiment. The only antennas available were specified between 8 GHz – 12 GHz and 12 GHz – 18 GHz. The latter pair was used in the experiments.

The experiments were performed with 3DPC on the rotating platform upright and at normal incidence to the antennas. $S_{21}$ was measured using the HP8722C network analyzer. The platform was then rotated either 10° or 15° and $S_{21}$ was measured again. This process was continued until an incidence angle of 45°. The 3DPC was then oriented sideways and the measurement procedure was repeated. In Figure 3.9b, the 3DPC is seen in upright orientation. Sideways orientation is achieved by rotating the 3DPC 90° counter clock wise.

The network analyzer was set to operate at a center frequency of 12.5 GHz and a span of 5 GHz. It was calibrated using the thru-reflect-line (TRL) method. Calibration is a three step process. First, one antenna transmits through free space and the other antenna receives (thru). A metallic
plate is inserted between the antennas and the antennas take turns transmitting and measures the reflection off the plate (reflect). Finally, a short delay is added between the antennas (usually a quarter wavelength delay), and transmission is measured again (line).

The position of the antennas, lenses, and 3DPC is calculated by making use of Gaussian beam design principles as described in [20]. The distance from the horn antenna aperture to the front face of the lens is 15 cm, while the distance from the opposite face of the lens to the sample is 30 cm. The beam waist at the sample is 2.7 cm and the Rayleigh range at the sample is 11.7 cm.

### 4.2 Experimental Results

The 3DPC was positioned upright and transmission was measured for various angles of incidence. The result is shown in Figure 4.3. The results for the 3DPC positioned sideways are shown in Figure 4.4.

![Graph](attachment:image.png)

**Figure 4.3:** Transmission plot for 3DPC oriented upright without any defects for multiple angles of incidence. There is a clear overlap of the bandgaps centered at 12.5 GHz.
Figure 4.4: Transmission plot for 3DPC oriented sideways for multiple angles of incidence.

In both cases there is an overlap of the bandgaps for the different incident angles and orientations. Given the size of our sample with relation to the beam width, incidence angles over 45° caused the edges of the plate to interfere severely with the beam and made the results unusable, as seen in Figure 4.5.

Figure 4.5: Figure showing the relationship between the beam and angle of incidence. (a) Normal incidence: The beam is completely focused on the sample. (b) 45° incidence: Due to the smaller cross section of the 3DPC, the beam interacts with the edges of the 3DPC.
Increasing sample size would allow for higher angles of incidence to be measured accurately. Unfortunately, it was not feasible due to machining, time, and cost constraints. As such only measurements up to 45° are shown.

**Figure 4.6: Intensity plot showing the bandgap in the 3DPC structure with the 3DPC oriented upright.**

Figure 4.6 and Figure 4.7 show an intensity plot of the bandgap of our 3DPC structure with the 3DPC oriented upright and sideways respectively. Here, the shift in gap to higher frequencies is much clearer with the increase in the angle of incidence. The yellow shading in the plots represents transmission near -10 dB and can be considered to be the edges of the bandgap. The bandgap exists between 11.6 GHz – 13.5 GHz for upright orientation and 11.4 GHz – 13.5 GHz for sideways orientation. The center of the gap is nearly 12.5 GHz in both cases. In the upright case, the percent bandwidth is calculated to be 15.2%, and in the sideways case it is 16.8%. 
Figure 4.7: Intensity plot showing the bandgap in the 3DPC structure with the 3DPC oriented sideways. Angles of incidence range from 0° - 45°.

The band diagram in 3.11 shows a bandgap spanning 12 GHz – 13 GHz. The difference here is due to the criteria MPB uses to qualify a bandgap, and is slightly different than how we have characterized it. However, the important point to note is that in both situations, the bandgap is centered at 12.5 GHz.

To further ensure that these experimental results have merit, an HFSS simulation was run for normal incidence for both upright and sideways orientations and the comparison can be seen in Figure 4.8 and Figure 4.9. The simulated data and the experimental data match well for normal incidence. In Figure 4.8, there is a shift in frequency between the simulated and experimental result. This can be due to a few factors such as the imperfections in fabrication and losses not being modeled.

For non-normal incidence, the method outlined by Remsky in [25] and discussed in detail in Section 2.3 was unsuccessful due to the complexity of the 3DPC structure. In order to achieve good accuracy, the number of mesh points created by HFSS was extremely large and the simulation was unable to be completed with the processing power available.
Figure 4.8: Comparison between HFSS simulation and experimental data for upright orientation at normal incidence

Figure 4.9: Comparison between HFSS simulation and experimental data for sideways orientation at normal incidence
4.3 Introduction of Defects

The next step was to introduce two different sheet defects into the 3DPC structure and observe the behavior. The defects were the same size as a single layer of the 3DPC (6"×6"×0.25") and one had a dielectric constant of 1 (Styrofoam) while the other had a dielectric constant of 12 (ECCOSTOCK HiK sheet without the holes). These defects were introduced at various locations in the layered stack and the results show that the position of the defect affects the measured S-parameters quite noticeably. The layers were numbered from 1-9 as seen in Figure 4.10 and the defects either replaced an entire layer or were added between two existing layers.

![Image](image.jpg)

**Figure 4.10:** The layers are numbered 1-9 with 1 being the "top" or "front" of the stack.

The first defect measurement took place with the Styrofoam added in between layers 3 and 4. The results are shown in Figure 4.11 and Figure 4.12 for the two orientations. Comparing them to the results in Figure 4.3 and Figure 4.4, it is evident that the size of the gap is reduced. Furthermore, the gap has shifted to higher frequencies and this shift is more pronounced for higher angles of incidence. The introduction of a localized state can be seen as a peak in the transmission near the near the 11.7 GHz mark (for normal incidence) and increases in frequency with the increase in incidence.
Figure 4.11: Transmission plot for 3DPC with Styrofoam defect added between layers 3 and 4 for upright orientation.

Figure 4.12: Transmission plot for 3DPC with Styrofoam defect added between layers 3 and 4 for sideways orientation.
It is important to note that with this added layer of Styrofoam, the thickness of our 3DPC has increased causing the transmission for 45° incidence to be noticeably affected by the edges and thus is not shown here.

When the layer at position 2 is replaced by Styrofoam, the left half of the bandgap seems to shrink in size. The size of the gap below -10dB transmission is now approximately 3 GHz while previously without any defects this value was closer to 3.5 GHz. This represents a loss of about 14% and is true for both orientations and is seen in Figure 4.13 and Figure 4.14.

![Transmission plot for 3DPC with Styrofoam defect replacing the layer at position 2 for upright orientation.](image)

**Figure 4.13:** Transmission plot for 3DPC with Styrofoam defect replacing the layer at position 2 for upright orientation.
Figure 4.14: Transmission plot for 3DPC with Styrofoam defect replacing the layer at position 2 for sideways orientation.

Inserting a Styrofoam layer between positions 6 and 7 provided almost identical results to those obtained by inserting the Styrofoam defect between 3 and 4 as seen in Figure 4.15 and Figure 4.16.
Figure 4.15: Transmission plot for 3DPC with Styrofoam defect inserted between position 6 and 7 for upright orientation

Figure 4.16: Transmission plot for 3DPC with Styrofoam defected inserted between position 6 and 7 for sideways orientation
Next, the layer at position 5 was replaced by the Styrofoam defect. The localized state is clearly visible and the transmission peak is 0 dB for both orientations at normal incidence as seen in Figure 4.17 and Figure 4.18. The symmetry in the location of the defect seems to be the reason for such a prominent localized mode when compared to the other cases. A comparison with HFSS at normal incidence for sideways orientation is shown in Figure 4.19. We notice that the curves are slightly offset in frequency, and this may be attributed to the imperfections in machining.

**Figure 4.17**: Transmission plot for 3DPC with Styrofoam defect replacing the layer at position 5 for upright orientation
Figure 4.18: Transmission plot for 3DPC with Styrofoam defect replacing the layer at position 5 for sideways orientation

Figure 4.19: Comparison between HFSS and Experiment at normal incidence for sideways orientation for the styrofoam defect replacing the layer at position 5.
The second defect (dielectric 12) is now used to replace the layer at position 5 to see how it affects the transmission. The results are shown in Figure 4.20 and Figure 4.21. Two prominent differences can be seen immediately. There is no localized mode and the bandgap has shrunk. This can be attributed to the lack of a dielectric contrast between the 3DPC and the defect.

Figure 4.20: Transmission plot for 3DPC with dielectric 12 defect replacing the layer at position 5 for upright orientation
Figure 4.21: Transmission plot for 3DPC with dielectric 12 defect replacing the layer at position 5 for sideways orientation

4.4 Possible Improvements to Experiments

Although good experimental results were obtained, there are still a few areas of improvement for the future. The first problem is that of sample size vs. beam size. If larger samples were available, results for higher angles of incidence would be obtained. This would significantly reduce the leakage of the incident wave from the side of the structure for higher angles of incidence. However, this would increase the cost of manufacturing the 3DPC both in terms of time and money. Each layer took about 3.5 hours of total machining time assuming all the setup was done beforehand. The edges were not machined down to the correct size for fear of damaging the plate. Perhaps doing so may have produced more consistent results for higher angles of incidence.

The results presented here have not been corrected for the presence of the fixture and a future improvement would be to use more advanced calibration techniques to remove the effect of the
fixture. This is more of a problem for higher angles of incidence, something that was not a significant issue here.

Another area that benefits from improvement is the choice in materials. There were many issues with machining the ECCOSTOCK HiK and despite the best possible efforts noticeable imperfections in the layers were present. A slightly softer material with a high dielectric would have greatly improved the speed and quality of the machining process. Unfortunately such materials were not easily available for this task.
5 Conclusion

In this work, photonic crystal (PC) structures were investigated in order to obtain a full three-dimensional (3D) bandgap. A quasi-3DPC multi-layer structure which was the result of the amalgamation of a Bragg reflector and a triangular lattice of air holes in a high dielectric medium was studied in detail. The concept was for the Bragg reflector to provide a 1D bandgap for transmission along the z-direction, while the triangular lattice of air holes would provide a 2D bandgap for transmission in the x-y plane. While there was overlap between the 1D and 2D bandgaps, a full 3D bandgap was non-existent.

A 3DPC structure proposed by Joannopoulos in [27] consisting of 3 layers and yielding an FCC lattice demonstrated a full 3D bandgap. A prototype of this structure was build using ECCOSTOCK HiK high dielectric material ($\varepsilon = 12$) in order to experimentally demonstrate the existence of a bandgap. However, fabricating the structure based on the original design was very difficult as the material was not easy to machine and posed many challenges. The original design was modified in order to machine it and the band diagram for the modified structure showed the existence of a full 3D bandgap.

Experiments on the machined 3DPC were performed with the use of two horn antennas, two collimating lenses, a rotating platform, a track, and a network analyzer. The analyzer was calibrated using the thru-reflect-line (TRL) method and transmission ($S_{21}$) was measured. The angle of incidence was changed by rotating the PC on the rotating platform and measurements up to 45° were obtained. The results showed the existence of a bandgap centered at 12.5 GHz and spanning 2 GHz. The measurements were taken for two different orientations of the PC.

Two types of planar defects were introduced into the structure, either replacing a single layer or inserted between two existing layers. The defects used were made of Styrofoam (dielectric constant of 1) or an unmachined ECCOSTOCK HiK sheet. With the Styrofoam defect, localized states would appear and were visible in the form of a peak in transmission ($S_{21}$). The location of the Styrofoam defect had an impact on how pronounced this localized state was. The Styrofoam defect replacing the middle layer of our 3DPC produced the most prominent localized state due to the symmetry of the resulting structure. On the other hand, the high dielectric defect produced
no localized state due to the lack of sufficient contrast between the PC and the defect. The effect of the high dielectric defect was the reduction in size of the bandgap.

5.1 Future Work

The results of these experiments are promising as they have shown that 3DPC structures can be manufactured for use in microwave applications. Possible work for the future may include using this structure as an antenna background for applications in point-to-point communications. The idea here might be to have all the backward radiated power from the antenna reflected by the 3DPC in the direction necessary.
References


