Electromagnetic Wave Scattering from a Two-Dimensional Periodic Array of Dielectric Cylinders with Applications to Photonic Crystals

by

Ma'kalon Em

B.S.E.E., Massachusetts Institute of Technology
June 1997

Submitted to the Department of Electrical Engineering and Computer Science in Partial Fulfillment of the Requirement for the Degree of

Master of Engineering

at the

Massachusetts Institute of Technology

September 1997

© Massachusetts Institute of Technology 1997
All rights reserved

Signature of Author

Department of Electrical Engineering and Computer Science
September 1997

Certified by

Professor Jin Au Kong
Thesis Supervisor
Professor of Electrical Engineering

Certified by

Dr. Kung Hau Ding
Thesis Supervisor
Research Scientist

Accepted by

Arthur C. Smith
Chairman, Departmental Committee on Graduate Students

OCT 29 1997
Electromagnetic Wave Scattering from a Two-Dimensional Periodic Array of Dielectric Cylinders with Applications to Photonic Crystals

by

Makkalon Em

Submitted to the Department of Electrical Engineering and Computer Science in Partial Fulfillment of the Requirement for the Degree of Master of Engineering

ABSTRACT

The focus of this thesis is on the simulation of electromagnetic wave propagation through two-dimensional photonic band gap structures. The structures being investigated are periodic array of circular dielectric cylinders. The cylinders are lossless with real permittivity and permeability. In the thesis, the finite-difference time-domain (FDTD) method is applied to calculate the transmission coefficients and the field spectra of electromagnetic waves from a finite two-dimensional array of cylinders and to obtain its photonic band gaps.

The FDTD method is reviewed in Chapter 2. A two-dimensional FDTD computer program with second order Mur absorbing boundary condition is developed for this study. In developing the computer simulation code, the total-field/scattered-field formulation is used to divide the field domain into the scattered-field domain and the total-field domain. A TM Gaussian incident field is used for studying the transmission spectra because of its wide frequency bandwidth. Furthermore, the Gaussian pulse plane wave is modulated so that it could be centered at various frequencies. Because the electromagnetic fields calculated in the FDTD algorithm is in time domain, signal processing algorithms based on Discrete Fourier Transform is introduced in Chapter 3 to obtain the electromagnetic fields in frequency domain.

The photonic band gaps are determined as a function of frequencies from the transmitted fields by either obtaining their spectra or transmission coefficients. The methodology used to obtain the transmitted fields for the band gap studies is presented. In particular, the transmitted fields are collected on a transmitted field plane transverse to the propagation direction of the incident field. The position of transmitted field plane is determined so that accurate FDTD results can be achieved. The minimum dimension of the total-field domain is also determined together with the dimension of the scattered-field domain.

Two different permittivities of cylinders are considered for the FDTD simulations. In the lower permittivity case, the contrast between the background, \( \varepsilon = \varepsilon_s \), and the scattering
objects, $\varepsilon_p = 4\varepsilon_o$, is smaller. In the higher permittivity case, the cylinder had permittivity $\varepsilon_p = 9\varepsilon_o$; the contrast between the background and the scattering objects is larger.

In the lower permittivity case, a $18 \times 9$ matrix of cylinders is simulated for the frequency range from $0 \text{ GHz}$ to $20 \text{ GHz}$. The transmission coefficients of the FDTD simulation results using 15 unit cells per wavelength are in good agreement with the results given in published literatures both in the magnitude of attenuation and the locations of the band gap centers.

For the higher permittivity case, the FDTD simulations are performed for two frequency ranges of $0 - 20 \text{ GHz}$ and $15 - 130 \text{ GHz}$. In the frequency range of $0 - 20 \text{ GHz}$, the photonic band structure is composed of a matrix of $18 \times 9$ cylinders. In the frequency range of $15 - 130 \text{ GHz}$, a matrix of $25 \times 7$ cylinders is used in the simulation. For both frequency ranges, it is found that excellent results are obtained when the simulations use 30 unit cells per wavelength comparing to those in the published literatures.

The sensitivity studies on the effect of the cylinder radius and lattice constant were performed on the photonic band structure consisting of a matrix of $18 \times 9$ cylinders with permittivity $\varepsilon_p = 4\varepsilon_o$. The deviations of radius or the lattice constant are assumed to be $\pm 5\%$ of the designed value. The transmitted field spectra of the deviated structures show the changes both in the magnitude and the locations of the band gaps.

The effect of the number of the cylinders on the band gaps is also studied. The number of cylinders along the transverse direction of the propagation is increased. The predicted magnitude of attenuation using a matrix of $36 \times 9$ cylinders has better agreement than using a smaller matrix of $18 \times 9$ cylinders compared to the results shown in the published literatures.

The defect modes with one or more cylinders removed from the matrix of $18 \times 9$ cylinders are studied for the photonic band structure with the permittivity $\varepsilon_p = 4\varepsilon_o$. In the studies, one cylinder, two non-adjacent cylinders, two adjacent cylinders, or three non-adjacent cylinders are removed from the middle of the matrix of cylinders. The results of defect mode studies show the localization of the resonant modes within one or more band gaps depending on the number of cylinders removed and the relative locations of the removed cylinders.

Thesis Supervisor: Professor Jin Au Kong
Title: Professor of Electrical Engineer

Thesis Supervisor: Dr. Kung Hau Ding
Title: Research Scientist
Acknowledgments

I would like to thank the following people:

Professor J.A. Kong for allowing me to do my thesis research in his group. His inspiring lectures excite many interests in electromagnetic wave researches.

Dr. K.H. Ding for his daily supervision of my research, for his mentoring, and for his patient when the results are not readily available.

Dr. Eric Yang for his maintenance of the computing facility.

Jerry Akerson, Chi On Ao, Sean Shih, Vincent Thomassier, Li-Fang Wang, and Yan Zhang. In one way or another, their wisdom and experience help me greatly. Special thanks to Jerry Akerson for his help on the finite-difference time-domain and his providing the FDTD computer programs.

Kit Wa-Lai, who passed away recently. Her smile and administrative works around the office will surely be missed by those who know her.

Last, I would like to thank all my friends at MIT who made life at MIT an enjoyable experience.
Contents

Acknowledgments .......................................................... 4

Table of Contents ......................................................... 5

List of Figures ............................................................ 8

1 Introduction ............................................................ 13

1.1 Background .................................................................. 13

1.2 Statement of the Problems .......................................... 16

1.3 Description of the Thesis............................................. 17

2 Finite-Difference Time-Domain Method .......................... 21

2.1 Maxwell's Equations in Two-Dimensions ..................... 22

2.2 FDTD Equations for the Two-Dimensional Yee Lattice ... 23

2.3 Total-Field/Scattered-Field Formulation ....................... 27
2.4 Stability of the Yee Algorithm ......................................................... 30

2.5 Second Order Mur Absorbing Boundary Condition .............................. 31

3 **Excitation Source and Signal Processing Algorithm** .......................... 35

3.1 Excitation Source .............................................................................. 35

3.2 Discrete Fourier Transform ............................................................... 36

3.3 Transmission Coefficient .................................................................. 38

4 **FDTD Numerical Simulation Results** .................................................. 43

4.1 FDTD Simulation Methodology ......................................................... 44

4.2 FDTD Simulation Results ................................................................. 46

4.2.1 FDTD Results for Lower Permittivity ........................................... 46

4.2.2 FDTD Results for Higher Permittivity .......................................... 48

(1) Frequency Range: 0 GHz to 20 GHz ................................................ 48

(2) Frequency Range: 15 GHz to 130 GHz ........................................... 51

5 **Sensitivity and Defect Studies on Band Gaps** .................................... 64

5.1 Sensitivity Studies on Radius and Lattice Constant ............................. 65

5.1.1 Effect of the Radius of Cylinder .................................................. 65

5.1.2 Effect of the Lattice Constant of Photonic Band Structure ............... 66

5.2 Effect of the Number of the Cylinders .............................................. 66
5.3 Defect Mode by Removing Cylinders ..............................................68

6 Summary and Future Work .............................................................87

Appendix: Stability Derivation for Three-Dimensional Cell .................92

References .......................................................................................97
List of Figures

1.1 One dimensional periodic structure of alternate permittivities $\varepsilon_1$ and $\varepsilon_2$. The periodicity is $P$. ................................................................. 19

1.2 Simulation problem space setup. The circles represent the cylindrical scatterers with radius $r$. The center-to-center distance between two adjacent cylinders is the lattice constant $d$ of the two-dimensional photonic band structure. The cylinders with permittivity $\varepsilon_p$ are located in a free space background of permittivity $\varepsilon_o$. The incident field is propagating from left to right. The transmitted field is collected along a plane perpendicular to the propagation direction. .............................................. 20

2.1 Two-dimensional Yee cell, TM polarization, and the sampling positions of the electric and magnetic fields. The cell is a square with $\Delta x = \Delta y = \Delta$. ......................... 33

2.2 The division of the computational domain into total-field region, and scattered-field region. The scattering objects are located within the total-field region. The absorbing boundary truncates the total computational domain................................................. 34

3.1 Incident Gaussian pulse vs. time steps with $\beta = 110, \Delta t = 1.17851$ ps second, and $f_o = 0$. The number of time steps is $n = 4096$. The pulse is centered at time step 265, and the pulse truncated width is 220 time steps.................................................... 39

3.2 Incident Gaussian pulse of Figure 3.1 in the frequency domain. The field spectrum is shown for the positive frequency. The spectrum is centered at $0 GHz$. .................. 40

3.3 Incident Gaussian pulse sinusoidally modulated with $f_o = 10 GHz$ vs. time steps with $\Delta t = 1.17851$ ps and $\beta = 110$. The pulse becomes a doublet which is centered at the time step equal to 265................................................................. 41

3.4 Incident Gaussian pulse of Figure 3.3 in the frequency domain. The field spectrum is centered at approximately $10 GHz$. .................................................. 42
4.1 Schematic diagram of the simulation problem space setup. The circles represent the cylindrical objects with radius $r$ and the lattice constant $d$. The cylinders with permittivity $\varepsilon_p$ are centered in the $y$-direction inside the total-field domain on a free space background of permittivity $\varepsilon_0$. The incident field is propagating in the $x$-direction and polarized in the $z$-direction. The transmitted field is collected along a plane perpendicular to the $x$-direction and parallel to the $y$-direction.

4.2 The field spectra vs. frequency. The square periodic photonic band structure consists of $18 \times 9$ cylinders with permittivity $\varepsilon_p = 4\varepsilon_0$, $\Delta = 0.5\ mm$, $\beta = 110$, and time steps $n = 2^{14}$ are used for the simulation. The Gaussian curve is for the incident wave spectrum. The transmitted field spectrum shows two band gaps centered at $7.5\ GHz$ and $14.5\ GHz$, respectively.

4.3 The transmission coefficient in dB determined from the spectra in Figure 4.2. The transmission coefficient shows the band gaps centered at $7.5\ GHz$ and $14.5\ GHz$ attenuated by $-30\ dB$ and $-40\ dB$, respectively.

4.4 The field spectra for the transmitted and incident waves. The square periodic photonic band structure consists of $18 \times 9$ cylinders with permittivity $\varepsilon_p = 9\varepsilon_0$, $\beta = 110$, $\Delta = 0.5\ mm$, and $n = 16384$ time steps are used for the simulation. The transmitted field spectrum shows three band gaps centered at $5\ GHz$, $10\ GHz$, and $14\ GHz$.

4.5 The transmission coefficient of the field spectra in Figure 4.4. The band gaps are centered at $5\ GHz$, $10\ GHz$, and $14\ GHz$ and attenuated respectively by $-40\ dB$, $-50\ dB$, and $-50\ dB$. The band gap centered at $15.5\ GHz$ is different from the expected gap obtained in [9, 11]. Also, there is an onset of sharp attenuation around $18\ GHz$.

4.6 The spectra for the transmitted and incident fields. The square periodic photonic band structure consists of $18 \times 9$ cylinders with $\varepsilon_p = 9\varepsilon_0$. The FDTD simulation parameters used are $\Delta = 0.25\ mm$, $\beta = 220$, and $n = 16384$ time steps. The Gaussian curve is the plot of the incident plane wave spectrum. The transmitted field spectrum shows the band gaps centered at $5.5\ GHz$, $10.5\ GHz$, and $14.5\ GHz$.

4.7 The transmission coefficient obtained from the field spectra in Figure 4.6. The band gaps centered at $5.5\ GHz$, $10.5\ GHz$, and $14.5\ GHz$ and attenuated respectively by $-37\ dB$, $-45\ dB$, and $-60\ dB$. The band gap at $16\ GHz$ is not as low as the band gap predicted in Figure 4.5. Also, the sharp attenuation around $18\ GHz$ disappeared.

4.8 The plot of spectra vs. frequency for a two-dimensional square lattice photonic band structure consisting of $25 \times 7$ cylindrical rods with $0.74\ mm$ in diameter and $1.87\ mm$ lattice constant. The FDTD simulation parameters used are $\Delta = 0.05\ mm$, $\beta = 200$, and $n = 2^{15}$ time steps. The band gap between $45\ GHz$ and $70\ GHz$ are evident. However, the expected band gap between $95\ GHz$ and $100\ GHz$ does not show clearly.
4.9 The transmission coefficient plot for the spectra in Figure 4.8. There are bumps around 4.5 GHz in the trough of the band gap. The band gap at 95 to 100 GHz is not clearly shown. The first band gap shows excellent agreement with References [5, 6, 8].

4.10 The field spectra for a two-dimensional square photonic band structure consisting of 25×7 cylindrical rods with 0.74 mm in diameter and 1.87 mm lattice constant. The unit cell dimension is Δ = 0.025 mm. The band gap at 95–100 GHz is more evident compared to Figure 4.8. This second band gap shows excellent agreement with Reference [5, 6, 8]. The total number of sample points in Figures 4.9 and 4.10 are half of the number of sample points in Figures 4.7 and 4.8.

4.11 The transmission coefficient obtained from the spectra in Figure 4.10. The attenuation at 45 to 70 GHz and 95 to 100 GHz are approximately

-50 dB and -30 dB, respectively.

5.1 The field spectra for the two-dimensional photonic band structure consisting of a matrix of 18×9 of cylinders. The permittivity of the cylinder is \( \varepsilon_p = 4\varepsilon_\text{o} \), and the lattice constant is \( d = 12.7 \text{ mm} \). The Gaussian curve is the incident field spectrum centered at 10 GHz. The dot, dot-dash, and solid curves are the spectra of the transmitted fields when the radius of cylinder is \( r = 4.8 \text{ mm} \), \( r = 4.56 \text{ mm} \), and \( r = 5.04 \text{ mm} \), respectively.

5.2 The plot of transmission coefficients obtained from Figure 5.1. The dot, dot-dash, and solid curves correspond to the transmission coefficients when the radius of cylinder is \( r = 4.8 \text{ mm} \), \( r = 4.56 \text{ mm} \), and \( r = 5.04 \text{ mm} \), respectively. When \( r = 4.56 \text{ mm} \), the band gaps are attenuated by -30 dB and -50 dB, and the centers of the band gaps shift by +0.5 GHz from the centers of the band gaps when \( r = 4.8 \text{ mm} \). When \( r = 5.04 \text{ mm} \), the band gaps are attenuated by -25 dB and -35 dB. The centers shift by -0.5 GHz from the centers of the band gaps when \( r = 4.8 \text{ mm} \).

5.3 The field spectra of a two-dimensional photonic band structure consisting of 18×9 cylinders. The permittivity of cylinder is \( \varepsilon_p = 4\varepsilon_\text{o} \), and the radius of cylinder is \( r = 4.8 \text{ mm} \). The dot, dot-dash, and solid curves correspond to the simulations when the lattice constant equals to \( d = 12.7 \text{ mm} \), \( d = 12.065 \text{ mm} \), and \( d = 13.335 \text{ mm} \), respectively.

5.4 The plot of transmission coefficients obtained from Figure 5.3. The dot, dot-dash, and solid curves correspond to the simulation when the lattice constant equals to \( d = 12.7 \text{ mm} \), \( d = 12.065 \text{ mm} \), and \( d = 13.335 \text{ mm} \), respectively. When \( d = 12.065 \text{ mm} \) the band gaps are attenuated by -25 dB and -35 dB. The centers of the band gaps shift by +0.5 GHz compared to the centers of the band gaps when \( d = 12.7 \text{ mm} \). When \( d = 13.335 \text{ mm} \) the band gaps are attenuated by -30 dB and -50 dB. The centers shift by -0.5 GHz compared to the centers when \( d = 12.7 \text{ mm} \).
5.5 The spectra for the transmitted and incident fields. The square periodic photonic band structure consists of $18 \times 9$ cylinders with $\varepsilon_p = 9 \varepsilon_n$. $\Delta = 0.5 \text{ mm}$, $\beta = 110$, and $n = 16384$ time steps are used for the simulation. The transmitted field spectrum shows three band gaps centered at $5\text{GHz}$, $10\text{GHz}$, and $14\text{GHz}$.................................74

5.6 The plot of transmission coefficients obtained from Figure 5.5. The band gaps centered at $5\text{GHz}$, $10\text{GHz}$, and $14\text{GHz}$ and are respectively attenuated by $-50 \text{ dB}$, $-60 \text{ dB}$, and $-60 \text{ dB}$. The magnitude of the transmission at $15.5 \text{GHz}$ is much lower than the results shown in References [9-11].................................................75

5.7 The spectra for the transmitted and incident fields. The square periodic photonic band structure consists of $36 \times 9$ cylinders with $\varepsilon_p = 9 \varepsilon_n$. Parameters $\Delta = 0.5 \text{ mm}$, $\beta = 110$, and $n = 16384$ time steps are used for the simulation. The transmitted field spectrum shows three band gaps centered at $5\text{GHz}$, $10\text{GHz}$, and $14\text{GHz}$.............76

5.8 The plot of transmission coefficients obtained from the field spectra in Figure 5.7. Three band gaps centered at $5\text{GHz}$, $10\text{GHz}$, and $14\text{GHz}$ and are respectively attenuated by $-50 \text{ dB}$, $-58 \text{ dB}$, and $-55 \text{ dB}$. The small band gap centered at $15.5 \text{GHz}$ is now attenuated by $-40 \text{ dB}$ and compared well to References [9-11].................................77

5.9 The configuration for defect mode studies. One or more cylinders with the coordinate specified by $(\text{column}, \text{row})$ are removed from the matrix. The incident field propagates from right to left and normal to column of cylinders.................................78

5.10 The plot of the transmitted field spectra for the defect mode when one cylinder at coordinate $(\text{column}, \text{row}) = (5, 9)$ is removed. The dot curve is the plot of the non-perturbed photonic band structure. The localizations of the resonance appear at $7.5 \text{GHz}$ and $15.5 \text{GHz}$ in the two band gaps........................................79

5.11 The plot of transmission coefficients of the defect mode when one cylinder at coordinate $(\text{column}, \text{row}) = (5, 9)$ is removed compared to the non-perturbed photonic band structure. The dot curve is the plot of the non-perturbed photonic band structure. The attenuations at the resonant frequencies of $7.5 \text{GHz}$ and $15.5 \text{GHz}$ are very small.........................................................80

5.12 The transmitted field spectrum of the defect mode when two non adjacent cylinders at coordinates $(\text{column}, \text{row}) = (5, 9)$ and $(\text{column}, \text{row}) = (5, 11)$ are removed. The dot curve is the plot of the non-perturbed photonic band structure. The localizations of the resonance appear $7.5 \text{GHz}$ and $15.5 \text{GHz}$ in the two band gaps. The resonances are very similar to the one defect mode..........................................81

5.13 The plot of transmission coefficients of the defect mode when two cylinders at coordinates $(\text{column}, \text{row}) = (5, 9)$ and $(\text{column}, \text{row}) = (5, 11)$ are removed. The dot curve is the plot of the non-perturbed photonic band structure. The attenuation at $15.5 \text{GHz}$ is large compared to one defect mode.........................................82

11
5.14 The transmitted field spectrum of the defect mode when two adjacent cylinders at coordinates \((\text{column, row}) = (5, 9)\) and \((\text{column, row}) = (4, 10)\) are removed. The localization of the resonance appears at 14.75 GHz in the second band gap. The resonance at the first band gap does not show clearly. 83

5.15 The plot of transmission coefficients of the defect mode compared to the non-perturbed photonic band structure. The removed cylinders are adjacent to each other and are located at \((\text{column, row}) = (5, 9)\) and \((\text{column, row}) = (4, 10)\). The resonance is localized at 14.75 GHz in the second band gap and is attenuated by \(-5\ dB\). The resonance at the first band gap does not show clearly. 84

5.16 The transmitted field spectrum of the defect mode when three non-adjacent cylinders at coordinates \((\text{column, row}) = (4, 2)\), \((\text{column, row}) = (5, 10)\), and \((\text{column, row}) = (5, 16)\) are removed. There is a resonance at 14.75 GHz in the second band gap. The resonance in the first band gap does not show clearly. 85

5.17 The plot of transmission coefficients when three non-adjacent cylinders at \((\text{column, row}) = (4, 2)\), \((\text{column, row}) = (5, 10)\), and \((\text{column, row}) = (5, 16)\) are removed. The attenuation of the resonance at 14.75 GHz in the second band gap is approximately \(-7\ dB\) 86
Chapter 1

Introduction

1.1 Background

The photonic crystals were first suggested and confirmed by Yablonovitch and colleagues [1-2]. The photonic crystals are made of arbitrarily shaped dielectric scatterers forming periodic lattice. Like electrons in atomic crystals, electromagnetic wave in a periodic dielectric structure exhibits frequency intervals over which propagation can not occur for any direction [1-2, 5-13]. In the conventional electronic band theory, behaviors of electrons are described by the Schrodinger equation. In contrast, in photonic band theory, Maxwell's equations with periodic dielectric functions are used to describe the behavior of electromagnetic waves. The periodicity of the dielectric structures can be one-, two-, or three-dimension. For example, one-dimensional photonic crystals are the well known multi-layers of dielectric slabs with alternate permittivities $\varepsilon_1$ and $\varepsilon_2$ (Figure 1.1). When the permittivities of the layers have large enough contrast, the photonic band gaps will exist [13].
The photonic band structure may have many practical scientific and engineering applications. For example, the photonic crystals promise to greatly improve the efficiency of the semiconductor laser devices [5, 11, 13, 17]. Using photonic band materials, one can fabricate dielectric wave guides and high-Q resonators for solid state laser devices [5, 11, 13, 17]. Currently, resonant cavities for integrated circuits are fabricated from high dielectric materials [13, 17]. The circuits are then shielded by metallic waveguides. Since the fields radiated from the cavities are attenuated with the inverse of distance, the conduction losses from the shielding can be appreciable. These losses can be avoidable if the cavities are embedded in the photonic band structures such that the field in the structures will attenuate exponentially [13, 17].

In the literature, the considered photonic band structures are usually infinite periodic dielectric structures. The analysis technique has been plane wave expansion of the wave equation and eigenvalue technique in solution [11-13, 17]. For the photonic band structures of finite extent, both experimental and numerical methods have been applied to study the band gaps. Various experiments have been conducted to study the band gaps at microwave frequency range [3-5, 10-11]. For instance, the coherent microwave transient spectroscopy (COMITS) experimental technique has been used in the studies of References [3-5]. This technique is based on the radiation and detection of picosecond-duration electromagnetic transients. COMITS consists of transmitting and receiving antenna elements. First, the reference wave form from the transmitter is detected and recorded at the receiver with no photonic crystal sample between the receiver and transmitter. Then the photonic crystals are placed in between the transmitting and the receiving antennas. The reference wave form is then incident on the photonic crystals. The complex transmission coefficient is obtained by dividing the Fourier transform of the received signal in the presence of the samples with the Fourier transform of the reference wave form in the absence of the samples. With the scatterers consisted of alumina-ceramic cylindrical rods of 0.74 mm in diameter and 100 mm in length, with permittivity $\varepsilon = 9\varepsilon_0$ and permeability...
\( \mu = \mu_0 \), Robertson and coworkers [5] spaced the center-to-center distance between two adjacent cylinders by 1.87 mm. Their photonic band gap structure has 7 rods deep in the direction of propagation and 25 rods transverse to the propagation direction. They observed the band gaps for both TE (polarization perpendicular to the axis of the cylinder) and TM (polarization parallel to the axis of the cylinder) cases. For the TM case, their experiment clearly showed the band gaps between 45 and 70 GHz. Also, there is a suggested gap at 100-125 GHz. For the TE case, the band gaps are between 60 and 70 GHz and between 95 to 125 GHz.

Another approach is based on using numerical methods to solve Maxwell's equations and to simulate the wave propagation through the photonic crystal structures. For example, Pendry and MacKannon [6-8] developed the transfer matrix method to compute the transmission and reflection coefficients. In the transfer matrix method, the periodic system is first subdivided into a number of parallel planes, and Maxwell's equations are discretized in the time domain. Proper approximation is then made to the propagation constants \( k_x \), \( k_y \), and \( k_z \) in terms of the lattice dimensions of the unit cell [6-8]. The discretized Maxwell's equations are then Fourier transformed to obtain similar equations in the frequency domain. A transfer matrix \( T \) relating fields on a previous plane of unit cells to fields on the next plane of unit cells is obtained as a result. This transfer matrix \( T \) is a function of permittivity, permeability, the position of the cells, and the lattice dimensions of a unit cell [6-8]. Generally, the unit cell is chosen to be cubic. In calculating the transmission and the reflection, the transfer matrices of the unit cells in the parallel plane are combined to form extended product [6-9, 11]. In practice, one notes that the numerical instability will be reached before all the transfer matrices can be multiplied. For this reason, the transfer matrix for the subsection of the structure is iteratively calculated as many times as possible before reaching instability. The strips are then stacked together using multiple scattering formula to calculate the transmission coefficient and the reflection coefficient [6-9, 11]. The transfer matrix method has been applied, using the photonic
band structure parameters in Reference [5], to predict the band gaps in Reference [6, 8]. The simulation results show good agreement with the experimental results [5-6, 8].

Other numerical techniques such as finite-difference time-domain (FDTD) [16, 18] and finite difference [19] method have also been applied to analyze the two-dimensional photonic crystals.

1.2 Statement of the Problems

The focus of this thesis is on the simulations of electromagnetic wave propagation through two-dimensional photonic band gap structures. The structures being investigated are periodic array of circular dielectric cylinders. The cylinders are lossless with real permittivity and permeability. The configuration for the simulations is illustrated in Figure 1.2 where \( d \) is the lattice constant, \( r \) is the radius of the cylinders, \( \varepsilon_p \) is the dielectric constant of the cylinders, and \( \varepsilon_o \) is the dielectric constant of the background. The lattice constant in Figure 1.2 is defined as the center-to-center distance between two adjacent cylinders. A square lattice is shown in Figure 1.2, the lattice constant is thus the same in both \( \hat{x} \) and \( \hat{y} \) directions. The permeability of the cylinders and the permeability of the free space are assumed to be the same in this study.

In the thesis, rather than using transfer matrix method, the finite-difference time-domain (FDTD) method is applied to solve Maxwell's equations when an electromagnetic wave propagates through a two-dimensional array of cylinders. The transmission spectrum is calculated from the transmitted signals to obtain its photonic band gaps. A two-dimensional FDTD computer program with second order Mur absorbing boundary condition is developed for this study. A Gaussian pulse plane wave modulated sinusoidally is used as an excitation source in the computer simulation. Signal processing algorithms based on Discrete Fourier Transform are implemented to obtain the photonic band gaps from the FDTD modeling. The simulation results from the FDTD model of photonic crystals will be presented for the structures studied by others using the transfer
matrix numerical method and the coherent microwave transient spectroscopy (COMITS) experiments. A parametric study is further performed in this thesis research to investigate the relationships between the band gaps and the photonic crystal parameters: the radius of the cylinders, the lattice constant, and the number of cylinders. The resonance for defect mode will also be studied for the structure in which one or more cylinders are removed from the array of cylinders.

1.3 Description of the Thesis

In this thesis, an analysis based on the FDTD technique is presented on the electromagnetic wave propagation through a two-dimensional photonic band structure of finite extent. A schematic diagram of the problem is shown in Figure 1.2. As shown in Figure 1.2, the photonic band structure consists of a matrix of cylinders of radius \( r \) and lattice constant \( d \). The incident field for the FDTD simulation is propagating from left to right with \( \vec{k}_{\text{inc}} = k \hat{x} \) and TM polarization. This incident electric field will be used for all the simulations presented in the thesis.

In Chapter 2, the two-dimensional FDTD algorithm is derived from Maxwell's equations for computer simulations. In developing the FDTD code, the computational domain is divided into the total-field and scattered-field regions, where the concept of computational space discretization is presented.

Chapter 3 discusses the properties of incident field in more detail. In particular, an incident field with wide frequency bandwidth is desirable for studying the transmission spectra. Therefore, a Gaussian pulse plane wave modulated sinusoidally is used as an excitation source in the computer simulation. Furthermore, since the FDTD method calculates the electromagnetic fields in the time domain, signal processing algorithms based on Discrete Fourier Transform is to be used to obtain the electromagnetic fields in the frequency domain from the electromagnetic fields in the time domain.
The transmitted fields will be calculated at the right end of the simulation problem space. The photonic band gaps are determined from the transmitted fields by either obtaining their spectra or transmission coefficients. Section 4.1 describes the methodology used in the simulations. The conditions for stable simulations are described here. Section 4.2 presents the transmission coefficient and spectrum results from the FDTD simulations for the two-dimensional photonic band structures with dielectric circular cylinders of lower and higher permittivities.

To study the relationship between the band gaps and the photonic band structures, sensitivity studies on the variation of the structure parameters are performed and presented in Chapter 5. These parameters include the radius of the cylinders, the lattice constant of the photonic band structure, and the fractional volume of cylinders. For the radius and lattice constant sensitivity studies, simulations are performed for the cylinders with ±5% deviation from the desired value. In the sensitivity study on the fractional volume, the number of cylinders in the transverse direction are increased so that the periodic system has larger extent. Chapter 5 concluded with the defect mode study when one or more cylinders are removed from the array of cylinders. The defect of missing cylinders is expected to produce resonant modes inside the band gaps.

Chapter 6 summarizes the FDTD results and suggested future works. One future work would be to apply periodic absorbing boundary to simulate the problem of photonic crystals. In such an attempt one can simulate more infinite-like periodic structures, compared to wavelength, without having to increase the dimension of the array of the cylinders.
Figure 1.1 One dimensional periodic structure of alternate permittivities $\varepsilon_1$ and $\varepsilon_2$. The periodicity is $P$. 
Figure 1.2 Simulation problem space setup. The circles represent the cylindrical scatterers with radius $r$. The center-to-center distance between two adjacent cylinders is the lattice constant $d$ of the two-dimensional photonic band structure. The cylinders with permittivity $\varepsilon_p$ are located in a free space background of permittivity $\varepsilon_\infty$. The incident field is propagating from left to right. The transmitted field is collected along a plane perpendicular to the propagation direction.
Chapter 2

Finite-Difference Time-Domain Method

The finite-difference time-domain (FDTD) method is a numerical technique in solving electromagnetic wave propagation and scattering problems using the discretized Maxwell's equations in the time domain. In this chapter, a brief description and formulation for the FDTD computation of two-dimensional electromagnetic wave scattering problems is presented. Section 2.2 describes the FDTD formulation for dielectric scattering materials. In particular, the two-dimensional time-marching equations for TM and TE waves are derived from Maxwell's equations. Section 2.3 describes the total-field/scattered-field formulation which is used to specify the computational domain. The dimension of the unit Yee cell and the time increment required for stable FDTD simulations are specified in Section 2.4. The second-order Mur absorbing boundary condition is presented in the last section of this chapter.
2.1 Maxwell's Equations in Two-Dimensions

Consider a source-free region where there is no electric charges or currents, Maxwell's curl equations are given by [21-22]

\[ \nabla \times \vec{E}(\vec{r}, t) = -\frac{\mu \partial \vec{H}(\vec{r}, t)}{\partial t} \]  
(2.1.1)

\[ \nabla \times \vec{H}(\vec{r}, t) = \frac{\varepsilon(\vec{r}) \partial \vec{E}(\vec{r}, t)}{\partial t} \]  
(2.1.2)

where \( \vec{E} \) is the electric field in volts per meter; \( \vec{H} \) is the magnetic field in amperes per meter; \( \mu \) is the magnetic permeability in Henrys per meter; and \( \varepsilon \) is the electric permittivity in Farads per meter.

In this thesis study, the electromagnetic field excitation and the photonic crystal lattice are assumed to have no variation in \( z \) direction. This assumption implies that all partial derivatives with respect to \( z \) equal to zero. Thus, the equations (2.1.1) and (2.1.2) decouple into the TM and TE polarizations. For TM polarization, \( E_z, H_x, \) and \( H_y \) are non-zero, and equations (2.1.1) and (2.1.2) reduce to [23, 27, 33]

\[ \frac{\partial H_x}{\partial t} = -\frac{1}{\mu} \left( \frac{\partial E_z}{\partial y} \right) \]  
(2.1.3)

\[ \frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_z}{\partial x} \right) \]  
(2.1.4)
\[
\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon} \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right) \quad (2.1.5)
\]

For TE polarization, the non-zero fields are \( E_x, \ E_y, \text{and} \ H_z \). Using duality [21-22], the equivalence of equations (2.1.3)-(2.1.5) is obtained:

\[
\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon} \left( \frac{\partial H_z}{\partial y} \right) \quad (2.1.6)
\]

\[
\frac{\partial E_y}{\partial t} = -\frac{1}{\varepsilon} \left( \frac{\partial H_z}{\partial x} \right) \quad (2.1.7)
\]

\[
\frac{\partial H_z}{\partial t} = -\frac{1}{\mu} \left( \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \right) \quad (2.1.8)
\]

It is noted that the TM and TE modes contain no common field components.

2.2 FDTD Equations for the Two-Dimensional Yee Lattice

The finite-difference time-domain (FDTD) method, initially reported by K. S. Yee in 1966 [42], has become a powerful numerical technique for solving Maxwell's equations. In Yee's algorithm, the electric and magnetic fields are discretized over cubic grids together with the finite difference approximation of the spatial derivatives \( \nabla = \hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y} + \hat{z} \frac{\partial}{\partial z} \) and the temporal derivatives (\( \partial t \)).

The partial derivatives are approximated using a central-difference scheme for second order accuracy [26]. In the central-difference technique, the derivative of a function \( f(\xi) \) at \( \xi_o \) is approximated as [26]
\[
\frac{\partial f(\xi)}{\partial \xi} \bigg|_{\xi = \xi_o} = \frac{f\left(\xi_o + \frac{\Delta \xi}{2}\right) - f\left(\xi_o - \frac{\Delta \xi}{2}\right)}{\Delta \xi} - \frac{(\Delta \xi)^2}{24} f^{(3)}(\xi_o)
\] (2.2.1)

where \( f^{(3)}(\xi_o) \) is the third derivative of \( f \) at \( \xi_o \). Retaining the leading order terms, the error associated with the central difference scheme is \( O\left((\Delta \xi)^2\right) \) [26].

Using Yee's notation [27, 35, 38], a discretized function \( F \) at the \( n-th \) time step and location \((i,j)\) is written as

\[
F^n(i,j) = F(i\Delta x, j\Delta y, n\Delta t)
\] (2.2.2)

where \( \Delta x \) and \( \Delta y \) are the cell dimensions and \( \Delta t \) is the time increment. In the FDTD, the computational domain is divided into unit cells. These discretized cells are called Yee cells. The dimensions of the cells are determined from the highest frequency of the desired field computation. Furthermore, the fields are spatially interleaved at half-space increments and are evaluated at alternate half-time steps. For the TM case, the interleave of the electric and magnetic fields in the Yee cell is shown in Figure 2.1.

There are three field components in the cell shown in Figure 2.1. The electric field \( E_z(i,j) \) is represented by a field orienting upward in the \( z \)-direction at the grid point \((i,j)\). The two components of the magnetic field \((H_x \text{ and } H_y)\) orthogonal to the electric field are located with their positions shift by one half-space increment in the Yee cell from the electric field's position. Thus, the magnetic fields are located at \((i-1/2,j),(i+1/2,j),(i,j-1/2), \text{ and } (i,j+1/2)\).

Applying equation (2.2.1) and the notation of (2.2.2), Maxwell's equations (2.1.3)-(2.1.8) can be casted in discretized form. For TM wave, we have Maxwell's equations in the FDTD form [26-27]:

24
\[
\frac{H_x^{n+1/2}(i,j) - H_x^{n-1/2}(i,j)}{\Delta t} = -\frac{1}{\mu} \left( \frac{E_x^n(i,j+1/2) - E_x^n(i,j-1/2)}{\Delta y} \right) \tag{2.2.3}
\]

\[
\frac{H_y^{n+1/2}(i,j) - H_y^{n-1/2}(i,j)}{\Delta t} = \frac{1}{\mu} \left( \frac{E_x^n(i+1/2,j) - E_x^n(i-1/2,j)}{\Delta x} \right) \tag{2.2.4}
\]

\[
\frac{E_z^{n+1}(i,j) - E_z^n(i,j)}{\Delta t} = \frac{1}{\varepsilon(i,j)} \left( \frac{H_y^{n+1/2}(i+1/2,j) - H_y^{n+1/2}(i-1/2,j)}{\Delta x} \right) \tag{2.2.5}
\]

\[
\frac{H_x^{n+1/2}(i,j) - H_x^{n+1/2}(i-1/2,j)}{\Delta y} \right) \tag{2.2.6}
\]

\[
\frac{E_y^{n+1}(i,j) - E_y^n(i,j)}{\Delta t} = \frac{1}{\varepsilon(i,j)} \left( \frac{H_z^{n+1/2}(i+1/2,j) - H_z^{n+1/2}(i-1/2,j)}{\Delta x} \right) \tag{2.2.7}
\]

\[
\frac{H_z^{n+1/2}(i,j) - H_z^{n-1/2}(i,j)}{\Delta t} = \frac{1}{\mu} \left( \frac{E_x^n(i+j+1/2) - E_x^n(i-j-1/2)}{\Delta y} \right) \tag{2.2.8}
\]
Rewriting equations (2.2.3)-(2.2.5) for TM wave, the time-advancing equations for the components of $E_z$, $H_x$, and $H_y$, are expressed as

$$E_z^{n+1}(i,j) = E_z^n(i,j) - \frac{H_x^{n+1/2}(i,j+1/2) - H_x^{n+1/2}(i,j-1/2)}{\Delta y \varepsilon(i,j)} \frac{\Delta t}{\varepsilon(i,j)} + \frac{H_y^{n+1/2}(i+1/2,j) - H_y^{n+1/2}(i-1/2,j)}{\Delta x \mu} \frac{\Delta t}{\mu} \tag{2.2.9}$$

$$H_x^{n+1/2}(i,j) = H_x^{n-1/2}(i,j) - \frac{E_z^n(i,j+1/2) - E_z^n(i,j-1/2)}{\Delta x \mu} \frac{\Delta t}{\mu} \tag{2.2.10}$$

$$H_y^{n+1/2}(i,j) = H_y^{n-1/2}(i,j) + \frac{E_z^n(i+1/2,j) - E_z^n(i-1/2,j)}{\Delta y \mu} \frac{\Delta t}{\mu} \tag{2.2.11}$$

Similar equations for the TE polarization are obtained from equations (2.2.6)-(2.2.8):

$$H_z^{n+1/2}(i,j) = H_z^{n-1/2}(i,j) + \frac{E_x^n(i,j+1/2) - E_x^n(i,j-1/2)}{\Delta y \mu} \frac{\Delta t}{\mu} - \frac{E_y^n(i+1/2,j) - E_y^n(i-1/2,j)}{\Delta x \mu} \frac{\Delta t}{\mu} \tag{2.2.12}$$

$$E_x^{n+1}(i,j) = E_x^n(i,j) + \frac{H_z^{n+1/2}(i,j+1/2) - H_z^{n+1/2}(i,j-1/2)}{\Delta y \varepsilon(i,j)} \frac{\Delta t}{\varepsilon(i,j)} \tag{2.2.13}$$
\[ E_y^{n+1}(i,j) = E_y^n(i,j) + \frac{H_z^{n+1/2}(i+1/2,j) - H_z^{n+1/2}(i-1/2,j)}{\Delta x} \frac{\Delta t}{\varepsilon(i,j)} \] (2.2.14)

At each cell, as shown in Figure 2.1, the updated electric field at the time step \( n + 1 \) is calculated from the electric field at the time step \( n \) and the magnetic field at the time step \( n + \frac{1}{2} \). Similarly, the magnetic field at the time step \( n + \frac{1}{2} \) is obtained from the electric field at the time step \( n \) and the magnetic field at the time step \( n - \frac{1}{2} \).

For the simulation, the computer program is implemented by defining the constant terms \( \Delta t/(\Delta y \cdot \varepsilon(i,j)) \), \( \Delta t/(\Delta x \cdot \varepsilon(i,j)) \), \( \Delta t/(\Delta y \cdot \mu) \), and \( \Delta t/(\Delta x \cdot \mu) \) in equations (2.2.9)-(2.2.14) so that these constants can be used repeatedly without having to redefine their values [26-27].

### 2.3 Total-Field/Scattered-Field Formulation

The computational domain for solving Maxwell's equations using FDTD must be truncated due to finite computer memory. A rectangular boundary is generally used to enclose the computational domain for the FDTD simulations. The electric and magnetic fields are specified in the computational domain. In this study, the total-field/scattered-field formulation [26-27, 30, 36] is adopted to specify the regions of the fields.

Figure 2.2 illustrates the FDTD total computational domain where it is divided into two regions of the total-field and the scattered-field. The total-field region is centered in the inner region of the computational domain. The scattering objects are located in the total-field region. The electric and magnetic fields in the total-field region include the incident wave as well as the scattered wave. These scattered fields arise from the interaction between the incident fields and the scattering objects. The interaction must satisfy Maxwell's equations and the boundary conditions where the tangential electric and magnetic fields are continuous at the interface of different materials. Here, it is assumed
that the incident electric and magnetic fields are known at all elementary cells and at all time steps, and the FDTD algorithm operates on the total field components [26-27]. The outer zone of the computational domain is denoted as the scattered-field region. Here, it is assumed that there is no incident wave. Thus, the fields in the scattered-region are the total fields minus the incident fields, and the FDTD algorithm operates on the scattered fields only. The outer boundary truncates the computational domain, and a desired type of absorbing boundary condition must be specified. The second order Mur absorbing boundary condition, which is used in this thesis, will be discussed in Section 2.5 of this chapter.

The total-field and scattered-field regions are separated by a virtual interface which relates the total fields and the scattered fields. In particular, the equations governing the fields in the total-field region is different from the equations governing the fields in the scattered-field region. However, these fields have to be specified such that they are consistent from the total-field region to the scattered-field region when the spatial difference is taken across this interface. Taflove has solved the problem of consistency, and in his book [26] he gives the corrections needed to be made to the fields in the scattered-field and total-field regions for one-, two-, and three-dimensional cases.

For example, consider the corrections needed to be made on equation (2.2.9) at the interface with \( j = j_o \) of Figure 2.1. The consistency is achieved by modifying \( E_z \) to be [23]

\[
E_{z,\text{tot}}^{n+1}(i, j_o) = E_{z,\text{tot}}^n(i, j_o) - \frac{H_{x,\text{tot}}^{n+1/2}(i, j_o + 1/2) - H_{x,\text{tot}}^{n+1/2}(i, j_o - 1/2)}{\Delta y} \cdot \frac{\Delta t}{\varepsilon(i, j_o)} \\
+ \frac{H_{y,\text{tot}}^{n+1/2}(i + 1/2, j_o) - H_{y,\text{tot}}^{n+1/2}(i - 1/2, j_o)}{\Delta x} \cdot \frac{\Delta t}{\varepsilon(i, j_o)} \\
+ \frac{\Delta t}{\Delta x \varepsilon(i, j_o)} H_{x,\text{inc}}^{n+1/2}(i, j_o - 1/2)
\]

(2.3.1)
where "tot" denotes the field in the total-field region, "scat" denotes the field in the scattered-field region, and "inc" denotes the incident field.

Several advantages in using the total-field/scattered-field formulation in the FDTD simulation have been noted in [26-27, 30, 36]. One advantage is that we are able to arbitrarily specify the incident field in the total-field region. The incident field of any form and duration can be applied at any incidence angle and polarization. Furthermore, the total-field formulation is advantageous when the total field is very small. For example, let's consider a special case of a strong scattered field which almost cancels the incident field. Thus, the summation of the incident field and scattered field is very small. The calculation of the scattered field is expected to bear some numerical error due to the approximation made in the FDTD formulation. If the scattered field is added to the incident field to find the total field, the small numerical error will be carried over and contributes a significant error in the total field value because the total field is very small in this case. Instead, if the total field is calculated directly, the numerical error caused by the FDTD approximation will be smaller compared to the scattered field formulation. In addition, using the total-field/scattered-field formulation, the simulation can be run for much longer time steps [26]. The reason is that it allows the simulation of the absorbing boundary conditions by extending the lattice to infinity in the scattered-field region, and the reflections at the truncation boundary are small.
2.4 Stability of the Yee Algorithm

In the Yee's algorithm, the time step $\Delta t$ required for a stable simulation is determined by the dimensions of a unit cell since, for any given time step, a wave can pass through only a single Yee cell. In the FDTD method, the wave propagates with a numerical phase velocity less than the speed of light in free space. Thus, the size of an unit cell is generally chosen to be much less than a wavelength to minimize the phase error. Also, the time step must be bounded for a stable algorithm [26-31]. The limit is set by the Courant stability criterion as, for a two-dimensional case,

$$
c\Delta t \leq \frac{1}{\sqrt{\left(\frac{1}{\Delta x}\right)^2 + \left(\frac{1}{\Delta y}\right)^2}}
$$

(2.4.1)

where $c$ is the speed of light in free space, $\Delta t$ is the elementary time increment, and $\Delta x$ and $\Delta y$ are the dimensions of a Yee cell. The exact relationship of the time step and the cell dimensions can be derived from Maxwell's equations. A derivation of the stability criterion for the three-dimensional case is given in Appendix.

For a square two-dimensional case where $\Delta x = \Delta y = \Delta$, the stability condition becomes

$$
c\Delta t \leq \frac{\Delta}{\sqrt{2}}
$$

(2.4.2)

We noted that in the discretization, the determination of the cell dimension $\Delta$ depends on the frequency applied and the dielectric properties of the scattering medium. Generally the cell dimension is chosen to be 10 cells per wavelength and inversely proportional to the square root of the permittivity of the scattering material.
\[ \Delta = \frac{\lambda_{\text{shortest}}}{10\sqrt{\varepsilon_p}} \]  \hspace{1cm} (2.4.3)

The shortest wavelength, \( \lambda_{\text{shortest}} \), is determined from the highest frequency of the simulation and the velocity of light in free space,

\[ \lambda = \frac{c}{f_{\text{highest}}} \]  \hspace{1cm} (2.4.4)

### 2.5 Second Order Mur Absorbing Boundary Condition

The numerical simulation of electromagnetic scattering problems is limited by the available computer memory and computational speed. This limitation requires a finite computational domain and an algorithm that would accurately model the outward-going scattered waves to infinity. Such truncation algorithms are referred as absorbing boundary conditions. The second order Mur absorbing boundary condition, which has been applied by many researchers [28, 41], works well for both normal or near normal incidence [41]. In this study, the second order Mur absorbing boundary condition will be applied to truncate the FDTD computational domain.

Mur derived the second order absorbing boundary based on the paper by Engquist and Majda for a one-way wave equation [35-36, 38]. For the two-dimensional case, let \( x = 0 \) be the boundary plane where the absorbing boundary conditions are to be applied in the simulation. The approximation to the one-way wave condition under the second order Mur is [26, 35-38, 41]

\[
\left[ \frac{1}{c} \frac{\partial^2}{\partial x \partial t} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} + \frac{1}{2} \frac{\partial^2}{\partial y^2} \right] F_{|x=0} = 0 \hspace{1cm} (2.5.1)
\]
where $F$ is the tangential electric or magnetic field at the truncation boundary. A time-marching equation for the tangential electric fields $E(0,j)$ can be derived by applying the central-difference scheme to equation (2.5.1). A discrete formulation of (2.5.1) becomes [26, 36, 41]

$$E_{z}^{n+1}(0,j) = -E_{z}^{n-1}(1,j) + \frac{c\Delta t - \Delta}{c\Delta t + \Delta} \left( E_{z}^{n+1}(1,j) - E_{z}^{n-1}(0,j) \right)$$

$$+ \frac{2\Delta}{c\Delta t + \Delta} \left( E_{z}^{n}(0,j) + E_{z}^{n}(1,j) \right)$$

$$+ \frac{(c\Delta t)^2}{2\Delta(c\Delta t + \Delta)} \left( E_{z}^{n}(0,j + 1) - 2E_{z}^{n}(0,j) + E_{z}^{n}(0,j - 1) + E_{z}^{n}(1,j + 1) - 2E_{z}^{n}(1,j) + E_{z}^{n}(1,j - 1) \right)$$

(2.5.2)

for TM polarization.
Figure 2.1 Two-dimensional Yee cell, TM polarization, and the sampling positions of the electric and magnetic fields. The cell is a square with $\Delta x = \Delta y = \Delta$. 
Figure 2.2 The division of the computational domain into total-field region, and scattered-field region. The scattering objects are located within the total-field region. The absorbing boundary truncates the total computational domain.
Chapter 3

Excitation Source and Signal Processing Algorithm

For the study of photonic band gap structures, one is interested in the electromagnetic wave propagation through a periodic arrangement of scattering objects and the transmitted waves as a function of frequency. In this thesis, the FDTD method described in Chapter 2 is applied to simulate the wave propagation through the photonic band materials. A Gaussian pulse wave will be used as the excitation source in the simulation because of its wide bandwidth. All fields are then computed by time stepping until they reach a steady state [27]. The discrete Fourier transform (DFT) signal processing algorithm is used to transform the time domain fields into the frequency domain.

3.1 Excitation Source

Because of its multiple frequency information, a Gaussian pulse wave modulated sinusoidally is used as an excitation source in the FDTD simulation for this study. This Gaussian pulse can be centered at any frequency with the use of a carrier frequency. The Gaussian pulse modulated sinusoidal wave $e(\tau)$ has a form of

$$e(\tau) = e_o e^{-\alpha(\tau-\Delta t)^2} \cos[2\pi f_o (\tau - \beta \Delta t)]$$

(3.1.1)
where \( e_0 \) is the amplitude, \( f_0 \) is the carrier frequency, and \( \beta \) measures the time steps from the peak value of the pulse to the truncated value of the pulse. In general, the timely-sampled input pulse signal lies in \( 0 \leq \tau \leq 2\beta \Delta t \). The value of \( \alpha \) is determined so that the truncation will not introduce unwanted high frequencies. In this study \( \alpha \) is usually chosen to be \((4/\beta \Delta t)^2\) [27]. For this \( \alpha \), the truncated value of the incident field is decayed by a factor of \( e^{-16} \) from its maximum value. The cosine term sinusoidally modulated the Gaussian pulse in time domain.

Figure 3.1 plots a sample Gaussian pulse defined by equation (3.1.1) with \( \beta = 110 \), and \( f_0 \) is set equal to zero. The dimension of a Yee square cell is \( \Delta = 0.5mm \) which corresponds to using \( \Delta t = 1.17851 \, ps \). The time delay \((\beta \Delta t)\) or the center of the pulse generally depends on the location where the field is measured. In Figure 3.1, \( \beta \Delta t \) is equal to \( 12.96362 \, ns \).

### 3.2 Discrete Fourier Transform

In the Yee algorithm, the electromagnetic fields are computed in the time domain at an evenly spaced time interval \( \Delta t \). However, in this study, we are interested in the transmission coefficient as well as the field spectrum as a function of frequency. The Fourier transform is applied to the transient electromagnetic fields to obtain the transmission coefficient and the field spectrum directly on a large bandwidth.

Consider a time dependent function \( h(t) \), the Fourier transform of \( h(t) \) is given by the integral equation [44-45]

\[
H(f) = \int_{-\infty}^{\infty} h(t) e^{j2\pi ft} \, dt \tag{3.2.1}
\]

where \( f \) is the frequency.
Suppose that there are \( N \) finite number of sampled values of function \( h(t) \) at \( t_k = k\Delta t \)

\[
h_k = h(t_k)
\]  \hspace{1cm} (3.2.2)

where \( \Delta t \) is the evenly sampled interval and \( k = 0, 1, 2, ..., N - 1 \). The Fourier transform \( H(f) \) is obtained by approximating the integral equation (3.2.1) by a discrete sum [44-45]

\[
H_n = H(f_n) = \sum_{k=0}^{N-1} h_k e^{i2\pi n'k\Delta t} = \Delta t \sum_{k=0}^{N-1} h_k e^{i2\pi n'k}
\]  \hspace{1cm} (3.2.3)

where \( f_n = n/(N\Delta t) \) is the discrete frequency at the sample point \( n = -N/2, ..., N/2 \). The summation in equation (3.2.3) is called the discrete Fourier transform (DFT) of \( h_k \). The discrete inverse Fourier transform, which recovers \( h_k \) from \( H_n \), is

\[
h_k = \frac{1}{N} \sum_{n=0}^{N-1} H_n e^{-i2\pi kn/N}
\]  \hspace{1cm} (3.2.4)

The Fast Fourier Transform (FFT) technique is usually used to perform the transformation in (3.2.3) and (3.2.4) [44].

The DFT of the pulse shown in Figure 3.1 is plotted in Figure 3.2 for the positive frequency. The magnitude of the field quantity in the frequency domain is termed the field spectrum in this thesis. It is shown that the pulse wave of Figure 3.1 is centered at 0 GHz in the frequency domain.

A sample Gaussian pulse modulated sinusoidal wave with a carrier frequency of \( f_o = 10 \, \text{GHz} \) is shown in Figure 3.3 in time domain and in Figure 3.4 in frequency domain. The time domain pulse shown in Figure 3.3 becomes a doublet for the same set of parameters as in Figure 3.1. The peak of the pulse in the frequency domain has been shifted to \( f_o = 10 \, \text{GHz} \) which is caused by the modulated cosine term in (3.1.1).
3.3 Transmission Coefficient

In the simulations performed in this study, a plane wave is generated by the excitation source located on the left side of total-field region in Figure 2.2. The incident wave travels rightward as a function of time. As the wave hits the scatterers, part of the wave will be reflected back leftward and part of the wave will pass through the photonic structure. The transmitted signal as a function of time can be collected at any desired points in the computational domain.

The transmitted fields in the total-field region are sampled on unit Yee cells along a plane, beyond the outermost scatterers, transverse to the propagation direction. This plane is called the transmitted field plane. The location of selected plane of transmitted fields will be described in more detail in Chapter 4 where the FDTD simulation of wave propagation through a photonic band structure is performed. The samples of the transmitted fields are first summed in time domain; the summed field is then transformed into frequency domain using the FFT method. On the same plane, the incident fields are also sampled, summed, and Fourier transformed into frequency domain. The transmission coefficient \( T(f) \) as a function of frequency is defined as the ratio of the transmitted field in frequency domain and the incident field in frequency domain

\[
T = \frac{\sum_j \tilde{E}_{\text{tot}}(i_o, j)}{\sum_j \tilde{E}_{\text{inc}}(i_o, j)} \tag{3.3.1}
\]

where \( \tilde{E}_{\text{tot}} \) and \( \tilde{E}_{\text{inc}} \) denote the total electric field and the incident electric field in the frequency domain, respectively. The plane of transmitted field is chosen at \( i = i_o \), and the summation is over the cell index \( j \) in the transverse direction. In taking the FFT of the time domain field, we also obtain the phase factor should it be desired.
Figure 3.1 Incident Gaussian pulse vs. time steps with $\beta = 110$, $\Delta t = 1.17851$ ps second, and $f_0 = 0$. The number of time steps is $n = 4096$. The pulse is centered at time step 265, and the pulse truncated width is 220 time steps.
Figure 3.2 Incident Gaussian pulse of Figure 3.1 in the frequency domain. The field spectrum is shown for the positive frequency. The spectrum is centered at $0\,GHz$. 
Figure 3.3. Incident Gaussian pulse sinusoidally modulated with $f_o = 10 \text{ GHz}$ vs. time steps with $\Delta t = 1.17851 \text{ ps}$ and $\beta = 110$. The pulse becomes a doublet which is centered at the time steps equal to 265.
Figure 3.4. Incident Gaussian pulse of Figure 3.3 in the frequency domain. The field spectrum is centered at approximately $10\,GHz$. 
Chapter 4

FDTD Numerical Simulation Results

In this chapter, the electromagnetic wave propagation through two-dimensional photonic band structures is simulated using the FDTD method with the second order Mur absorbing boundary condition. These structures are made of periodic array of dielectric circular cylinders. The cylinders are lossless with real permittivity and permeability. In the wave propagation simulations, the permeability of the cylinders is assumed to be the same as the free space permeability. Two different permittivities of the cylinders are considered in this chapter. In the lower permittivity case, the contrast between the background, $\varepsilon = \varepsilon_\infty$, and the scattering objects, $\varepsilon_p = 4\varepsilon_\infty$, is smaller. In the higher permittivity case, the cylinder has permittivity $\varepsilon_p = 9\varepsilon_\infty$, the contrast between the background and the scattering objects is larger. The FDTD simulation results of the transmission spectra are presented in Section 4.2.
4.1 FDTD Simulation Methodology

Figure 4.1 illustrates the setup for the FDTD wave propagation simulations. The dark solid outer boundary is the second order Mur absorbing boundary which truncates the computational domain. The inner rectangular region is the total-field region. The area between the absorbing boundary and the total-field region is the scattered-field region, in which only the scattered fields are calculated. The two-dimensional scattering objects, which are represented by the circular cylinders with radius \( r \) and permittivity \( \varepsilon_r \), are located within the total-field region. These cylindrical objects are periodically positioned with the same lattice constant \( d \) in both directions. The axis of the cylinders is pointing in the \( z \)-direction out of the paper. The dark solid line on the left side of the total-field region represents the incident field plane. The incident field is propagating rightward in the \( x \)-direction and is polarized in the \( z \)-direction. The incident field interacts with the scattering objects producing the total and scattered fields. The transmitted fields are collected on the transmitted field plane, which is normal to the \( x \)-direction located on the right side of the total-field region. This transmitted field plane is located \( L_1 \) unit cells away from the last column of cylinders and \( L_2 \) unit cells away from the interface between the total-field region and the scattered-field region. The interface between the total-field region and scattered-field region is \( D \) unit cells away from the absorbing boundary.

In this study, the scattered-field and total-field regions are both discretized into square Yee unit cells of the dimension \( \Delta x = \Delta y = \Delta \) as shown on upper right corner in Figure 4.1. The minimum number of computational cells required in the total-field region is determined from the dimensions of the cylinder radius \( r \), the lattice constant \( d \), and the number of the cylinders. For instance, if the number of the cylinders is \( l \) in the \( x \) or \( y \)-direction, then \( M \) minimum number of unit cells in the \( x \) or \( y \)-direction is determined by

\[
M \geq \text{INT}\{(l-1) \cdot d + 2 \cdot r\} + 1
\]  

(4.1.1)
where the symbol \( \text{INT}\{x\} \) denotes the integer part of \( x \). In all the simulations performed in this study, the minimum number of the unit cells in the \( x \)- and \( y \)-directions is chosen to be the integer in the curly bracket plus at least 10 unit cells.

The dimensions of the scattered-field region are determined by the permittivity of the cylinder. The results of FDTD simulations become more accurate when \( D \) is larger. However, if \( D \) is too large, the simulation would take much longer time and would require more computer memory. For this reason, the dimension of \( D \) is chosen optimally. In this thesis research, \( D \) is chosen to be 20 or 50 unit cells when the permittivity of cylinder is \( \varepsilon_p = 9\varepsilon_0 \). When the permittivity of cylinder is \( \varepsilon_p = 4\varepsilon_0 \), \( D \) is then chosen equal to 10 unit cells.

The dimension of the total computational domain is determined by adding \( D \) and the minimum number of unit cells required for the total-field region. With the known dimensions in the \( x \) and \( y \) directions, the matrix of periodic cylinders are positioned inside the total-field region. A subroutine is developed to perform the placement of cylinders and the discretization of the photonic band structure.

In constructing the photonic band structures, the cylinders are arranged to make sure that they do not overlap with the scattered-field region, the incident field plane, and the transmitted field plane. In addition, the matrix of cylinders are placed such that they are centered in the \( y \)-direction. In the \( x \)-direction, for better simulation results, the transmitted field plane need to be located many unit cells away from the last column of the cylinders and many unit cells away from the total-field/scattered-field interface. Incident field plane is located within the total-field region and on the left-hand side of the first column of cylinders. However, to save some computational memory, the incident field plane is placed as close to the first column of cylinders as possible given that they do not overlap. Consequently, the matrix of cylinders will not center in the \( x \)-direction. In particular, the columns of cylinders are constructed in the following way. After determining the minimum number of unit cells, the locations of the centers in the \( x \)-direction are determined. An
additional $L_1 + L_2$ number of unit cells are added to the minimum number of unit cells in the total-field region. The transmitted field plane is located $L_1$ unit cells behind the last column of the cylinders and $L_2$ unit cells in front of the total-field/scattered-field interface. In the simulation, $L_1 = L_2$ is chosen to be 10 unit cells when $\varepsilon_\rho = 4\varepsilon_o$. When $\varepsilon_\rho = 9\varepsilon_o$, $L_1$ and $L_2$ are chosen from 40 to 150 unit cells to get good performance.

### 4.2 FDTD Simulation Results

The appearance of the photonic band gaps depends on the dielectric properties of the scattering objects. Two different permittivities of the cylinder will be studied using the methodology described in Section 4.1. One case is of lower permittivity contrast with $\varepsilon_\rho = 4\varepsilon_o$. In this case, the range of frequency simulated is $0 - 20 \, GHz$. The other case is for the higher permittivity contrast with $\varepsilon_\rho = 9\varepsilon_o$. For the second case, the frequency ranges simulated are $0 - 20 \, GHz$ and $15 - 130 \, GHz$. In all cases, the background permittivity is of free space $\varepsilon_o$. The incident electric field is polarized in the $z$-direction and propagates in the $x$-direction (TM polarization).

#### 4.2.1 FDTD Results for Lower Permittivity

In this case, the permittivity of the cylinders is $\varepsilon_\rho = 4\varepsilon_o$. The radius of the cylinders is $r = 4.8 \, mm$. The lattice constant of the two-dimensional square lattice photonic band structure is $d = 12.7 \, mm$. This is equivalent to a 0.449 filling ratio, defined as the cross-section area of the cylinder divided by the square of the lattice constant.

For this photonic band structure, the band gaps have been calculated using transfer matrix technique [11]. In Reference [11], the transmission coefficients were computed as a function of frequency from $0 - 20 \, GHz$. Two band gaps centered at $8 \, GHz$ and $15.5 \, GHz$ were found.

The minimum dimension of a unit cell required for stability in the FDTD simulation is determined from the highest frequency value of interest. Here, $\Delta = 0.5 \, mm$ is chosen. For
this value, there are approximately 15 unit cells per wavelength. The physical radius of the cylinders and the lattice constant of the photonic band structure are converted into an equivalence number of unit cells using the cell dimension. Thus, the radius and the lattice constant of this photonic band structure are equivalent to 9.6 unit cells and 25.4 unit cells for the given physical radius and lattice constant dimensions, respectively.

A matrix of $18 \times 9$ (18 rows in the y-direction and 9 columns in the x-direction) cylinders are placed inside the total-field region. To make sure that all the scattering objects are located within the total-field region, the minimum number of unit cells required for the total-field computational domain are determined using the formula (4.1.1) in Section 4.1. In the y-direction, this is equal to 470 unit cells. With $L_1 = L_2 = 10$ unit cells, the minimum number of unit cells in the x-direction is 230. The dimension of scattered-field region is $D = 10$ unit cells. Thus, in this case the total computational domain is divided into $490 \times 280$ unit cells.

A Gaussian pulse wave is applied to simulate the wave propagation through the photonic band structure. The incident wave propagates rightward in the x-direction and polarized in the z-direction. The excitation Gaussian pulse is described by the parameters $\beta = 110, \quad \Delta t = \Delta / (c \sqrt{2}) = 0.11785 \text{ ps}, \quad \alpha = (4/\beta \Delta t)^2 = 9.52066 \times 10^{20}, \quad \text{and} \quad f_o = 10 \text{ GHz}$. The spectrum of the incident wave has approximately $20 \text{ GHz}$ in width. This incident field spectrum is centered at $10 \text{ GHz}$. With these described parameters, the simulation is observed to be stable up to $n = 2^{15}$ time steps.

Figures 4.2 and 4.3 plot the FDTD simulation results for the field spectra and transmission coefficients, respectively. The dot-dash Gaussian curve in Figure 4.2 is the spectrum of the incident Gaussian pulse. The dot curve is for the transmitted field. The transmitted field spectrum shows two band gaps centered at $7.5 \text{ GHz}$ and $14.5 \text{ GHz}$. The transmission coefficients are determined from the spectra in Figure 4.2 and are plotted in decibel ($\text{dB}$) $[10 \log(|\text{transmission coefficient}|)]$ in Figure 4.3. The plot of transmission coefficients shows that the transmitted signals within the band gaps are approximately
attenuated by $-30\, \text{dB}$ and $-40\, \text{dB}$ at $7.5\, \text{GHz}$ and $14.5\, \text{GHz}$, respectively. The trough of the band gap at $14.5\, \text{GHz}$ is not smooth, which might be due to the discretization of the computational domain. The oscillations shown before and after the onset of the band gaps are caused by the discretization too. The shapes of the band gaps will become smoother if uses smaller $\Delta$ in the simulation.

The FDTD results of transmission coefficients in $\text{dB}$ as a function of frequency are in good agreement with the results obtained in Reference [11]. The level of transmitted signal within the band gaps calculated using the FDTD technique compares very well except that in [11] the photonic band gaps are centered around $8\, \text{GHz}$ and $15.5\, \text{GHz}$. The difference in the center place of band gap might be due to the dimension of the unit cell used in the FDTD simulation. Smaller dimension of the unit cell could improve the results of the FDTD simulation. This improvement will be demonstrated in the FDTD simulation results for higher permittivities cases in the next section.

4.2.2 FDTD Results for Higher Permittivity

In the high permittivity case the permittivity of the cylinders is $\varepsilon_p = 9\varepsilon_o$. Two FDTD simulations are performed to find the band gaps at two different frequency ranges. The first frequency range is $0\,\text{–}\,20\,\text{GHz}$, and the second frequency range is $15\,\text{–}\,130\,\text{GHz}$. Two different photonic band structures are simulated for these cases. For the frequency range of $0\,\text{–}\,20\,\text{GHz}$, the cylinder radius is $r = 4.8\,\text{mm}$, and the lattice constant is $d = 12.7\,\text{mm}$. For the case of $15\,\text{–}\,130\,\text{GHz}$, the radius is $r = 0.37\,\text{mm}$, and the lattice constant is $d = 1.87\,\text{mm}$.

1) **Frequency Range: 0 GHz to 20 GHz**

In this case, the square lattice photonic band structure has the same lattice constant and radius as the structure described in Section 4.2.1. The lattice constant of the photonic band structure and the radius of the cylinders are $d = 12.7\,\text{mm}$ and $r = 4.8\,\text{mm}$, respectively. Again, the filling ratio is 0.449.
Two FDTD simulations were performed using different cell dimensions. In the first simulation, the dimension of the unit cells is $\Delta = 0.5\ mm$, which is approximately equivalent to 15 unit cells per wavelength. In the second simulation, the dimension is $\Delta = 0.25\ mm$, which is approximately equivalent to 30 unit cells per wavelength for the FDTD simulation. The physical lattice constant and radius are converted into 25.4 unit cells for lattice constant and 9.6 unit cells for radius when $\Delta = 0.5\ mm$. Similarly, the lattice constant and the radius are respectively 50.8 unit cells and 19.2 unit cells when $\Delta = 0.25\ mm$. The minimum number of unit cells required for the total-field domain, where a matrix of $18 \times 9$ cylinders are placed, is determined for different dimensions of unit cells. The dimension of $D$ is 40 unit cells, and the dimension of $L_1 = L_2$ is 20 unit cells.

First, consider the FDTD simulation with a coarse discretization of $\Delta = 0.5\ mm$. With the dimensions of $L_1 = L_2$ and $D$ given above, the FDTD computational domain is equal to $550 \times 360$ unit cells ($550$ in the $y$-direction and $360$ in the $x$-direction). The $\hat{z}$-polarized, $\hat{x}$-directed excitation Gaussian pulse is described by the parameters $\beta = 110$, $\Delta t = \Delta / \left( c \sqrt{2} \right) = 1.17851\ ps$, $\alpha = \left( 4 / \beta \Delta t \right)^2 = 9.52066 \times 10^{-20}$, and $f_o = 10\ GHz$. The spectrum of the incident wave has approximately $20\ GHz$ in width. This incident field spectrum is centered at $10\ GHz$. With the parameters given above, the FDTD simulation reaches a stable result with $n = 2^{14}$ time steps.

Figures 4.4 and 4.5 plot the FDTD simulation results using $\Delta = 0.5\ mm$. The incident Gaussian pulse spectrum is shown in Figure 4.4. The transmitted field spectrum shows three band gaps centered at $5\ GHz$, $10\ GHz$, and $14\ GHz$. The plot of transmission coefficients shows that the transmitted signals within the band gaps are approximately attenuated by $-40\ dB$ at $5\ GHz$, $-50\ dB$ at $10\ GHz$, and $-50\ dB$ at $14\ GHz$. The transmission coefficient plot also shows a small band gap centered at $15.5\ GHz$ with $-50\ dB$ attenuation. The results of attenuation at $5\ GHz$ and $15.5\ GHz$ are lower than the results obtained by References [9, 11]. The results in the References [9, 11] had the band
gaps centered at approximately 5.5 GHz, 10.5 GHz, 15 GHz, and 16.5 GHz, which are about 1.0 GHz deviation compared with the FDTD simulation results presented here. Furthermore, in Figure 4.4 the transmission coefficient predicted by FDTD drops sharply around 18 GHz, since there exists another band gap at the vicinity of 20 GHz [9, 11]. The onset of the sharp attenuation around 18 GHz is caused by the shifted centered positions of band gaps using $\Delta = 0.5 \, mm$ in the discretization of Yee algorithm. Next, improved predictions will be shown by using smaller $\Delta$.

The FDTD simulation results for the band gaps for higher permittivity contrast can be improved by decreasing the dimension of unit cell used in the Yee algorithm. Consider the FDTD simulation with $\Delta = 0.25 \, mm$. The lattice constant and the radius respectively become $d = 50.8$ unit cells and $r = 19.2$ unit cells. With the dimensions of $L_1 = L_2 = 20$ unit cells and $D = 40$ unit cells, the FDTD computational domain is now divided into $1000 \times 580$ unit cells (1000 in the y-direction and 580 in the x-direction). Because the dimension of unit cell is now half of the previous one, the new $\beta$ must be doubled to retain the same pulse width of 20GHz in the frequency domain. Thus, the $\hat{z}$-polarized, $\hat{x}$-directed excitation Gaussian pulse is described by the parameters $\beta = 220$, $\Delta t = \Delta / (c \sqrt{2}) = 1.17851 \, ps$, $\alpha = (4 / \beta \Delta t)^2 = 9.52066 \times 10^{20}$, and $f_n = 10 \, GHz$. With $\Delta = 0.25 \, mm$ and the described parameters, the FDTD simulation results reach the stable state when $n = 2^{14}$ time steps.

Figures 4.6 and 4.7 plot the FDTD simulation results for the field spectra and the transmission coefficient. The photonic band gaps are now centered at 5.5 GHz, 10.5 GHz, and 14.5 GHz with attenuation of $-40 \, dB$, $-45 \, dB$, and $-60 \, dB$, respectively. The fine structure of the band gap is centered at 16 GHz now instead of 15.5 GHz. Thus, by decreasing the dimension of the unit cell by a factor of two, the band gap obtained are in very good agreement with the results given in References [9, 11], in both magnitudes of the transmitted signals and the locations of the band gaps. Furthermore, the sharp attenuation at 18 GHz disappears when $\Delta = 0.25 \, mm$ is used.
This suggests that a finer grid mesh is needed to get a better resolution on the band gap prediction.

\( (2) \textbf{Frequency Range: } 15 \text{ GHz to } 130 \text{ GHz} \)

In this case, the two-dimensional periodic photonic band structure has circular cylinders with permittivity \( \varepsilon_p = 9\varepsilon_o \), 0.74 mm in diameter, and the lattice constant 1.87 mm. The array of cylinders consists of 7 rods in the x-direction and 25 rods in the y-direction. Two FDTD simulations are performed for the frequency range from 15 GHz to 130 GHz.

In the first simulation, the square cell dimension \( \Delta = 0.05 \text{ mm} \) is used. The lattice constant and radius correspond to 37.4 unit cells and 7.4 unit cells, respectively. The FDTD simulation is performed with the dimensions \( L_1 = D = 50 \) unit cells and \( L_2 = 100 \) unit cells. The total computational domain is divided into 1030 unit cells in the y-direction and 510 unit cells in the x-direction.

Similarly, a \( \hat{z} \)-polarized incident wave is applied and propagates in the x-direction. The excitation Gaussian pulse is described by the parameters \( \beta = 200 \), \( \Delta t = \Delta / (c\sqrt{2}) = 1.17851 \text{ ps} \), \( \alpha = (4/\beta\Delta t)^2 = 2.88000 \times 10^{22} \), and \( f_o = 55 \text{ GHz} \) when \( \Delta = \Delta x = \Delta y = 0.05 \text{ mm} \). The spectrum of the incident wave has approximately 110 GHz in width. This incident field spectrum is centered at 55 GHz. We observe that with \( \Delta = 0.05 \text{ mm} \) and the parameters described above, the simulation results have good stability for at least \( n = 2^{15} \) time steps.

Figure 4.8 plots the spectra of transmitted and incident fields from the FDTD simulation. There is a band gap at the frequency interval of 45 – 70 GHz. The attenuation of this band gap is about \(-65 \text{ dB} \) as shown in Figure 4.9. The plot of the transmission coefficient shows bumps around 45 GHz in the trough of the band gap which might be due to the choice of the unit cell dimension.
Figure 4.1 Schematic diagram of the simulation problem space setup. The circles represent the cylindrical objects with radius $r$ and the lattice constant $d$. The cylinders with permittivity $\varepsilon_p$ are centered in the y-direction inside the total-field domain on a free space background of permittivity $\varepsilon_0$. The incident field is propagating in the x-direction and polarized in the z-direction. The transmitted field is collected along a plane perpendicular to the x-direction and parallel to the y-direction.
Figure 4.2 The field spectra vs. frequency. The square periodic photonic band structure consists of $18 \times 9$ cylinders with permittivity $\varepsilon_p = 4\varepsilon_o$. $\Delta = 0.5 \text{ mm}$, $\beta = 110$, and time steps $n = 2^{14}$ are used for the simulation. The Gaussian curve is for the incident wave spectrum. The transmitted field spectrum shows two band gaps centered at $7.5 \text{ GHz}$ and $14.5 \text{ GHz}$, respectively.
Figure 4.3 The transmission coefficient in dB determined from the spectra in Figure 4.2. The transmission coefficient shows the band gaps centered at 7.5 GHz and 14.5 GHz attenuated by $-30\, dB$ and $-40\, dB$, respectively.
The FDTD results using $\Delta = 0.05\ mm$ show excellent agreement for the band gap at the frequency interval $45 - 70\ GHz$ compared to References [5-6, 8]. However, the band gap at $95 - 100\ GHz$ does not show clearly. The band gap at $95 - 100\ GHz$ becomes more evident when the FDTD simulation is run with a smaller unit cell dimension. In particular, the dimension of the unit cell $\Delta = 0.025\ mm$ is used. The lattice constant and radius become $d = 74.8$ unit cells and $r = 14.8$ unit cells, respectively. The transmitted field plane is located with the distances $L_1 = 50$ unit cells and $L_2 = 100$ unit cells. The dimension of the scattered-field region is set equal to $D = 50$ unit cells. The FDTD computational domain is now divided into $2000 \times 730$ unit cells in the row $\times$ column directions, respectively.

The $\hat{z}$-polarized, $\hat{x}$-directional excitation Gaussian pulse is now described by the parameters $\beta = 320$, $\Delta t = \Delta/(c\sqrt{2}) = 0.058926\ ps$, $\alpha = (4/\beta \Delta t)^2 = 4.5 \times 10^{22}$, and $f_o = 60\ GHz$. The spectrum of the incident wave has approximately $120\ GHz$ in width. This incident field spectrum is centered at $60\ GHz$. With $\Delta = 0.025\ mm$ and the described parameters, the FDTD simulation is run for $n = 2^{14}$ time steps. Excellent stability is achieved at this time step.

Figures 4.10 and 4.11 show the FDTD simulation results when the dimensions of the unit cells are $\Delta = 0.025\ mm$. The bump in the trough of the first band gap are now disappeared. This first band gap becomes smoother and more symmetric. Comparing to the results in References [5-6, 8], the second band gap at $95 - 100\ GHz$ agrees very well. The magnitude of the second gap is not as low as the first band gap as predicted by the experiment [5]. Furthermore, the FDTD simulation shows a band gap at the vicinity of $150\ GHz$ which is in agreement with the suggested band gap experiment in Reference [5].
Figure 4.4 The field spectra for the transmitted and incident waves. The square periodic photonic band structure consists of $18 \times 9$ of cylinders with permittivity $\varepsilon_p = 9\varepsilon_o$, $\beta = 110$, $\Delta = 0.5 \text{mm}$, and $n = 16384$ time steps are used for the simulation. The transmitted field spectrum shows three band gaps centered at $5 \text{GHz}$, $10 \text{GHz}$, and $14 \text{GHz}$. 
Figure 4.5 The transmission coefficient of the field spectra in Figure 4.4. The band gaps are centered at 5GHz, 10GHz, and 14GHz and attenuated respectively by −40 dB, −50 dB, and −50 dB. The band gap centered at 15.5 GHz is different from the expected gap obtained in [9, 11]. Also, there is an onset of sharp attenuation around 18 GHz.
Figure 4.6 The spectra for the transmitted and incident fields. The square periodic photonic band structure consists of 18x9 cylinders with $\varepsilon_p = 9\varepsilon_o$. The FDTD simulation parameters used are $\Delta = 0.25\text{mm}$, $\beta = 220$, and $n = 16384$ time steps. The Gaussian curve is the plot of the incident plane wave spectrum. The transmitted field spectrum shows the band gaps centered at $5.5\text{GHz}$, $10.5\text{GHz}$, and $14.5\text{GHz}$. 
Figure 4.7 The transmission coefficient obtained from the field spectra in Figure 4.6. The band gaps centered at 5.5 GHz, 10.5 GHz, and 14.5 GHz and attenuated respectively by 
-37 dB, -45 dB, and -60 dB. The band gap at 16 GHz is not as low as the band gap predicted in Figure 4.5. Also, the sharp attenuation around 18 GHz in Figure 4.5 is disappeared.
Figure 4.8 The plot of spectra vs. frequency for a two-dimensional square lattice photonic band structure consisting of $25 \times 7$ cylindrical rods with 0.74 mm in diameter and 1.87 mm lattice constant. The FDTD simulation parameters used are $\Delta = 0.05$ mm, $\beta = 200$, and $n = 2^{15}$ time steps. The band gap between 45 GHz and 70 GHz are evident. However, the expected band gap between 95 GHz and 100 GHz does not show clearly.
Figure 4.9 The transmission coefficient plot for the spectra in Figure 4.8. There are bumps around 45 GHz in the trough of the band gap. The attenuation of the band gap at 95 to 100 GHz is not clearly shown. The first band gap shows excellent agreement with References [5, 6, 8].
Figure 4.10 The field spectra for a two-dimensional square photonic band structure consisting of $25 \times 7$ cylindrical rods with 0.74 mm in diameter and 1.87 mm lattice constant. The unit cell dimension is $\Delta = 0.025$ mm. The band gap at 95 – 100 GHz is more evident compare to Figure 4.8. This second band gap shows excellent agreement with References [5, 6, 8]. The total number of sample points in Figures 4.9 and 4.10 are half of the number of sample points in Figures 4.7 and 4.8.
Figure 4.11 The transmission coefficient obtained from the spectra in Figure 4.10. The attenuations at 45 to 70 GHz and 95 to 100 GHz are approximately $-50 \text{ dB}$ and $-30 \text{ dB}$, respectively.
Chapter 5

Sensitivity and Defect Studies on Band Gaps

The dimensions of the scatterers and the lattice constant in the photonic band structure are expected to deviate from the actual desired values when the structure is fabricated. These deviations might affect the photonic band gaps both in the magnitude of attenuation and the locations of the band gaps. For these reasons, sensitivity studies are performed on the photonic band structures using the developed two-dimensional FDTD simulation code. First, the effect on the band gaps when the lattice constant or the radius of cylinder is deviated from the designed values is studied. Here, the lattice constant and the radius of cylinder are assumed to deviate from the desired values by ±5%. Second, the effect on the band gaps is studied for the case where the number of rows of cylinders in the FDTD simulation is increased. In particular, one is interested in the change of band gaps when the finite extent of the photonic band structure becomes larger. In addition to the sensitivity study, the effect on the band gaps when one or more cylinders are removed from the matrix of cylinders is also studied. Such defects are expected to produce resonant modes in the band gap regions [9-13].
5.1 Sensitivity Studies on Radius and Lattice Constant

The sensitivity studies on the effect of the cylinders radius and lattice constant are performed on the photonic band structure consisting of a matrix of $18 \times 9$ of cylinders with permittivity is $\varepsilon_r = 4\varepsilon_o$. The parameters used in this simulation is the same as the parameters used in Section 4.2.1, where the cell dimensions is $\Delta = 0.5\ mm$, and the excitation source has $\beta = 110$ and $f_o = 10\ GHz$.

5.1.1 Effect of the Radius of Cylinder

The deviation of radius is assumed to be $\pm 5\%$ of the designed radius, $r = 4.8\ mm$ in this case. Two FDTD simulations are performed on the cylinders with $r = 4.56\ mm$ (5% smaller) and $r = 5.04\ mm$ (5% larger). The lattice constant is still kept the same as $d = 12.7\ mm$. Thus, the filling ratios become 0.4050 and 0.4948 for the smaller cylinder case and larger cylinder case, respectively.

A matrix of $18 \times 9$ cylinders are placed inside the total-field region. With $L_1 = L_2 = 10$ unit cells and $D = 10$ unit cells, the FDTD computational domain is discretized into $490 \times 280$ unit cells when $r = 4.8\ mm$, $480 \times 270$ unit cells when $r = 4.56\ mm$, and $490 \times 280$ unit cells when $r = 5.04\ mm$.

Figures 5.1 and 5.2 show the field spectra and transmission coefficients, and compare the three cases of cylinders with different radii. The dot, dot-dash, and solid curves, in Figures 5.1 and 5.2, are for $r = 4.8\ mm$, $r = 4.56\ mm$, and $r = 5.04\ mm$, respectively. Compared the deviated results to the actual result, we can see that the transmitted signals within the band gaps have higher attenuation (peak attenuations at $-30\ dB$ and $-50\ dB$) for $r = 4.56\ mm$, and the centers of the band gaps shift by $+0.5\ GHz$ from the centers of the band gaps when $r = 4.8\ mm$. On the other hand, the transmitted signals within the band gaps have lower attenuation (peaked at $-25\ dB$ and $-35\ dB$) for $r = 5.04\ mm$ compared to those of $r = 4.8\ mm$, and the centers of the band gaps shift by $-0.5\ GHz$ from the centers of $r = 4.8\ mm$. 

65
5.1.2 Effect of the Lattice Constant of Photonic Band Structure

Similar studies are performed on the effects of the variations of the lattice constant on the band structures. The deviation of the lattice constant is also assumed to be $\pm 5\%$ of the desired lattice constant $d = 12.7\ mm$. Two FDTD simulations with the lattice constant $d = 12.065\ mm$ and $d = 13.335\ mm$ are performed and compared to the structure with the lattice constant $d = 12.7\ mm$. The radius of the cylinders is fixed with $r = 4.8\ mm$, and the filling ratios are 0.4973 and 0.4070 for smaller and larger lattice constants, respectively.

A matrix of $18 \times 9$ cylinders are placed inside the total-field region. With $L_1 = L_2 = 10$ unit cells and $D = 10$ unit cells, the FDTD computational domain is discretized into $490 \times 280$ unit cells when $d = 12.7\ mm$, $460 \times 270$ unit cells when $d = 12.065\ mm$, and $500 \times 280$ unit cells when $d = 13.335\ mm$.

The field spectra and transmission coefficients for the simulations are plotted in Figures 5.3 and 5.4. The dot, dot-dash, and solid curves correspond to the simulations when the lattice constant equals to $d = 12.7\ mm$, $d = 12.065\ mm$, and $d = 13.335\ mm$, respectively. When $d = 12.065\ mm$ the transmitted signals at the two band gaps are attenuated respectively by $-25\ dB$ and $-35\ dB$ which are higher than those for $d = 12.7\ mm$. The centers of the band gaps shift by $+0.5\ GHz$ compared to the band gaps for $d = 12.7\ mm$. However, when $d = 13.335\ mm$ the transmitted signals at the two band gaps are attenuated by $-30\ dB$ and $-50\ dB$ which are lower than those for $d = 12.7\ mm$. The centers of the band gaps now shift by $-0.5\ GHz$ compared to the band gaps for $d = 12.7\ mm$.

5.2 Effect of the Number of Cylinders

The transmission spectra obtained by using the FDTD simulations for the photonic band structure consisting of $18 \times 9$ cylinders with permittivity $\varepsilon = 4\varepsilon_0$ or $\varepsilon = 9\varepsilon_0$ agree
well with the results shown in References [9-11]. The difference between the results of these two cases is that the band gaps predicted by the FDTD method for the lower permittivity case ($\varepsilon = 4\varepsilon_0$) is much smoother than the higher permittivity ($\varepsilon = 9\varepsilon_0$). One way to obtain smoother transmission spectra for structures with higher dielectric contrast is to increase the number of the cylinders, in particular, the number of cylinders along the transverse direction of the propagation in the FDTD simulations. This is in effect makes the dimension of the photonic band structure in the transverse direction larger compared to the wavelength.

Two simulations, one with structure $18 \times 9$ cylinders and the other with $36 \times 9$ cylinders, using $\Delta = 0.5 \text{ mm}$, $\beta = 110$, and $n = 16384$ time steps are performed. Other conditions for these two simulations are the same as the conditions described in Section 4.2.2 for the case of $0 - 20 \text{ GHz}$ frequency range. Note the difference in the numbers of cylinders in the x-direction between these two cases. With $L_1 = L_2 = 20$ unit cells and $D = 40$ unit cells, the computational domain is discretized into $550 \times 360$ unit cells when the matrix is $18 \times 9$ cylinders, and the computational domain is discretized into $940 \times 360$ unit cells when the matrix is $36 \times 9$ cylinders.

Figures 5.5 and 5.6 plot the results for the field spectra and transmission coefficient for the FDTD simulation when the photonic band structure consists of a matrix of $18 \times 9$ cylinders. In Figures 5.7 and 5.8, the results are plotted for the structure with $36 \times 9$ cylinders. It is noted that the curves of the band gaps are smoother when the matrix is bigger with $36 \times 9$ cylinders. In all cases, the band gaps are centered at $5 \text{ GHz}$, $10 \text{ GHz}$, and $14 \text{ GHz}$. In addition, the small band gap centered at $15 \text{ GHz}$ in Figure 5.6 is attenuated about $-50 \text{ dB}$, which is much lower relative to other band gaps in the same figure. However, the simulated signal at this same small band gap attenuated about $-40 \text{ dB}$ when the array of $36 \times 9$ cylinders is used in the FDTD simulation. The results using $36 \times 9$ array of cylinders are much better than the results using $18 \times 9$ array of cylinders when compared with the results shown in References [9, 11]
5.3 Defect Mode By Removing Cylinders

A photonic band structure is termed as defect if there is a perturbation to the periodicity of the lattice. In a defect photonic band structure, the defect mode frequency occurs in the photonic band gap range [11-13]. Because of this property of the defect, there is a resonant frequency inside the band gaps. This resonant frequency of the defect mode has many applications. For instance, a non-metallic high-Q cavity can be made from the photonic band structure to improve the solid state devices for laser applications [11-13].

For the photonic band structure studied in this thesis research, the simplest perturbation is when one or more cylinders are removed from the matrix of cylinders. The FDTD simulations for the defect mode are performed using the configuration shown in Figure 5.9, where one or more cylinders will be removed from the \((\text{column, row})\) coordinate. The incident field is propagating from right to left, and normal to the transverse cylinders.

The photonic band structure parameters are those used in the simulations in Section 4.2.1: the permittivity of the cylinders is \(\varepsilon_p = 4\varepsilon_o\), the radius of the cylinders is \(r = 4.8 \text{ mm}\), and the lattice constant is \(d = 12.7 \text{ mm}\). The dimensions of the unit cells are \(\Delta = 0.5 \text{ mm}\). A matrix of \(18 \times 9\) cylinders are placed inside the total-field region. With \(L_1 = L_2 = 10\) unit cells and \(D = 10\) unit cells, the total computational domain is divided into \(490 \times 280\) unit cells. The excitation Gaussian pulse is described by the parameters \(\beta = 110\), \(\Delta t = \Delta/(c\sqrt{2}) = 1.17851 \text{ ps}\), \(\alpha = (4/\beta \Delta t)^2 = 9.52066 \times 10^{20}\), and \(f_o = 10 \text{ GHz}\). The simulation is run for \(n = 2^{15}\) time steps.

Figures 5.10 and 5.11 show the transmission spectra for the defect mode when one cylinder at the coordinate \((\text{column, row}) = (5, 9)\) is removed. Compared with the dot curve where the periodicity of photonic band structure is not perturbed, the defect mode shows resonant frequencies within the band gaps. The first band gap has resonance localized at \(7.5 \text{ GHz}\). The localization of the second resonance appears at \(15.5 \text{ GHz}\) in the second
band gap. As shown in Figure 5.11, the attenuations at the resonance frequencies of 7.5 GHz and 15.5 GHz are very small.

Figures 5.12 and 5.13 plot the results of the defect mode when two non-adjacent cylinders at coordinates \((column, row) = (5, 9)\) and \((column, row) = (5, 11)\) are removed from the array. The resonance for this defect mode is very similar to the defect mode when one cylinder is removed from the matrix of cylinders. In particular, the first resonance occurs at also 7.5 GHz. The second resonance at 15.5 GHz is smaller in magnitude than magnitude of the resonance with one defect. The reason for such similarity is that in the second case the removed cylinders are not adjacent. Therefore, there is no interacting between the modes. The overlaps of the interacting modes is negligible [9, 11].

The defect mode with two adjacent cylinders removed is also studied. Figures 5.14 and 5.15 plot the results where the two removed cylinders located at \((column, row) = (5, 9)\) and \((column, row) = (4, 10)\). Because the removed cylinders are adjacent to each other, the modes interact. As the result of the interaction, the resonance is different from the removal of two non-adjacent cylinders. There appears to be a resonance at 8 GHz in the first band gap. However, this resonance is not clear. In the second band gap, the resonance clearly localizes at 14.75 GHz.

The FDTD simulation is further performed when three non-adjacent cylinders are removed from the array. In particular, the cylinders at \((column, row) = (4, 2)\), \((column, row) = (5, 10)\), and \((column, row) = (5, 16)\) are removed. Figures 5.16 and 5.17 plot the results of the simulation. These results are very similar to the simulation results when two adjacent cylinders are removed (Figures 5.14 and 5.15). There appears to be a resonance in the first band gap localized at 8 GHz. However, this resonance is not clear either. The second band gap shows a clear resonance at 14.75 GHz.
Figure 5.1 The field spectra for the two-dimensional photonic band structure consisting of a matrix of $18 \times 9$ of cylinders. The permittivity of the cylinder is $\varepsilon_p = 4\varepsilon_o$, and the lattice constant is $d = 12.7 \, mm$. The Gaussian curve is the incident field spectrum centered at 10 $GHz$. The dot, dot-dash, and solid curves are the spectra of the transmitted fields when the radius of cylinder is $r = 4.8 \, mm$, $r = 4.56 \, mm$, and $r = 5.04 \, mm$, respectively.
Figure 5.2 The plot of transmission coefficients obtained from Figure 5.1. The dot, dot-dash, and solid curves correspond the transmission coefficients when the radius of cylinder is $r = 4.8 \text{ mm}$, $r = 4.56 \text{ mm}$, and $r = 5.04 \text{ mm}$, respectively. When $r = 4.56 \text{ mm}$, the band gaps are attenuated by $-30 \text{ dB}$ and $-50 \text{ dB}$, and the centers of the band gaps shift by $+0.5 \text{ GHz}$ from the centers of the band gaps when $r = 4.8 \text{ mm}$. When $r = 5.04 \text{ mm}$, the band gaps are attenuated by $-25 \text{ dB}$ and $-35 \text{ dB}$. The centers shift by $-0.5 \text{ GHz}$ from the centers of the band gaps when $r = 4.8 \text{ mm}$. 
Figure 5.3 The field spectra of a two-dimensional photonic band structure consisting of $18 \times 9$ cylinders. The permittivity of cylinder is $\varepsilon_p = 4\varepsilon_o$, and the radius of cylinder is $r = 4.8\ mm$. The dot, dot-dash, and solid curves correspond to the simulations when the lattice constant equals to $d = 12.7\ mm$, $d = 12.065\ mm$, and $d = 13.335\ mm$, respectively.
Figure 5.4 The plot of transmission coefficients obtained from Figure 5.3. The dot, dot-dash, and solid curves correspond to the simulation when the lattice constant equals to \( d = 12.7 \text{ mm} \), \( d = 12.065 \text{ mm} \), and \( d = 13.335 \text{ mm} \), respectively. When \( d = 12.065 \text{ mm} \) the band gaps are attenuated by \(-25 \text{ dB} \) and \(-35 \text{ dB} \). The centers of the band gaps shift by \(+0.5 \text{ GHz} \) compared to the centers of the band gaps when \( d = 12.7 \text{ mm} \). When \( d = 13.335 \text{ mm} \) the band gaps are attenuated by \(-30 \text{ dB and } -50 \text{ dB} \). The centers shift by \(-0.5 \text{ GHz} \) compared to the centers when \( d = 12.7 \text{ mm} \).
Figure 5.5 The spectra for the transmitted and incident fields. The square periodic photonic band structure consists of $18 \times 9$ cylinders with $\varepsilon_p = 9\varepsilon_0$, $\Delta = 0.5 \text{ mm}$, $\beta = 110$, and $n = 16384$ time steps are used for the simulation. The transmitted field spectrum shows three band gaps centered at $5\text{GHz}$, $10\text{GHz}$, and $14\text{GHz}$.
Figure 5.6 The plot of transmission coefficients obtained from Figure 5.5. The band gaps centered at 5 GHz, 10 GHz, and 14 GHz and are respectively attenuated by −50 dB, −60 dB, and −60 dB. The magnitude of the transmission at 15.5 GHz is much lower than the results shown in References [9-11].
Figure 5.7 The spectra for the transmitted and incident fields. The square periodic photonic band structure consists of \(36 \times 9\) cylinders with \(\varepsilon_p = 9\varepsilon_o\). Parameters \(\Delta = 0.5 \text{ mm}, \ \beta = 110\), and \(n = 16384\) time steps are used for the simulations. The transmitted field spectrum shows three band gaps centered at \(5 \text{ GHz}, 10 \text{ GHz},\) and \(14 \text{ GHz}\).
Figure 5.8 The plot of transmission coefficients obtained from the field spectra in Figure 5.7. Three band gaps centered at 5 GHz, 10 GHz, and 14 GHz and are respectively attenuated by −50 dB, −58 dB, and −55 dB. The small band gap centered at 15.5 GHz is now attenuated by −40 dB and compared well to References [9-11].
Figure 5.9 The configuration for defect mode studies. One or more cylinders with the coordinate specified by \((\text{column, row})\) are removed from the matrix. The incident field propagates from right to left and normal to column of cylinders.
Figure 5.10 The plot of the transmitted field spectra for the defect mode when one cylinder at coordinate \((column, row) = (5, 9)\) is removed. The dot curve is the plot of the non-perturbed photonic band structure. The localizations of the resonance appear at 7.5 GHz and 15.5 GHz in the two band gaps.
Figure 5.11  The plot of transmission coefficients of the defect mode when one cylinder at coordinate \((column, row) = (5, 9)\) is removed compared to the non-perturbed photonic band structure. The dot curve is the plot of the non-perturbed photonic band structure. The attenuations at the resonant frequencies of 7.5 GHz and 15.5 GHz are very small.
Figure 5.12 The transmitted field spectrum of the defect mode when two non adjacent cylinders at coordinate \((\text{column, row}) = (5, 9)\) and \((\text{column, row}) = (5, 11)\) are removed. The dot curve is the plot of the non-perturbed photonic band structure. The localizations of the resonance appear 7.5 \(GHz\) and 15.5 \(GHz\) in the two band gaps. The resonances are very similar to the one defect mode.
Figure 5.13 The plot of transmission coefficients of the defect mode when two cylinders at coordinate \((column, row) = (5, 9)\) and \((column, row) = (5, 11)\) are removed. The dot curve is the plot of the non-perturbed photonic band structure. The attenuation at 15.5 GHz is large compared to one defect mode.
Figure 5.14 The transmitted field spectrum of the defect mode when two adjacent cylinders at coordinates \((\text{column}, \text{row}) = (5, 9)\) and \((\text{column}, \text{row}) = (4, 10)\) are removed. The localization of the resonance appears at 14.75 GHz in the second band gap. The resonance at the first band gap does not show clearly.
**Figure 5.15** The plot of transmission coefficients of the defect mode compared to the non-perturbed photonic band structure. The removed cylinders are adjacent to each other and are located at \((column, row) = (5, 9)\) and \((column, row) = (4, 10)\). The resonance is localized at 14.75 GHz in the second band gap and is attenuated by \(-5\, dB\). The resonance at the first band gap does not show clearly.
Figure 5.16 The transmitted field spectrum of the defect mode when three non-adjacent cylinders at coordinates $(column, row) = (4, 2)$, $(column, row) = (5, 10)$, and $(column, row) = (5, 16)$ are removed. There is a resonance at $14.75 \text{ GHz}$ in the second band gap. The resonance in the first band does not show clearly.
Figure 5.17 The plot of transmission coefficients when three non adjacent defect cylinders at $(column, row) = (4, 2)$, $(column, row) = (5, 10)$, and $(column, row) = (5, 16)$ are removed. The attenuation of the resonance at $14.75 \, GHz$ in the second band gap is approximately $-7 \, dB$. 
Chapter 6

Summary and Future Work

The focus of this thesis is on the simulation of electromagnetic wave propagation through two-dimensional photonic band gap structures. The structures investigated in this thesis are periodic array of circular dielectric cylinders. The cylinders are lossless with real permittivity and permeability. In the thesis, the finite-difference time-domain (FDTD) method is applied to calculate the transmission coefficients and the field spectra of electromagnetic waves from a finite two-dimensional array of cylinders and to obtain its photonic band gaps.

The FDTD method is reviewed in Chapter 2. A two-dimensional FDTD computer program with second order Mur absorbing boundary condition is developed for this study. In developing the computer simulation code, the total-field/scattered-field formulation is used to divide the field domain into the scattered-field domain and the total-field domain. Chapter 3 discusses the properties of the Gaussian incident field. This incident field is desirable for studying the transmission spectra because of its wide frequency bandwidth. Furthermore, the Gaussian pulse plane wave is sinusoidally modulated so that it could be centered at various frequencies. Because the FDTD algorithm calculated the
electromagnetic fields in time domain, signal processing algorithms based on Discrete Fourier Transform is introduced in Chapter 3 to obtain the electromagnetic fields in frequency domain.

The photonic band gaps are determined as a function of frequencies from the transmitted fields by either obtaining their spectra or transmission coefficients. In Chapter 4, the methodology used to obtain the transmitted fields for the band gap studies is presented. In particular, the transmitted fields are collected along a transmitted field plane transverse to the propagation direction of the incident field. The position of transmitted field plane is determined so that accurate FDTD results can be achieved. The minimum dimension of the total-field domain is also determined together with the dimension of the scattered-field domain.

Two different permittivities of cylinders are considered in the thesis for the FDTD simulations. In the lower permittivity case, the contrast between the background, $\varepsilon = \varepsilon_o$, and the scattering objects, $\varepsilon_p = 4\varepsilon_o$, is smaller. In the higher permittivity case, the cylinders had permittivity $\varepsilon_p = 9\varepsilon_o$; the contrast between the background and the scattering objects is larger.

In the lower permittivity case, a $18 \times 9$ matrix of cylinders is simulated for the frequency range from 0 GHz to 20 GHz. With $\Delta = 0.5 mm$, the radius and the lattice constant are respectively equivalent to 9.6 unit cells and 25.4 unit cells. Setting $L_1 = L_2 = 10$ unit cells and $D = 10$ unit cells, the total computational domain is divided into $490 \times 280$ unit cells for a $18 \times 9$ matrix of cylinders. A TM Gaussian pulse wave with parameters $\beta = 110$, $\Delta t = 1.17851 \text{ ps}$, $\alpha = 9.52066 \times 10^{20}$, $f_o = 10 \text{ GHZ}$, and the spectral width of 20 GHz is used as the incident field. The transmitted field spectrum predicts two band gaps centered at 7.5 GHz and 14.5 GHz, respectively. The transmitted signals within the band gaps are attenuated by $-30 \text{ dB}$ and $-40 \text{ dB}$ at 7.5 GHz and 14.5 GHz, respectively. Comparing to the results given in Reference [11], the
transmission coefficients of the FDTD simulation results using 15 unit cells per wavelength are quite good.

For the higher permittivity case, the FDTD simulations are performed for two frequency ranges of $0-20\ GHz$ and $15-130\ GHz$. For both frequency ranges, it is found that excellent results are obtained when the simulations use 30 unit cells per wavelength. In the frequency range $0-20\ GHz$, $\Delta = 0.25\ mm$ is used in the simulation. With the dimensions of $L_1 = L_2 = 20$ unit cells and $D = 40$ unit cells, the total FDTD computational domain is divided into $1000 \times 580$ unit cells. A TM excitation Gaussian pulse is then described by the parameters $\beta = 220$, $\Delta t = 1.17851\ ps$, $\alpha = 9.52066 \times 10^{20}$, and $f_0 = 10\ GHz$. Three band gaps are presented at $5.5\ GHz$, $10.5\ GHz$, and $14.5\ GHz$ with attenuations of $-40\ dB$, $-45\ dB$, and $-60\ dB$, respectively. For frequency range of $15-130\ GHz$, $\Delta = 0.025\ mm$ is used in the simulation. With $L_1 = 50$ unit cells, $L_2 = 100$ unit cells, and $D = 50$ unit cells, the total FDTD computational domain is divided into $2000 \times 730$ unit cells. Two band gaps are observed at frequency intervals $45-70\ GHz$ and $95-100\ GHz$. Comparing to References [5-6, 8], the FDTD simulations show excellent agreement with them. Furthermore, another band gap appears at the vicinity of $150\ GHz$ as suggested in References [5-6, 8].

The sensitivity studies on the effect of the cylinders radius and lattice constant are performed on the photonic band structure consisting of a matrix of $18 \times 9$ cylinders with permittivity $\varepsilon_p = 4\varepsilon_o$. The deviation of radius or the lattice constant is assumed to be $\pm 5\%$ of the designed value. The transmitted field spectra show changes both in the magnitude and the locations of the band gaps. In particular, it is found that the centers of the band gaps shift by $\pm 0.5\ GHz$.

The effect of the number of the cylinders on the band gaps is also studied and presented in Chapter 5. The number of cylinders along the transverse direction of the propagation is increased to make the photonic band structure looks more infinite-like in the transverse direction. The results for the simulation using $36 \times 9$ matrix of cylinders are...
noted to be smoother than using a matrix of $18 \times 9$ cylinders. The magnitude of attenuation using a matrix of $36 \times 9$ cylinders has a better agreement than the magnitude of attenuation predicted using a matrix of $18 \times 9$ cylinders compared to References [9, 11].

The defect modes with one or more cylinders removed from the matrix of cylinders are studied for the photonic band structure with the permittivity $\varepsilon_p = 4\varepsilon_n$. The defect mode of one cylinder removed from the middle of the matrix of $18 \times 9$ cylinders shows resonant frequencies within both band gaps. The first band gap has resonance localized at $7.5 \, \text{GHz}$. The localization of the second resonance appears at $15.5 \, \text{GHz}$ in the second band gap.

The results of the defect mode of two cylinders removed from the array depend on where the removed cylinders are. When two non-adjacent cylinders are removed, the resonance for this defect mode is very similar to the one defect mode. The first resonance occurs at $7.5 \, \text{GHz}$, and the second one is localized at $15.5 \, \text{GHz}$. When two adjacent cylinders are removed from the middle of the matrix of cylinders, the results show dramatic contrast from the defect mode when two non-adjacent cylinders are removed. The second band gap shows a resonance localized at $14.75 \, \text{GHz}$. The resonance in the first band gap does not show clearly.

The FDTD simulation is also performed when three non-adjacent cylinders are removed from the middle of the matrix of cylinders. The results are very similar to the case of two removed adjacent cylinders in the matrix of cylinders. The resonance in the first band gap is not clearly shown. The second band gap has a clear resonance at $14.75 \, \text{GHz}$.

In this thesis only the square photonic band structure is studied using the FDTD simulation with the second order Mur absorbing boundary. The simulation results have an excellent agreement with other numerical and experimental results shown in the published literatures. In future work, the FDTD technique should be used to study the triangular photonic band structure and compare the results to the results using other numerical method and experimental technique. The FDTD results for the triangular photonic band structure are expected to produce similar results to the square photonic band structure [11].

90
Furthermore, in the square photonic band structure, the square cylinders can used in the FDTD simulation instead of the circular cylinders. In both cases, the results are expected to be similar [14].

In simulating the wave propagation through two-dimensional periodic photonic band structure using the FDTD technique, the results agree very well with the results using other numerical methods [6-9, 11]. The FDTD simulations also agree very well with the experiment done by other [5]. Furthermore, one observes that the number of cylinders used in the simulation affects the results of the simulation. In particular, the results are better when the number of cylinders in the transverse direction is increased. This is because the photonic band structure now looked more infinite-like. Therefore, it is desirable if the FDTD simulation can simulate finite photonic band structure as if it is infinite. In future work, to achieve this desired effect, the FDTD simulations with periodic boundary should be performed to study the photonic band gaps.
Appendix

Stability Derivation for Three-Dimensional Cell

The stability criterion of the Yee algorithm for a three-dimensional problem has been derived by Taflove and Brodwin [26, 43]. Consider the normalized Maxwell's equations with $\mu = 1$, $\epsilon = 1$, $\sigma = 0$, $c = 1$, and $i^2 = -1$

$$\nabla \times \overline{H} = \frac{\partial \overline{E}}{\partial t} \quad (A.1)$$

$$-\nabla \times \overline{E} = \frac{\partial \overline{H}}{\partial t} \quad (A.2)$$
Multiplying equation (A.1) by $i$ and add the result to equation (A.2), one obtains

$$i\nabla \times (H + iE) = \frac{\partial}{\partial t}(H + iE)$$

(A.3)

An eigenvector $\vec{V} = H + iE$ satisfies [26, 43]

$$\frac{\partial \vec{V}}{\partial t} = \Lambda \vec{V}$$

(A.4)

$$i\nabla \times \vec{V} = \Lambda \vec{V}$$

(A.5)

Equation (A.4) is approximated using centered-difference approximation (2.2.1) and rearranged to obtain

$$\frac{\vec{V}^{n+1/2} - \vec{V}^{n-1/2}}{\vec{V}^n} = \Lambda \Delta t$$

(A.6)

A quadratic equation is obtained by letting $p = \frac{\vec{V}^{n+1/2}}{\vec{V}^n}$ and substituting it into equation (A.6)

$$p^2 - (\Lambda \Delta t)p - 1 = 0$$

(A.7)

The solution to equation (A.7) is

$$p = \frac{\Lambda \Delta t}{2} \pm \sqrt{\left(\frac{\Lambda \Delta t}{2}\right)^2 + 1}$$

(A.8)
In equation (A.8), the stability required that $|\rho| \leq 1$ so that equation (A.6) is bounded. This requirement for stability is achieved when [26, 43]

$$\text{Re}\{\Lambda\} = 0 \quad (A.9)$$

and

$$|\text{Im}\{\Lambda\}| \leq 2/\Delta t \quad (A.10)$$

Now consider the solution of the eigenvector of the form $\vec{V}(l,m,n) = \vec{V}_o e^{i(k_x l \Delta x + k_y m \Delta y + k_z n \Delta z)}$. Applying the centered-difference approximation (2.2.1) to the $\nabla$ operator in equation (A.5), and, for simplicity, considering only the $\hat{x}$ component of the field, one obtains

$$i \cdot \hat{x} \frac{e^{i(k_x (\Delta x + \Delta x/2) + k_y m \Delta y + k_z n \Delta z)} - e^{i(k_x (\Delta x - \Delta x/2) + k_y m \Delta y + k_z n \Delta z)}}{\Delta x} \times \vec{V}^n = \Lambda \vec{V}^n \quad (A.11)$$

The exponential term simplifies and is equal to $2i \sin\left(\frac{k_x l \Delta x}{2}\right)$. Rewriting equation (A.11) and separating it into $x$-, $y$-, and $z$-component in term of sine one has

$$\begin{bmatrix} \sin(\delta k_y) \Delta y V_z - \sin(\delta k_z) \Delta z V_y \\ \Delta y \end{bmatrix} = -\frac{\Lambda}{2} V_x \quad (A.12)$$

$$\begin{bmatrix} \sin(\delta k_z) \Delta z V_x - \sin(\delta k_x) \Delta x V_z \\ \Delta z \end{bmatrix} = -\frac{\Lambda}{2} V_y \quad (A.13)$$
\[
\begin{bmatrix}
\sin(\delta k_x) \\
\Delta x
\end{bmatrix} V_y - \begin{bmatrix}
\sin(\delta k_y) \\
\Delta y
\end{bmatrix} V_x = -\frac{\Lambda}{2} V_z
\]  

(A.14)

where \( \delta k_x = (k_x l \Delta x)/2, \delta k_y = (k_y m \Delta y)/2, \) and \( \delta k_z = (k_z n \Delta z)/2.\)

Equations (A.12) and (A.13) combine to give equation (A.15) in terms of \( V_y, \) and \( V_z.\)

\[
\begin{bmatrix}
\sin(\delta k_y) \sin(\delta k_z) \\
\Delta y \Delta z
\end{bmatrix} + \frac{\Lambda}{2} \begin{bmatrix}
\sin(\delta k_x) \\
\Delta x
\end{bmatrix} V_z = \left[ \frac{\Lambda^2}{4} + \frac{\sin^2(\delta k_z)}{\Delta z^2} \right] V_y
\]

(A.15)

Similarly, equations (A.12) and (A.14) combine to form an equation in terms of \( V_y, \) and \( V_z.\)

\[
\begin{bmatrix}
\sin(\delta k_y) \sin(\delta k_z) \\
\Delta y \Delta z
\end{bmatrix} - \frac{\Lambda}{2} \begin{bmatrix}
\sin(\delta k_x) \\
\Delta x
\end{bmatrix} V_z = \left[ \frac{\Lambda^2}{4} + \frac{\sin^2(\delta k_y)}{\Delta y^2} \right] V_y
\]

(A.16)

From equations (A.15) and (A.16), \( V_y \) and \( V_z \) are eliminated to solve for \( \Lambda \) in terms of \( k_x, k_y, k_z, \delta x, \delta y, \) and \( \delta z.\)

\[
\Lambda^2 = -4 \left[ \frac{\sin^2(k_x l \Delta x)}{2 \Delta x^2} + \frac{\sin^2(k_y m \Delta y)}{2 \Delta y^2} + \frac{\sin^2(k_z n \Delta z)}{2 \Delta z^2} \right]
\]

(A.17)
The solutions to equation (A.17) exist for all \( k_x, k_y, \) and \( k_z \) when

\[
\text{Re}\{\Lambda\} = 0 \quad \text{(A.18)}
\]

and

\[
|\text{Im}\{\Lambda\}| \leq 2\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}} \quad \text{(A.19)}
\]

Combining equations (A.9)-(A.10), (A.18)-(A.19), and de normalized the result back by a factor of \( c \), the stability condition becomes

\[
c\Delta t \leq \frac{1}{\sqrt{(1/\Delta x)^2 + (1/\Delta y)^2 + (1/\Delta z)^2}} \quad \text{(A.20)}
\]
References


