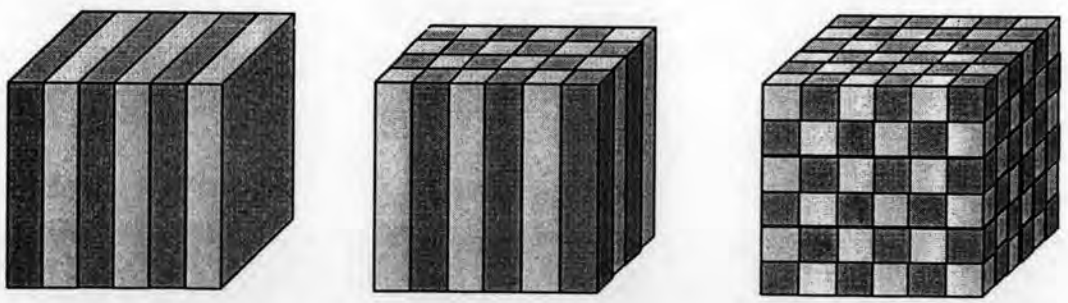
CHAPTER 1

INTRODUCTION

1.1 Photonic crystals and research background

Researches on photonic crystals (PCs) are recently active in arena of numerical analysis, material design, nanotechnology, and applications in photonic circuits. As numerical analysis tools is one of powerful tool for designing new photonic crystal structure in many application, this work aims to present efficient numerical analysis tool based on the finite element method for analyzing band gap characteristics of 2-dimensional photonic crystals. This chapter provides the introduction of the photonic crystals, and review of numerical tools for analyzing 2-dimensional photonic crystals.

Photonic crystals (PCs) are periodic dielectric structures, which can exhibit a photonic band gap (PBG). Inside the frequency gap, there will be no available mode so that the light is forbidden to propagate. In other words, the incident optical wave to PCs within that certain range of frequency is reflected by PCs. This main property of PCs gives a clue that PCs can control the propagation of the optical wave. The length of the periodicity is in the order of the corresponding photon wavelength. The periodic forms of a photonic crystal structure can be classified into 1-dimensional PCs, 2-dimensional PCs, and 3-dimensional PCs. Figure 1.1(a-c) show examples of PC's structures in 1-dimension, 2-dimension, and 3-dimension, respectively. Most applications of PCs nowadays are based on 2-dimensional PCs (2D PCs) due to nontrivial Brillouin zones, topological sensitivity, a minimum index contrast, and capability to be used to demonstrate most proposed PC devices [1]. Examples of 2-dimension PCs in reality for triangular lattice structures and square lattice structures are shown in Figure 1.2.



(a) Periodic in 1-dimension (b) Periodic in 2-dimension (c) Periodic in 3-dimension

Figure 1.1 Illustrations of photonic crystals (PCs) in (a) 1-dimension, (b) 2-dimension, and (c) 3-dimension [1].

The range of frequency band gap is a desirable data for designing structure of PCs in many applications. The range of frequency band gap can be obtained from the graph called "band gap characteristic of periodic PCs". The graph of band gap characteristic shows relation between a wave vector and corresponding frequencies of each eigenmodes. Because of periodicity of the structure in the PCs, it is necessary to employ the concept of a reciprocal lattice, Bloch theorem, and Brillouin zone in order to simplify the numerical calculation of the band gap characteristic [2-8].

Figure 1.2(a-b) show examples of a square lattice PC and a triangular lattice PC, respectively. Typical graphs of band gap characteristics are computed by MPB software, which is available at http://ab-initio.mit.edu/mpb/download.html. Figure 1.3(a-b) show examples of the graphs of band gap characteristics for a square lattice PC and a triangular lattice PC. The band gap characteristics are useful for indicating the frequency band where the wave cannot propagate through the PC. The horizontal axis in band gap characteristic graph designates the wave vectors where their values are given by the irreducible Brillouin zone. The Brillouin zone can be named as a wave vector zone. The irreducible Brillouin zone lies inside the first Brillouin zone. The first Brlillouin zone is the minimum wave vector zone in one periodicity, which is also called as a unit cell. The irreducible Brillouin zone is the reduced area of the unit cell that can be placed sufficiently by symmetric rotation and translation inside the unit cell. The unit cell can be found by applying the Weigner-Seitz cell algorithm [10]. The irreducible Brillouin zone inside the unit cell of the square lattice can be depicted by a triangle Γ-X-M-Γ as shown in the inset of Figure 1.2(a) while in case of triangular lattice, this zone are given by a triangle Γ-M-K-Γ as shown in the inset of Figure 1.2(b).

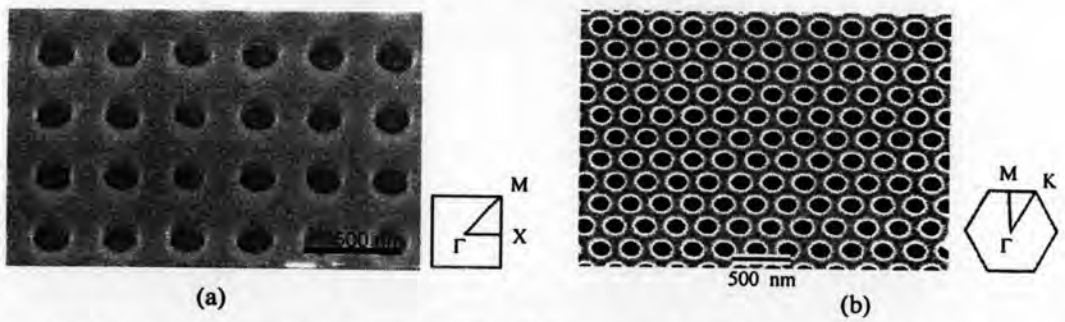
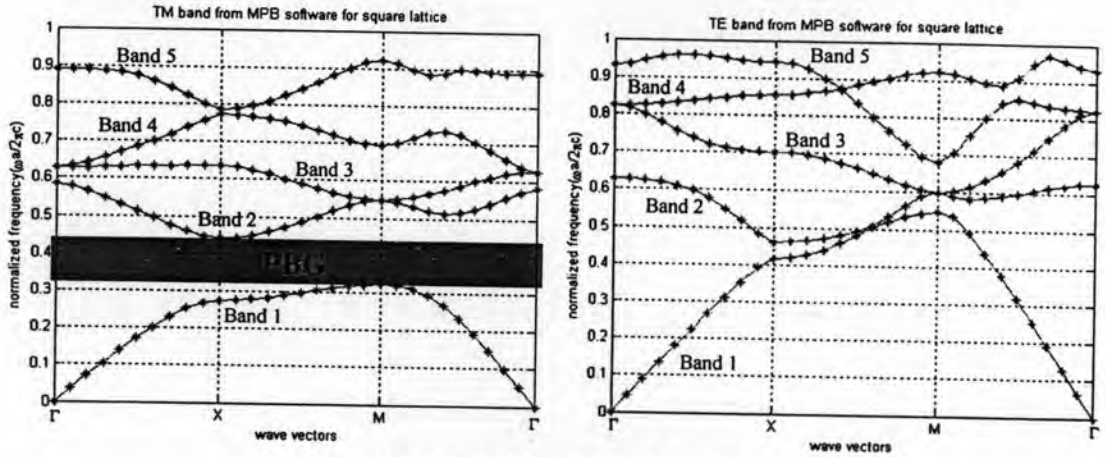


Figure 1.2 Two dimensional of photonic crystals with (a) a square lattice [29] and (b) a triangular lattice PCs [31] in case of holes embedded on dielectric medium.

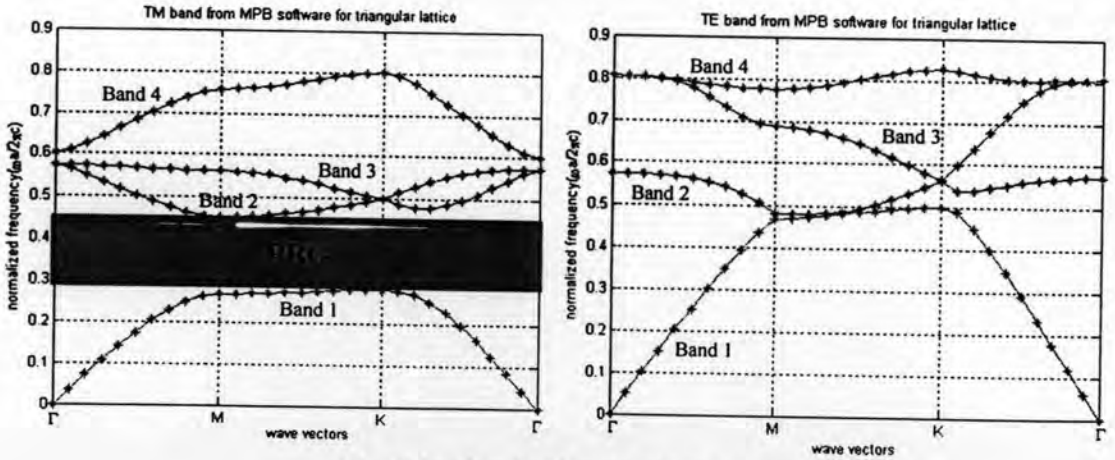
Given one 2D PC, its band gap characteristic can be obtained numerically by semi-analytical method, such as plane wave expansion method (PWE) [4], or other numerical methods for instance, the finite element method (FEM) [3,6,8] and the finite difference frequency domain method (FDFD) [7]. In PWE, the periodic structures are modeled with perfect periodic structure. The typical models used in PWE are cylindrical dielectric rods surrounded by air medium, or cylindrical air holes embedded in dielectric medium. Figure 1.3 shows two types of band gap characteristics of the square lattice PC and the triangular

lattice PC, which are computed by PWE method using MPB software. The structures of both cases are dielectric rods embedded on air medium. The dielectric constant of the rods for the case of square and the triangular lattice PCs are 8.9 and 11.4, respectively with r/a=0.2. The parameter r is the radius of the rod and a is the length of the periodicity, which is called as a lattice constant or a pitch, measured from a pair of the closest lattice points.

These band gap characteristics are computed by specifying the in-plane wave vector $\vec{k}$. The direction of vector $\vec{k}$ is in the plane of periodicity. The input values of vector $\vec{k}$ vary according to the edge of the irreducible BZ formed by points Γ, X, and M as shown in Figure 1.2(a) for square lattice PCs, and by points Γ, M, and K in Figure 1.2(b) for triangular lattice.



(a) a dielectric rod with ε_r=8.9 in air medium



(b) a dielectric rod with ε_r=11.4 in air medium

Figure 1.3 Examples of the band gap characteristics from (a) a square lattice and (b) a triangular lattice PCs for both TM mode (left side) and TE mode (right side)

As shown in Figure 1.3, there are forbidden bands of frequency in TM mode where there is no related wave vector for the modes to propagate. The lowest frequency

has an existing mode, which is strongly concentrated in the higher dielectric medium i.e. the dielectric rods in this case. The lowest frequency band is also called the "dielectric band". On the other hand, the higher frequency modes tend to concentrate in the lower dielectric medium, which normally is an air medium so that the related bands are common to be called the "air band". The modes that concentrate in higher dielectric constant offer the lower mode frequency than others. This condition initializes the frequency splitting and creates the band gap. This behavior can be understandable from the formulation where the solutions are obtained.

The function of the band gap characteristics as shown in Figure 1.3 is a guide map of frequency selection. At a defined wave vector $\bar{k}$ which consists of component in x-direction k_x and component in y-direction k_y, a set of frequencies are obtained. When a pair of a wave vector and a frequency is found on a particular band, the mode exists and the optical wave can propagate through the periodic structures. In this case, the ability of reflection of the structures disappears. If this condition is not desired, then this phenomenon becomes a loss where the wave is escaping out from the structures. On the other hand, when a frequency is chosen inside the band gap for a defined range of wave vectors, there is no intersection between them on the band curves. Therefore, no extended mode is available in the structure and such optical wave becomes evanescent at the interface between the incident plane and the structures. This is the use of the provided band gap characteristics.

1.1.1 Applications of 2D PCs

The main beneficial feature of 2D PCs is the ability to control the propagation of the light besides its small (nano-scale) size and large possibilities in modifying the geometry of the PC structures for their applications. Large contributions of 2D PCs yield some optical devices such as lasers, couplers and most of optical devices used in optical networks [2,3]. The usages of 2D PCs are obtained by modifying the structures into functional defect structures. The defects in 2D PCs can be defined into two major categories, i.e. line defects and point defects where these defects will break the periodicity of the structure. The existence of the defects localizes modes within a very narrow frequency band inside the band gap.

1.1.1.1 2D PCs with line defects

The line defects in 2D PCs have a function as a waveguide where the optical wave can travel through from the source device to the destination device. Line defects in 2D PCs can be made by removing some holes or rods in line periodicity so that an empty row of holes/rods exists as in Figure 1.4(a). The PC waveguide can be designed more to give advanced functions and purposes such as a Mach Zehnder photonic crystal waveguide [26] in Figure 1.4 and a bending waveguide [30] in Figure 1.5.

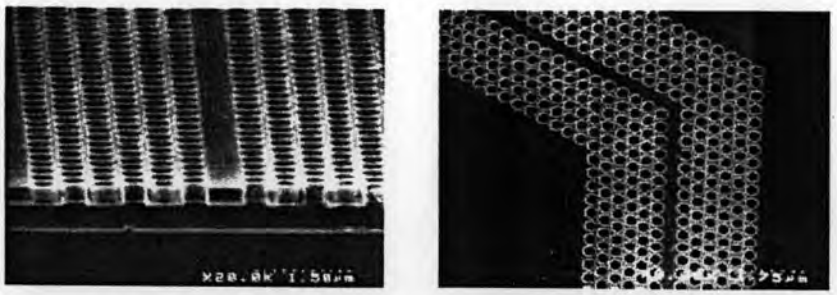


Figure 1.4 SEM micrograph of (a) the cross section of the triangular-structure waveguide suspended in air and (b) SEM micrograph of 60 bend in the triangular lattice [30]

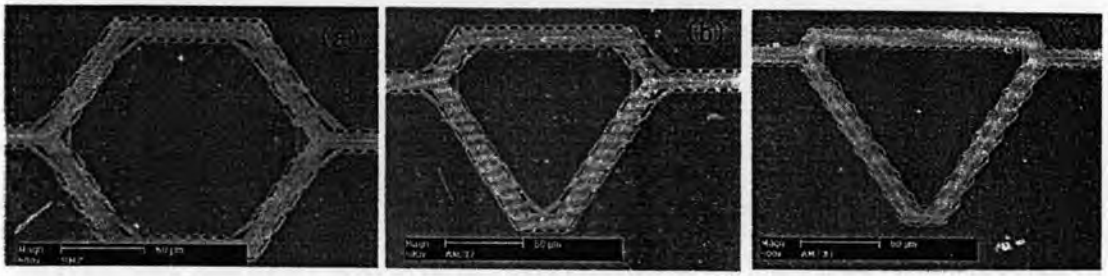


Figure 1.5 Examples of Mach-Zehnder photonic crystal waveguide with path length differences of (a) 0 μm (b) 75 μm and (c) 121 μm [26].

In the principle, the optical wave launches with a frequency inside the band gap through the line defect, the line defect becomes a waveguide where the light can propagate through, while the PC structures in the both sides of the defect act as a reflector so that the light can be confined inside the guide. At the interface between the waveguide and the PC structure, the light will be evanescent. The stronger the reflection of the structure makes the light more confined and the loss is reduced where the light is attenuated more quickly inside the structures. The width of the line defect here is in a wavelength scale, which is measured properly so that the optimal confinement can be obtained.

1.1.1.2 2D PCs with point defects

The point defects in a 2D PC make the structure act as a resonant cavity where the light can be confined in the PC. This defect will create a defect mode which has frequency exists inside the band gap. Such a defect mode in 2D PCs will only trap the light in a very narrow frequency band with a low loss and the high quality factor, Q. The Q factor is a measure of how many oscillations take place in a cavity before they damp and dissipate from the original excitation. The principal effect of a point defect placed in a 2D PC occurs when a mode with a frequency inside the PBG is excited in the structures.

The light will be localized inside the defect. The localization occurs because the periodic structures surrounding the defect will reflect the light back into the defect.

The defect frequencies, where the defect modes are available, can be calculated numerically. The defect frequencies are chosen to give the most suitable mode for the application. In this case, the efficiency and the accuracy of the numerical tools need to be focused inside the interested band gap range (frequency gap). In order to make a straightforward analysis, once the band gap ranges is captured that normally happen in lower bands of the band gap characteristic, the investigation of the defect frequencies can be taken and the higher bands may be ignored for this purpose. An example of point defects in a 2D PC of triangular lattice by removing a bundle of holes in dielectric medium is shown in Figure 1.6.

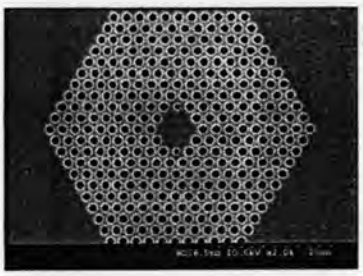


Figure 1.6 An example of 2D PCs in laser applications [27]

1.1.2 Some numerical methods for analyzing PCs

The band gap characteristics of 2D PCs are obtained numerically. Several methods have been proposed so far such as the plane wave expansion method (PWE) [4], the finite difference time domain method (FDTD) [5], the compact finite difference frequency domain method (FDFD) [7] and the finite element method (FEM) [3,8]. The PWE is a semi-analytical numerical method providing a higher accuracy for the solution than the numerical methods do. This method employs the Fourier series expansion to model the periodic structures. Due to the fixed periodicity of the expansion, it limits the structure model only for which having an ideal periodicity although there is an improvement in this method called a super cell method used when the defect exists. However, this method will not be suitable to model the practical structure efficiently where there are defects in the design structure of the PCs, or when the structure is distorted due to fabrication process. In computation aspect, PWE is a memory consuming method due to full matrices in system equation.

In comparison to those limitations of the PWE, there are numerical methods that can yield sparse matrices in system equation and have the flexibility to model irregular shape of PCs. For the application to any arbitrary shape and geometry structure of PCs, the finite element method (FEM) is one of powerful and versatile method. The FEM is suitable in modeling of the structure efficiently. The finite difference method and PWE method are less flexible in modeling the arbitrary shape than the FEM due to the grid-based discretization [5,7,8].

1.2 Research Motivation

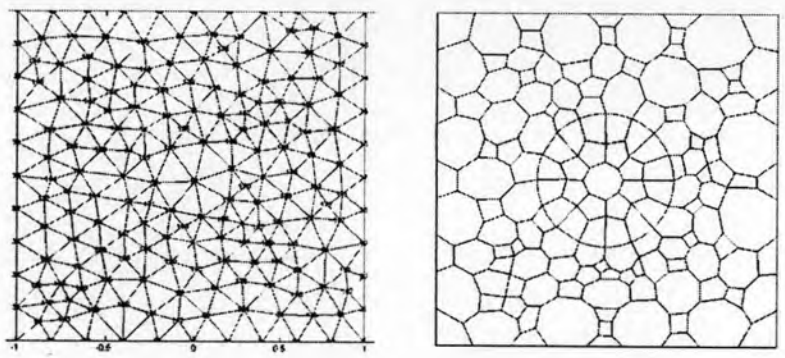
Research on PCs nowadays already has been in an advanced step in exploring the application and designing desirable forms of PCs. The PCs can be implemented in photonic integrated circuit (PIC) devices to support the next generation PIC in nanotechnology world [2,9]. This PC-based PIC operates at the frequency referenced by the band gap characteristic of the PC. If the frequency is selected inside the band gap, then the optical wave is forbidden to propagate through the PC structure. The structure will reflect the wave and it is very useful for guiding wave in order to keep it from escaping or a leakage wave where the loss comes from. Therefore, the operating wavelength or the operating frequency of the devices is chosen by considering from the band gap characteristic. Since the band gap is the most important property of PCs, the analysis of the band gap characteristic using numerical tools is advantageous as a starting point in design process.

An improvement of the performance of the available numerical tools is challenging research topics. The improvement can be expressed in terms of accuracy, computation time and memory consumption of the numerical calculation. The desired numerical tools should be efficient to calculate the property of the PCs. The finite element method (FEM) is a numerical tool for finding approximated solutions of a boundary value problem [3,8,12,15]. The concept of the finite element method starts with dividing the domain of the boundary value problem into finite number of small domain called "element". The process of dividing domain into elements is called "discretization". For the problem of analyzing 2D PC, the domain of the problem is the unit cell of the periodic structure. This unit cell is typically discretizised into triangular shape element. The interpolation of approximate solution is determined from the shape of element and the order of polynomial of the interpolation functions. The researches on interpolation functions for arbitrary polygonal element have been conducted so far. One of the proposed interpolation functions for polygonal element is Wachspress shape function proposed by E.L. Wachspress in 1975 [13, 18]. Recently, there is an improvement in FEM using generalized irregular polygonal elements using Wachspress shape functions that offer some advantages [13, 16-21], which is not yet applied in the finite element analysis of electromagnetic field. To open a chance in improving the finite element method, the research in this thesis is focused on implementing the Wachspress shape function to the finite element analysis of band gap characteristics. Some benefits of using the polygonal FEM can be explained as follows [13, 18]:

1. Greater flexibility in meshing due to the utilization of generalized polygonal elements. It means that during the domain discretization, not only one type of elements used to build the meshing but also those of other types can be combined together. Finally, the mesh may consist of triangles, quadrangles, hexagons, or any n-gons whose sizes meet the meshing requirements as shown in Figure 1.7. Those polygons can be convex or concave shapes based on the interpolation function that is used.
2. Useful to connect between two different n-gonal element types as shown also in Figure 1.7. The polygonal meshes show that the conformity is established among the

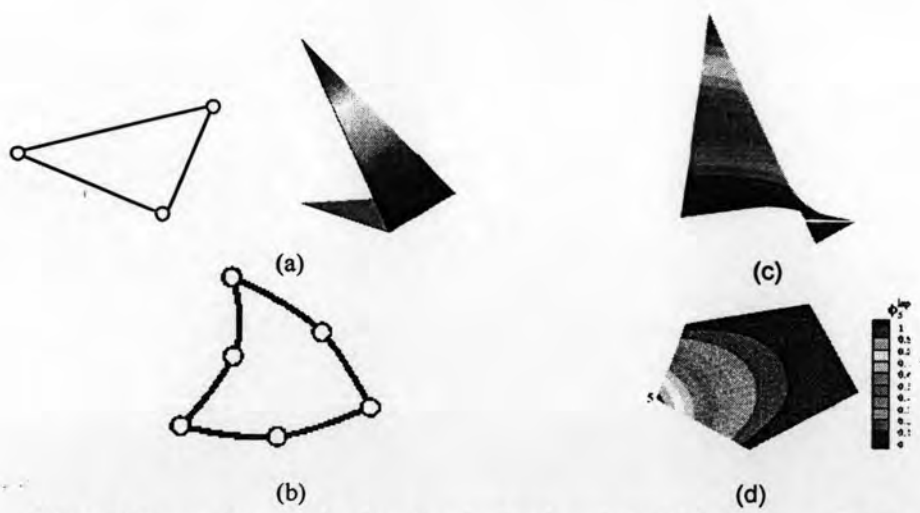
polygonal elements when arbitrary convex polygonal elements are employed so that the greater flexibility is available.

3. Higher accuracy due to the higher order interpolation function inside the element. The order of the function is determined by the number of vertices in the polygonal element. When number of vertices is larger, the order of the interpolation function becomes higher providing higher accuracy of the solutions. The difference between the triangular interpolation functions for first order (linear) and second order polynomials of polygonal interpolation functions is illustrated in Figure 1.8.
4. Suitable in material design and in the modeling of polycrystalline materials as in Figure 1.9.



(a) (b)

Figure 1.7 Examples of mesh designs using (a) triangular elements and (b) polygonal elements



(a) (c)

(b) (d)

Figure 1.8 The difference between the shape function in triangular FEM for (a) linear and (b) second order elements, and (c-d) the polygonal shape function given from side view and top view, respectively [13,18].

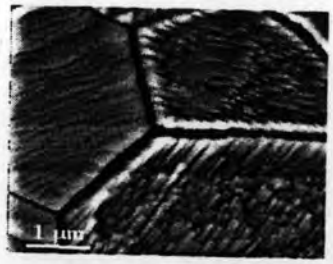


Figure 1.9 An atomic force micrograph of the sintered surface of a polycrystalline aluminum oxide ceramic [Source: http://mimp.mems.cmu.edu/~ordofmag/aluminum.htm]

Based on the benefits of the polygonal FEM, the performance of the method for calculating the band gap characteristic of 2D PCs is expected to be more efficient and more accurate than the conventional FEM method based on using triangular element. The Wachspress shape function is written in the form of a rational basis function based on an area calculation [16, 18].

As far as we know, the implementation of the polygonal FEM to calculate the band gap characteristic of 2D PCs is never investigated before. This thesis will show the performance of the method with a FEM formulation derived directly from the Helmholtz's equation. In this research, the Bloch's function will be imposed on the boundary of the calculation domain as a periodic boundary condition (PBC) as in [7]. The detail about the FEM formulation is presented in Chapter 2.

1.3 Thesis Objectives

This thesis mainly aims to:

1. Propose new finite element formulation which utilize polygonal element for analyzing band-gap characteristic of two-dimensional photonic crystals.
2. To compare the results to those of previous works in order to analyze the accuracy

1.4 Outlines of Thesis

This thesis is divided into five chapters and organized as follows:

Chapter 1 Introduction,

This chapter presents the overview of this thesis including the background of the problems, the motivations, the main objectives, and the organization of the thesis.

Chapter 2 Finite Element Methods for Analyzing A Band Gap Characteristic of Two Dimensional Photonic Crystals,

In this chapter, some related theories to this work are presented. The basic concept of PCs along with some examples of the applications, and the band gap characteristic will be explained and also how to determine the unit cell of the 2D PCs using the Weigner Seitz cell algorithm will be described. The concept of Brillouin zone is explored more in the case of square and triangular lattice constants. This chapter is assigned to give the details of FEM process in order to calculate the band gap characteristic of the 2D PCs for the conventional or the triangular FEM. The aim here is to provide the basic knowledge of the FEM before it is improved with the polygonal FEM. The theory of FEM will first focus on the triangular FEM for the linear/first order and the second order elements until the solution is obtained. The concept of a barycentric coordinate or an area coordinate will be presented here as used in the construction of the shape function. The Maxwell's and the Helmholtz's equations in scalar forms are presented here as the governing equations used as the mathematical model of the boundary value problems. Since the problem is deal with a periodic structure, sampled in a unit cell, the boundary condition used in this problem called periodic boundary conditions (PBC) will be introduced.

Chapter 3 Polygonal Finite Element Method,

This chapter will explain more about this polygonal FEM. How to construct the shape function in polygonal elements becomes the main topic here as the main difference with the conventional FEM. This chapter discusses about the brief history of the polygonal shape function as the interpolation function for generalized irregular polygonal elements. The numerical integration in this polygonal FEM is slightly different with the conventional FEM explained here. The method to compare results with the previous ones of the conventional method in term of the accuracy will be described here. The accuracy will be observed in term of an L2 (norm-2) as explained in [16, 18].

Chapter 4 Numerical Examples and Result Validation,

In this chapter, the results of the calculation are presented. The results include the ones from the linear triangular FEM for the square and the triangular lattice constants. The increased order of the element yields the second order results for both of them which are also presented here. The results are of the conventional FEM will be compared with ones from PWE obtained from the MPB software for the validation. The accuracy of the results will be investigated. The improvement with the polygonal FEM yields some results which are also validated with the previous results and observed for the accuracy in case of square lattice and triangular lattice PCs. Some parameters in the polygonal FEM will be investigated for ones which have the largest contribution in increasing the accuracy such as the number of n-gon elements and also the technique in the numerical integration. The aim of this chapter is to show the performance of the polygonal FEM in case of calculating the band gap characteristic of 2D PCs. Additional examples are the use

of hybrid polygonal FEM which is a combination of linear elements and higher order elements. Examples of the method in application to calculate the non-ideal geometry of the unit cell are also investigated as the case of cracked rod and deformed rod in the unit cell.

Chapter 5 Discussions and Conclusions,

This last chapter will finally conclude the whole of the works and provide some recommendations of the future works of this research.