Chapter 1

Introduction

1.1 Photonic Crystal

Photonic band gap (PBG) materials have been a fast developing field in micro-optics and quantum physics in the last decade. The physical characteristics and device fabrications of photonic crystals (PCs) have attracted increasing interest because they have photonic band structures similar to electronic band structures, potential usefulness in controlling light propagation around the band corner, and potential application for various optical devices.[1-6] These structures were originally proposed by John and Yablonovitch to realize new optical principles—the light is localized and trapped in the bulk material and the spontaneous emission is complete forbidden over a broad frequency range.[7,8] The band-structure concepts of solid-state physics are applied to electromagnetism, leading to the invention of artificial electromagnetic crystal structures.

Photonic band gap structures and defect or cavity structures are shown in Fig. 1.1. The photonic crystals are artificially arranged periodic dielectric media in 1D, 2D and 3D with periodicity in the operating wavelength scale (~um). It is an analogous to semiconductor with periodic structures in atomic scale (~nm). The formation of electronic band gap is due to the periodic potential for electrons in semiconductor; while the formation of photonic band gap is due to the periodic dielectric constants for photons in photonic crystal. Because of Bragg-like diffraction from the atoms in the semiconductor lattice, the electronic gap is opened. The electrons with energies in the gap range can not propagate in the semiconductor in any direction. The photons propagated in the periodic potential are also strongly affected by the mechanism of Bragg-like scattering. The photonic gap is opened when the dielectric contrast between columns and background material is different enough. The photons can not exist in the photonic band gap. The difference in band structures between bulk material and photonic band gap material has shown in Fig. 1.2.

The periodic potential and lattice constant are fixed in the electronic crystal, so the width and position of energy gap will be fixed. However, the lattice constant and periodic potential in the photonic crystal can be changed, thereby allowing the width and position of photonic band gap to be controlled with proper designs of PBG materials. The existence of photonic band gap is highly dependent on the lattice geometry, column shape and dielectric contrast. In particular, the lattice parameter in the photonic crystal is comparable to the wavelength of the electromagnetic wave, allowing estimating the size of photonic crystal for a specific range of frequencies for applications.

Although the features of photonic band gap are more analogous to electronic band gap, there are differences between them.[9] It is well known that electrons have spin 1/2 and are fermions, and exist interactions with other electrons. The electronic band structure is obtained by solving Schrödinger equation with the periodic potential of the crystal. The equation is treated in the scalar wave approximation. However, the photons have spin 1 and are bosons, and no interactions between photons. The photonic band structure is obtained by solving Maxwell equation with the periodic dielectric constant. The equation has to solve with a vector wave approximation. In addition, the photons have several advantages over electrons. The photons propagated in a dielectric material have a much greater speed than electrons in a metallic wire. The bandwidth of dielectric materials in PCs is larger than that of metals. Therefore, this characteristic is helpful to realize a large bandwidth telecommunications.

1.2 Photonic Band Gap

For the two-dimensional or three-dimensional photonic crystal, an electromagnetic wave can be decomposed into the E-polarization and H-polarization modes. For a polarization mode, a photonic crystal may exhibit the frequency regions where electromagnetic waves can not propagate in any direction. These frequency regions are called photonic band gap for this polarization mode. An complete PBG exists if the band gaps for both H-polarization and E-polarization modes are present and they overlap each other. The light incident on an complete PBG material with a frequency in the gap region will be backscattered from the material, independent of the angle of incidence.

The reasons why the PBGs appear in the photonic crystal are complex, so the designs of photonic crystal for obtaining desired PBG are with thumb of rules. Generally, the formation of photonic band gap is a result of interplay between the macroscopic Bragg scattering and the microscopic Mie scattering. Bragg scattering has the strong relation with the periodicity and geometry of lattice, while the Mie scattering has the strong the relation with the shape of individual columns.[10,11] The refractive index contrast affects mainly the strength of the two scattering mechanisms. One of the conditions for the appearance of a PBG is that the density of dielectric scatters be chosen such that the Mie scattering resonance of a single unit cell of PC has the same frequency with the Bragg resonance of the periodic array. We use a simple example of one-dimensional structure to illustrate these conditions. As shown in Fig. 1.3, the width of square wells is a and the space between wells is L. Assume the refractive index is n inside each well and is unity outside. The Bragg scattering condition is given by $\lambda = 2L$, where λ is the wavelength in the vacuum. The Mie scattering resonance reaches the maximum when the reflection coefficient is maximum. That is, the quarter wavelength has to design to fit into the well. The Mie scattering condition is given by $\lambda/4n = 2a$. Combining these two conditions yields the optimal volume filling fraction $pf = 2a/L = 1/(2n)$. These concepts may provide a guiding to predict the properties of light in the photonic crystals.

The features of complete PBG provide an opportunity to confine and control the propagation of waves. Some photonic crystals for applications such as laser diode and LED are shown in Fig. 1.4. Most of the promising applications of PBG materials depend on the widths and locations of their complete PBGs. The gap width in a PBG material is determined by the refractive index contrast of the two materials and by the filling factor of the high-index material. The location of the gap is determined by the lattice constant of the PC. We should note that gap width and gap position strongly relate with the sizes of columns and lattice parameter, and consequently affect the possibility for fabricating photonic crystals. The polarization-independent photonic band gap is obtained with properly designed dielectric constants, structural symmetry and filling ratio for PCs.

Many three-dimensional and two-dimensional PCs with band gaps in microwave region have been fabricated.[12-17] The frequency at which band gap occurs is directly related to the size of columns. The photonic crystal with the band gap in the microwave regime has columns a few millimeters in size. However, the band gap in the visible regime requires precise fabrication of columns on the order of $0.25\mu m$. The fabrication of such small size for three-dimensional PCs is exceedingly difficult by using standard photolithographic and etching techniques. Instead, the fabrication requirements are not stringent for two-dimensional PCs. Unlike three-dimensional photonic crystal structures, the two-dimensional photonic crystal structures can be fabricated easily. Several attempts have successfully fabricated 2D photonic crystals with IR band gaps and even visible frequency gaps.[18,19]

The absence of normal modes of EM waves inside PBG can give rise to unusual physical phenomena, such as the suppressed dipole-dipole interaction between atoms and the photon-atom bound states.[20,22] The enhancement of the density of state of EM waves near PBG corner can improve the performance of optoelectronic devices. Thus, the search for photonic crystals generating PBG in two or three dimensions has attracted a lot of attention. A large photonic band gap is needed in various applications such as the optical waveguide, defect cavity, defect-mode photonic crystal lasers.[23-27] Defects in photonic crystals are easily created by either adding other dielectric materials to or removing dielectric material from a chosen unit cell in the periodic lattice. This defect can create a local mode of EM wave in PBG and act like a microcavity. Thus it is possible to tune the defect modes to any frequency in PBG by designing the size, the shape, and the dielectric constant of the defect. In particular, a large PBG for the defect-mode photonic crystal laser leads to a large spontaneous emission factor, therefore, the spontaneous emissions can be suppressed efficiently and a narrow resonant peak can be obtained in the defect-mode laser. Recently, a large spontaneous emission factor (0.06) has been observed experimentally in the defect-mode photonic crystal laser.[28] A large PBG is essential if we wish to obtain a photonic crystal defect cavity with a narrow resonant peak.

The larger photonic bang gap is, the greater the forbidden region of the frequency spectrum. For two different photonic crystals possessing the same size of complete PBG, it may be advantageous from a fabrication standpoint to chose the one that has the large PBG occurring at high normalized frequency, $\omega a / 2\pi c$, where ω is the frequency, a is the lattice constant, and c is the speed of light in vacuum. For a given filling ratio, the size of columns is a, thus the photonic crystal with band gap at higher $\omega a / 2\pi c$ should be easier to fabricate. As a result, many have already been made to design various kinds of photonic crystal structures in an effort to obtain a large PBG.

There are two approaches to increase the PBG in the two-dimensional PCs. One is to increase the PBG for either E-polarization or H-polarization modes, and the other is to increase the PBG overlapping the E-polarization and H-polarization band gaps. The most severe limit to the PBG width comes from the degeneracy of photonic bands at high symmetry point in the Brillouin zone. Several methods have been suggested for lifting the band degeneracy and obtaining the complete PBG, which involve varying the contrast of dielectric contrast ratio, design of lattice element and filling ratio.[29-31] Additionally, the symmetry of photonic crystal also plays an important role in opening complete PBG.[32] For example, attempts inserted small circular rods in the original circular rods in square lattice, honeycomb structure and in group 4mm photonic crystals to reduce the symmetry of original structure, leading to a larger PBG.[33-35] The noncircular rods, such as square, triangular, hexagonal, were recently utilized to lift the band degeneracy in 2D lattices, but fail to open new complete PBGs or create PBGs larger than those using circular rods.[36-38] Although these noncircular rods can not efficiently enlarge complete PBG, it may provide more opportunities to reduce symmetry of PCs by deforming and rotating rods. The rectangular, elliptic rods embedded with square or triangular lattices through a rotational angle have obtained a large complete PBG.[39-41] In short, the PBG size can be increased by lowering the symmetries of lattice and columns. However, the effects of structural and rotational symmetries associated with the deformed and rotation of rods on E-polarization and

H-polarization band gaps of the photonic crystals have not been studied thoroughly.

1.3 Scope and Outline

This work mainly focuses on how to model and simulate photonic crystals, to explore their properties and investigate the effects of geometric parameters on the band structure. Three topics, the calculations for obtaining large PBG, the investigations of formed PBG in the square lattice and the effects of structural and rotational symmetry of hollow structures on the PBG are studied in this thesis. The plane-wave method (PWM) is employed in this thesis to calculate the band structures and field patterns of photonic crystals. The dissertation is organized as follows.

Chapter 2 discusses the theoretical framework used to study photonic crystal. The so-called master equation for photonic crystal is derived by using Maxwell's equation and Bloch theorem. Some operations for deriving the dielectric function for a given lattice element are discussed.

Chapter 3 presents the results how the structural and rotational symmetries affect the band structures of photonic crystal. The calculated results have shown that the increasing dielectric contrast and reducing the rotational and structural symmetries can obtain a sizable complete PBG in high normalized frequency. Moreover, the correlations between photonic structures and rods' symmetry can be reasonably explained, and the scattering mechanisms are systematically examined.

It is well known that the complete PBG for square lattice exists in the case of dielectric square columns, but closes when the rods are designed with circular cross section of the columns.[42,43] This is interesting that the isolated-dielectric rods can appear an complete PBG by the use of square rod without including dielectric veins. The types of boundary of dielectric rods may strong affect the band structures in the square lattice. In the chapter 4, we consider the 2D photonic crystals with dielectric N-polygonal rods as inclusions in the square lattice. The band structures depending on the polygonal structure have also been examined. The results show that the band structures of polygonal rod in the square lattice approach the same to that of the circular rod when the value of N is above eight whether isotropic and anisotropic dielectric rods used. The results may provide a guiding for fabricating the photonic crystals. Additionally, the reasons why an complete PBG appears in the square rods but closes in the circular rod in square lattice can be understood.

The standard fabrication of PCs is the electrochemical etching of holes in a slab material. The etching process may result in a rough and porous interface between rods and background matrix. The interface can be described by an effective medium, and its dielectric constant may be different. In the chapter 5, theoretical calculations are presented to investigate the influence of the interfacial layers on PBG in photonic crystals. In addition, three deformed and two rotational hollow Te (tellurium) rods are constructed to study the effects of structural and rotational symmetry on the gap widths of E- and H-polarization bands in photonic crystals. The H-polarization band gaps are strongly affected by the interaction between the fields of the rods as the rods are deformed and affected by the reduction in the rotational symmetry as whole rods are rotated. Only the shapes of the rods affect the E-polarization band gaps as the rods are either deformed or rotated. Moreover, H-polarization modes determine the complete PBG width as the rods are rotated, whereas E-polarization modes determine the complete PBG width as the rods are deformed. Theses results are useful in understanding the properties of the formed PBGs and provide a path for designing proper photonic crystal structures with desired PBGs. Finally, the summary and conclusion of the research are given in the chapter 6.

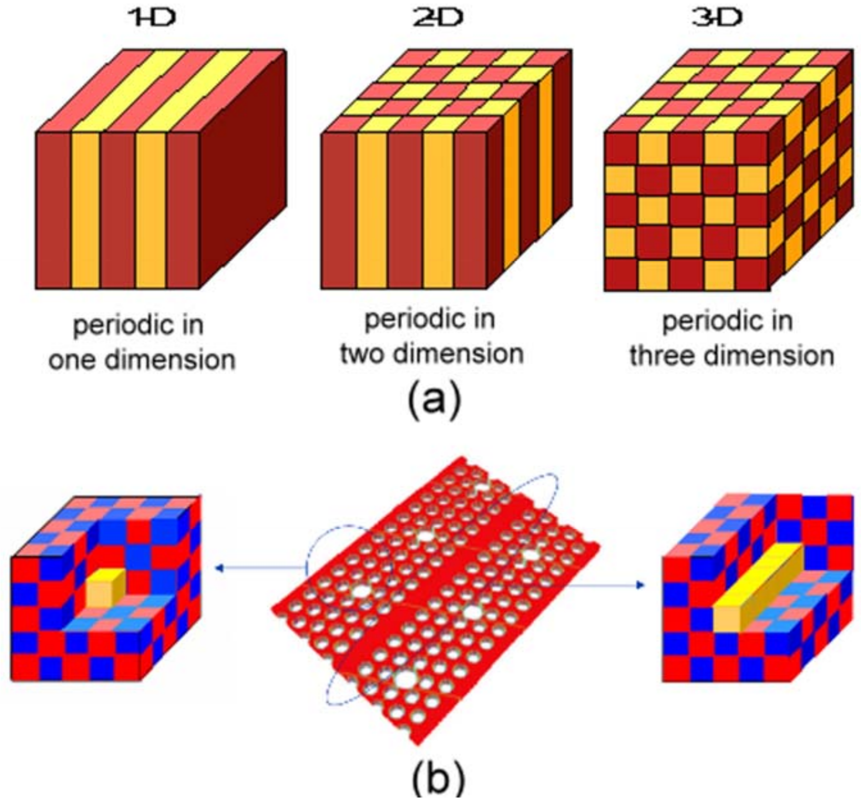


Figure 1.1 Schematic drawing of (a) periodic photonic crystals and (b) defect and cavity photonic crystals.

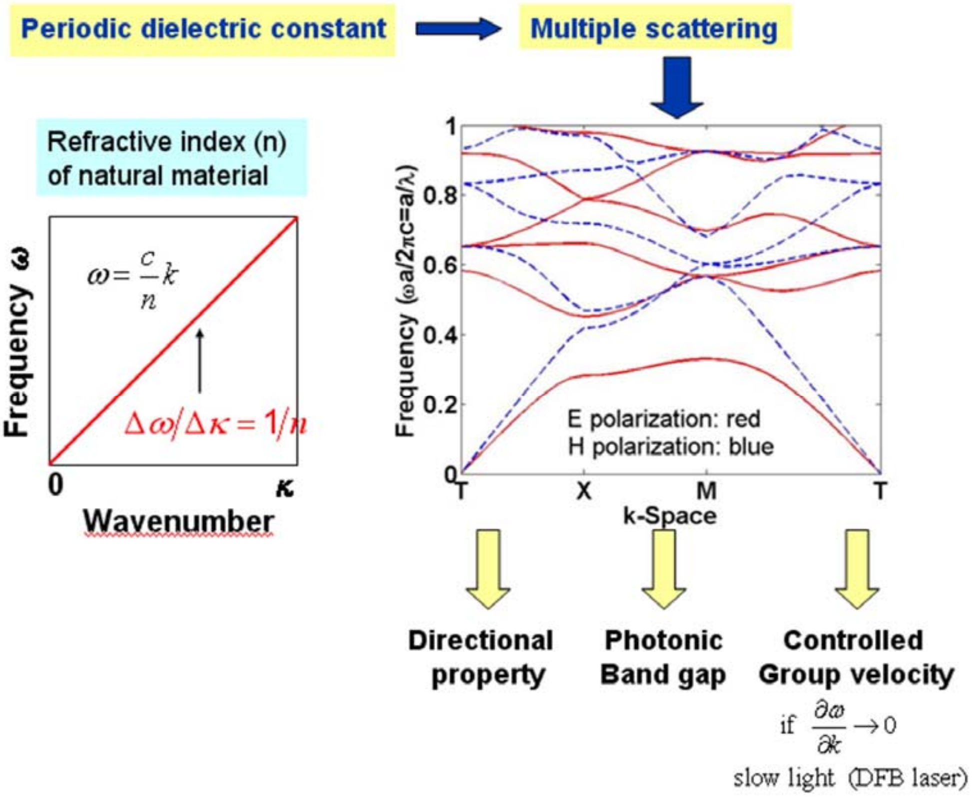


Figure 1.2 The comparison in optical properties between bulk material and photonic band gap material.

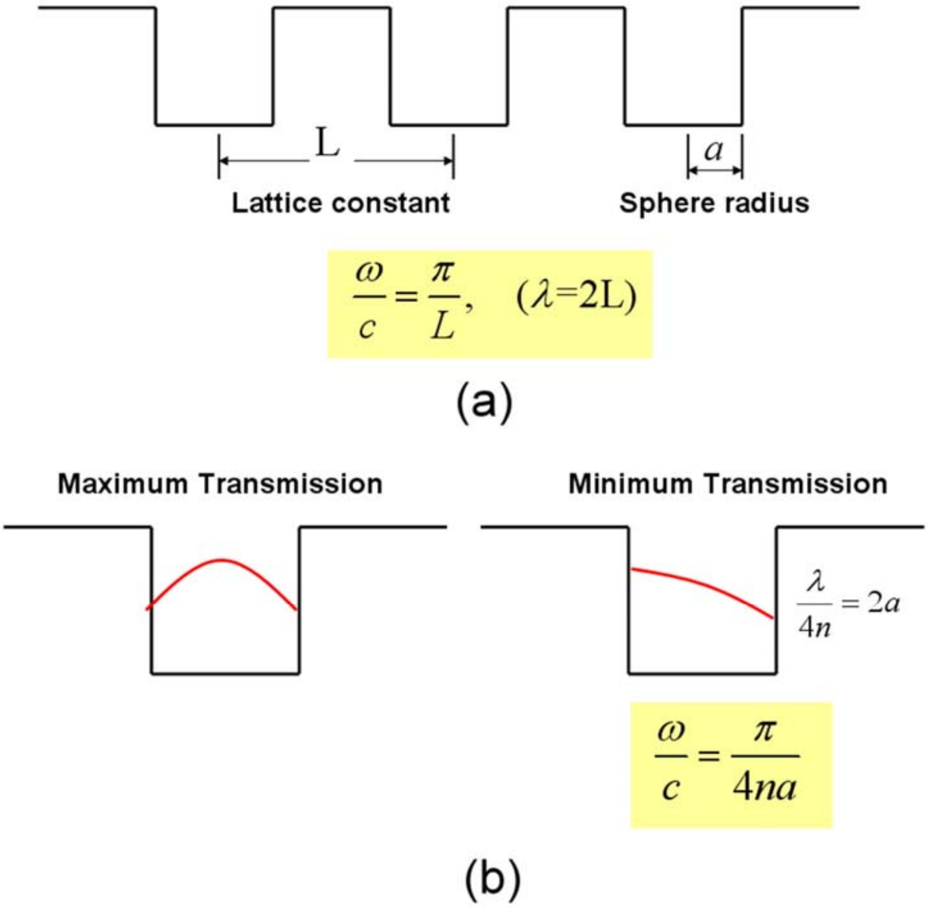
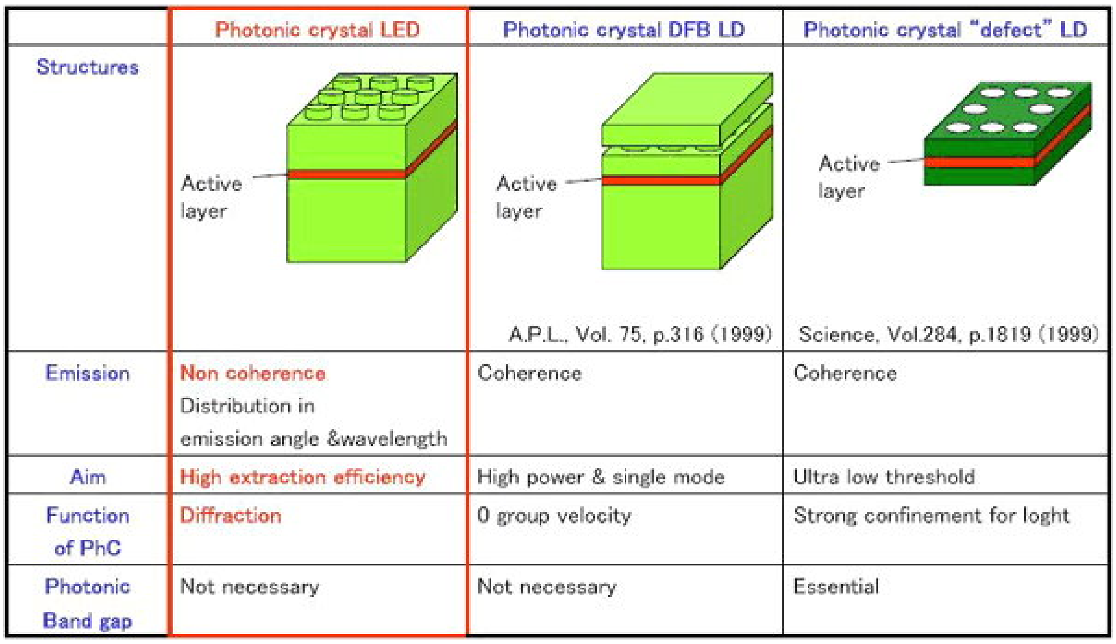


Figure 1.3 The representation of (a) macroscopic and (b) microscopic resonance. Cite from *J. Opt. B: Quantum Semiclass. Opt.* **5** R43-R82 (2003).



	Photonic crystal LED	Photonic crystal DFB LD	Photonic crystal "defect" LD
Structures	Active layer	Active layer A.P.L., Vol. 75, p.316 (1999)	Active layer Science, Vol.284, p.1819 (1999)
Emission	Non coherence Distribution in emission angle &wavelength	Coherence	Coherence
Aim	High extraction efficiency	High power & single mode	Ultra low threshold
Function of PhC	Diffraction	0 group velocity	Strong confinement for loght
Photonic Band gap	Not necessary	Not necessary	Essential

(cite from http://www.digitimes.com.tw/)

Figure 1.4 The advantage and function of photonic crystals on the LED and LD.