COMPUTATIONAL METHODS FOR THE ANALYSIS AND DESIGN OF PHOTONIC BANDGAP STRUCTURES

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Abstract

In the present thesis, computational methods for the analysis and design of photonic bandgap structure are considered. Many numerical methods have been used to study such structures. Among them, the plane wave expansion method is very often used. Using this method, we show that inclusions of elliptic air holes can be used effectively to obtain a larger complete band gap for two-dimensional (2D) photonic crystals. An optimal design of a 2D photonic crystal is also considered in the thesis using a combination of the plane wave expansion method and the conjugate gradient method. We find that a maximum complete 2D band gap can be obtained by connecting dielectric rods with veins for a photonic crystal with a square lattice of air holes in GaAs.

For some problems, such as defect modes, the plane wave expansion method is extremely time-consuming. It seems that the finite-difference time-domain (FDTD) method is promising, since the computational time is proportional to the number of the discretization points in the computation domain (i.e., it is of order $N$). A FDTD scheme in a nonorthogonal coordinate system is presented in the thesis to calculate the band structure of a 2D photonic crystal consisting of a skew lattice. The algorithm can easily be used for any complicated inclusion configuration, which can have both the dielectric and metallic constituents. The FDTD method is also applied to calculate the off-plane band structures of 2D photonic crystals in the present thesis. We also propose a numerical method for computing defect modes in 2D crystals (with dielectric or metallic inclusions). Compared to the FDTD transmission spectra method, our method reduces the computation time and memory significantly, and finds as many defect modes as possible, including those that are not excited by an incident plane wave in the FDTD transmission spectra method. The FDTD method has also been applied to calculate guided modes and surface modes in 2D photonic crystals using a combination of the periodic boundary condition and the perfectly matched layer for the boundary treatment. An efficient FDTD method, in which only real variables are used, is also proposed for the full-wave analysis of guided modes in photonic crystal fibers.

Keywords: Photonic crystals, Photonic band-gap materials, Photonic band structures, Off-plane band structures Cavities, Defect modes, Waveguides, Guided modes, Surface modes, Optical fibers, Numerical analysis, Optimal design, Finite-difference time-domain method, Plane wave expansion method, Periodic boundary condition, Perfectly matched layer
Preface

This work has been carried out at the Division of Electromagnetic Theory, Royal Institute of Technology during 1999 and 2000. The thesis consists of an introduction and eight research papers. My intention with this thesis is to develop computational methods for the analysis and design of photonic bandgap structures.

I would like to express my gratitude to my supervisor and co-author Doc. Sailing He for his excellent guidance (not just scientific). His advice and encourage have been of vital importance during my research work.

I also wish to thank all my colleagues at the division for their companionship, with special thanks to Prof. Staffan Ström and Dr. Henrik Holter for uncountable fruitful discussions.

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List of papers


IV. Min Qiu and Sailing He, ‘FDTD algorithm for computing the off-plane band structure in a two-dimensional photonic crystal with dielectric or metallic inclusions’, Physics Letter A, in press


Specification of my contributions to the included papers

I. In paper I, I carried out the numerical implementation of the plane wave expansion method, and I also performed the numerical simulations.

II. In paper II, I implemented the plane wave expansion method and the conjugate gradient method for photonic crystals. I also contributed with the idea of connecting dielectric rods with veins. I performed the numerical simulations for the paper.

III. In paper III, I suggested the use of the nonorthogonal finite-difference time-domain method, and developed the application of the method to compute the band structures of photonic crystals. I carried out the numerical implementation and I also performed the numerical simulations.

IV. In paper IV, I developed the finite-difference time-domain method for off-plane band structures of two-dimensional photonic crystals. I also performed the numerical simulations.

V. In paper V, I implemented the finite-difference time-domain method for computing the defect modes in photonic crystals. I also performed the numerical simulations.

VI. In paper VI, I generated the finite-difference time-domain method for guided modes in the photonic crystal waveguides. I related the guided modes to those in conventional metallic waveguides. I also performed the numerical simulations.

VII. In paper VII, I carried out the numerical implementation of the finite-difference time-domain method, and I also performed the numerical simulations.

VIII. I am the single author of paper VIII.
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1. Introduction

The discovery of photonic band-gap (PBG) materials and their use in controlling light propagation is a new and exciting development [1-3]. It has vast implications for material science, electrical engineering, optics, and physics. According to the world leading scientific journal Science, ‘new light on photonics’ is one of the ten top breakthroughs of the year 1999 (Dec. 1999, Science). Science [4] states that ‘Semiconductors transformed the communication and computing industries by channeling electrons faster than giant old vacuum tubes could. And many observers expect that in the 21st century these industries will be transformed again, by photonic crystals, latticelike structures that have the potential to manipulate photons as semiconductors do electrons – but at the speed of light.’

A photonic crystal (PC) is a periodic arrangement of dielectric or metallic materials, and is an optical analogy to a conventional crystal. A conventional crystal can provide an energy band gap to prevent an electron from propagating through the crystal. A photonic crystal provides a possibility to control and manipulate the propagation of light. When electromagnetic waves propagate in a photonic crystal, there is a relation between the wave vectors and the frequencies, i.e., a dispersion relation. This relation leads to the band structure of the photonic crystal. If, for some frequency range, no light of any polarization can propagate in a photonic crystal, the crystal is said to have a complete photonic band gap (PBG) [3]. In such a photonic crystal, no light modes, even the light stemming from spontaneous emission [1], can propagate if the frequency is within that PBG range. It has been shown that one can indeed design and construct such photonic crystals with photonic band gaps, preventing light with specific frequencies from propagating in certain directions.

If a single defect is introduced in an otherwise perfect photonic crystal, a mode (or group of modes) may be found at a frequency (or some frequencies) within the PBG. It is crucial to understand the nature of such localized modes for potential applications of doped photonic crystals in lasers [5], resonators [6], and wavelength division multiplexing (WDM) [7].
If one introduces a line defect (i.e., a waveguide) into a photonic crystal, one can guide light (whose frequencies are within the photonic band gap) from one location to another since the light cannot propagate in the surrounding PC. The transmission losses in a PC waveguide are very low for a wide range of frequencies, and vanish for specific frequencies, even through e.g. a sharp bend of $90^\circ$ [8].

Another way to guide light is by photonic crystal fibers, in which a single defect is introduced into two-dimensional (2D) photonic crystals, and the light is guided through the defect in the third dimension. Light may be confined to the vicinity of a low-index region in photonic crystal fibers. Optical fibers based on this waveguide mechanism support guided modes with extraordinary properties. It is different from the conventional optical fibers based on the well-known mechanism of total internal reflection. A photonic crystal fiber can be engineered to support only the fundamental guided mode at all frequencies, to be used as a large-mode-area fiber for fiber amplifiers or high-intensity light transmission, etc [9].

Photonic crystals may support surface modes (in which light is localized at a surface) for both two-dimensional and three-dimensional (3D) cases [3]. The study of surface modes in a PBG structure is important for e.g. reducing radiation losses for photonic crystal lasers and photonic crystal antennas [10].

A variety of methods have been used to calculate photonic band structures. Among these there are plane wave expansion method [11], multiple-scattering theory (Korringa-Kohn-Rostoker method) [12], tight-binding formulation [13], transfer matrix method [14], finite difference method [15,16], generalized Rayleigh identity method [17], averaged field approach [18-20] etc. These studies have shown many important properties of photonic crystals. Each method has its advantages and disadvantages, and one may choose a suitable method depending on particular problems.

The present thesis focuses on the investigation of some basic properties of photonic crystals, on the design novel two-dimensional photonic crystals, and on the development of methods to study photonic crystals. The methods used in the thesis are the plane wave expansion method and finite-difference time-domain (FDTD) method. An outline of the thesis is as follows. Section 2 gives the properties and some applications of photonic crystals. Section 3 contains a detailed description of the FDTD method, which is the main method used in the thesis to study in-plane and off-plane
band structures, defect modes, guided modes, surface modes, and fiber modes of two-dimensional photonic crystals. Section 4 is a short introduction to the plane wave expansion method, which is used to design a novel two-dimensional photonic crystal. Section 5 provides a summary of the papers that constitute the main part of the thesis.
2. Properties and applications of photonic crystals

In this section we give a short introduction to some basic properties and some applications of photonic crystals.

2.1. Photonic band structures

A crystal is a periodic arrangement of atoms or molecules. Therefore, a crystal presents a periodic potential to an electron propagation through it. In particular, the lattice might introduce gaps into the energy band structure of the crystal, so that electrons are forbidden to propagate with certain energies. The optical analogy of a conventional crystal is a photonic crystal, in which the periodicity is due to the periodic arrangement of dielectric or metallic materials. The dielectric ‘potential’ may produce many of the same phenomena for photons as the atomic potential does for electrons. Figure 1 shows two examples of three-dimensional photonic crystals, where (a) is the first photonic crystal which has a complete band gap [21], and (b) is a photonic crystal obtained by stacking Alumina rods [22].

![Figure 1](image1.png)

**Figure 1.** Examples of three-dimensional photonic crystals. (a) The first photonic crystal which has a complete band gap (E. Yablonovitch etc., 1991, *Source: http://www.ee.ucla.edu/labs/photon*). (b) A photonic crystal obtained by stacking Alumina rods (K. M. Ho etc. 1994, *Source: http://http://www.public.iastate.edu/~cmpexp/groups/hp/pbg.html*).
When electromagnetic waves propagate in a photonic crystal, there is a relation between the wave vectors and the frequencies, i.e., dispersion relation. This relation is called the *band structure* of the photonic crystal. A two-dimensional photonic crystal is periodic along a plane (e.g. xy-plane) and homogeneous along the third direction (e.g. z-direction). Therefore, propagating modes in the crystal must be oscillatory in the z-direction, with a wave vector $k_z$ (or $\beta$). If $k_z=0$, an electromagnetic wave can be decomposed into the $E$-polarization and $H$-polarization modes. If, for some frequency range, the electromagnetic waves cannot propagate in the photonic crystal for a given polarization, we say that the crystal has a photonic band gap for that polarization. If, for some frequency range, the electromagnetic waves cannot propagate in the photonic crystal for any polarization, we say that the crystal has a complete 2D photonic band gap.

We illustrate these concepts by some examples. Consider a two-dimensional square lattice of dielectric rods in air, in which the dielectric ‘atoms’ are isolated. The radius of the rod is $R=0.31a$ ($a$ is the lattice constant). The dielectric constant of the rods is $\varepsilon=11.4$. Figure 2 shows the band structures of the photonic crystal for both polarizations. One can see from Fig. 2 that there are three large band gaps for the $E$ polarization around frequencies 0.300, 0.450 and 0.700 ($\omega a/2\pi c$), respectively. However, there is no band gap for the $H$ polarization when the frequency is less than 0.800 ($\omega a/2\pi$). Therefore, there is no complete band gap for such a photonic crystal.

![Figure 2. Band structures of a square lattice of dielectric rods in air. The radius of the rods is $R=0.31a$. The dielectric constant of the rods is $\varepsilon=11.4$.](image-url)
Consider another two-dimensional photonic crystal, a square lattice of dielectric veins, in which the dielectric ‘atoms’ are connected. Figure 3 shows the band structures for this case with half vein width $d=0.120a$. From Fig. 3 one can see that there is a band gap for the $H$ polarization around the frequency $0.350 \ (\omega a/2\pi c)$, but there is no band gap for the $E$ polarization. Therefore, it appears that $E$ polarization band gaps are

Figure 3. Band structures of a square lattice of dielectric veins in air. The half vein width is $d=0.120a$. The dielectric constant of the veins is $\varepsilon=11.4$.

Figure 4. Band structures of a triangular lattice of air holes. The radius of the holes is $R=0.47a$. The dielectric constant of the background is $\varepsilon=11.4$. 
favored in a lattice of isolated high-\(\varepsilon\) regions, and \(H\) polarization band gaps are favored in a connected lattice. This is a rule of thumb for photonic band gaps [3].

To design a photonic crystal with a large complete two-dimensional band gap, one needs to make a compromise so that the high-\(\varepsilon\) regions of the structure are isolated to a considerable degree and linked only by narrow regions. This is usually achieved by using a triangular lattice of air holes. Figure 4 shows the band structures of a triangular lattice of air holes. The radius of the holes is \(R=0.47a\). The dielectric constant of the background is \(\varepsilon=11.4\). For such a photonic crystal, there is complete two-dimensional photonic band gap for both polarizations around the frequency 0.50 (\(\omega a/2\pi\)).

Paper I shows that elliptic air holes can be used effectively as inclusions to obtain a large complete band gap for two-dimensional photonic crystals. In paper II, we show how to use the rule of thumb for photonic band gaps and the conjugate gradient method to optimal design a two-dimensional square lattice photonic crystal which has a very large complete band gap. Paper III shows how to use the FDTD method to calculate the band structures of two-dimensional photonic crystals, also in the case of complicated inclusions.

Above we have shown the properties of band structures of two-dimensional photonic crystals in the case when \(k_z=0\). However, wave propagation out of the \(xy\)-plane is very important for studies of PC antennas, PC lasers and PC optical fibers, etc. In Paper IV, we show how to calculate the off-plane \((k_z\neq0)\) band structures of two-dimensional photonic crystals using the FDTD method.

### 2.2. Metallic photonic crystals

Metallic photonic band gap systems have received far less attention than dielectric photonic crystals. However, it has been suggested that periodic metallic structures have important applications, such as cavities [23], waveguides [24-25], and antennas [26-27]. Furthermore, metallic photonic crystals, with careful design, have robust photonic band gaps. Chan et al. [28,29] have designed a three-dimensional photonic crystal constructed by metallic ‘photonic atoms’, which are spheres with a dielectric core, a metal coating, and an outer insulating layer (a system made up of nontouching solid metal sphere will have qualitatively similar behavior). As long as the sphere filling ratio
Properties and applications

exceeds a threshold, robust photonic band gap exist in any periodic structure, such as face-centered cubic (FCC), body-centered cubic (BCC), the diamond structure, and even simple cubic (SC).

Metals, however, offer new challenges for the theoretical investigation of photonic crystals. From Maxwell's equations, the equivalent complex relative permittivity for a metal is \( \varepsilon_r(\omega) = 1 + i\sigma/\omega \) (for \( e^{-i\omega t} \) time dependence), whose imaginary part is proportional to \( \omega^{-1} \). For the plane wave method, such a metallic case is much more complicated than the case of purely dielectric materials, since it requires one is able to solve a generalized nonlinear eigenvalue problem. One may use a perturbative plane-wave approach [30] to solve this problem. However, such an approach requires the diagonalization of an equivalent, enlarged matrix, which increases the computational time and memory requirements. In Ref. [31], the relative permittivity for the metal was assumed to be real and have a simple form \( \varepsilon_r(\omega) = 1 - \omega_p^2/\omega^2 \) (\( \omega_p \) is the plasma frequency of the conduction electrons), and consequently Maxwell's equations can be transformed into a standard eigenvalue system after some manipulation. However, such a model for the frequency dependence of the permittivity is relevant only for high frequencies (far above the highest resonant frequency of the electrons).

Papers III-VIII show how to use the FDTD method to study photonic crystals, which may have metallic inclusions. The FDTD method can be applied to some complicated cases such as a photonic crystal whose inclusions contain both dielectric and metallic components.

### 2.3. Photonic crystal cavities

If a single defect is introduced in an otherwise perfect photonic crystal, a mode (or group of modes) may be found at a frequency (or some frequencies) within the PBG. The defect behaves like a cavity surrounded by reflecting walls, since the waves with these frequencies cannot propagate in the otherwise perfect crystal. Photonic crystal cavities, which usually have very high quality factors, can be compact and support only few modes.

Channel dropping filters, which can access one channel of a wavelength division multiplexed (WDM) signal while leaving other channels undisturbed, are essential
components of photonic integrated circuits and optical communication systems [7]. Resonant filters are attractive candidates for channel dropping, since they can potentially be used to select a single channel with a very narrow linewidth. A schematic picture of a resonant-cavity channel dropping filter is shown in Fig. 5. Since photonic crystal cavities are very efficient, one can naturally use them as components of channel
drop filters, which may achieve very high quality factors. Figure 6 shows a theoretical simulation of a photonic crystal channel drop filter structure with two cavities [32]. The quality factor $Q$ is larger than 1000. A transmission of essentially 100% between two waveguides can occur by choosing a suitable photonic crystal cavity.

There are also many other potential applications of photonic crystal cavities, such as lasers [5], resonators [6], antennas [33], waveguides [34], etc. Therefore, it is crucial to understand the nature of such localized defect modes. In paper V, we develop a method to calculate the defect modes based on the FDTD scheme.

2.4. Photonic crystal waveguides

Two main designs are commonly used to guide electromagnetic waves along a line: metallic pipe waveguides, and dielectric waveguides for infrared and visible light. Metallic waveguides provide lossless transmission only for microwaves, while dielectric waveguides have large losses at corners.

If one introduces a line defect (i.e., a waveguide) into a photonic crystal which has a photonic band gap, one can guide light (whose frequencies are within the photonic band gap) from one location to another since the light has nowhere else to go. Both theoretical simulations and experimental studies have shown that the transmission losses in a PC waveguide are very low for a wide range of frequencies, and vanish for specific frequencies, even through a $90^\circ$ sharp bend. Figure 7 shows the electric field pattern when an electromagnetic wave propagates through a photonic crystal waveguide sharp bend with essentially a 100% transmission [8]. For metallic photonic crystal waveguides, studies also show that an 85% transmission efficiency can be achieved even through a $90^\circ$ sharp bend with just a three unit cell thickness [24].

The study of guided modes in photonic crystal waveguides is very important for understanding the high transmission through sharp bends, and other properties [35,36]. Many studies have been carried out concerning guided modes in two-dimensional (2D) dielectric PBG crystals (see e.g. [37,38]). However, very few studies can be found in the literature concerning guided modes in metallic photonic band gap waveguides. Danglot et al. [39] have presented a modal analysis of a T-stub guiding structure patterned on a two-dimensional metallic photonic crystal. In paper VI, we study guided modes in a two-dimensional metallic photonic band gap crystal by the FDTD method. The relation
between the photonic crystal waveguide and the conventional metallic waveguide is also studied.

![Image](http://ab-initio.mit.edu/photons/index.html)

Figure 7. The electric field pattern when an electromagnetic wave propagates through a photonic crystal waveguide sharp bend. The photonic crystal is a square lattice of dielectric rods in air. The radius of dielectric rods is $R=0.18a$. The dielectric constant of the rods is $\varepsilon=11.4$. (Source: [http://ab-initio.mit.edu/photons/index.html](http://ab-initio.mit.edu/photons/index.html), the Joannopoulos Research Group at MIT)

2.5. **Surface modes in photonic crystals**

Real photonic crystals are necessarily bounded. Therefore, all real photonic crystals have surfaces. Theoretical and experimental studies have shown that photonic crystals may support surface modes (in which light is localized at the surface plane) for both two-dimensional and three-dimensional cases [3]. The study of surface modes in a PBG structure is important for e.g. reducing radiation losses for photonic crystal lasers and photonic crystal antennas [10]. In Paper VII, surface modes in two-dimensional dielectric and metallic photonic crystals are studied using the FDTD method. The
influence of the surface waves on the radiation pattern of a dielectric photonic crystal antenna has also been studied.

### 2.6. Photonic crystal fibers

Optical fibers are widely used in areas covering telecommunications, sensor technology, spectroscopy, and medicine [40]. A conventional optical fiber has a central core with a refractive index greater than that of the surrounding cladding, and is based on the principle of total internal reflection.

![Figure 8](http://www.bath.ac.uk/Departments/Physics/groups/opto/pcf.html, the Optoelectronics Group at University of Bath, UK.)

Figure 8. (a) A scanning electron micrograph (SEM) image of a photonic band-gap fibre. The region with the extra air hole in the centre acts as the core, in which light is guided by a photonic band-gap. The fibre is about 40 microns across. (b) The end of a PBG fibre, as seen under an optical microscope. The other end of the fibre is illuminated with white light. Only the region around the core is shown.

A special class of optical fibers is photonic crystal fibers [9], which is obtained by introducing a single defect into two-dimensional photonic crystals, and the light is guided through the defect in the third dimension. Optical fibers based on this waveguide
mechanism support guided modes with extraordinary properties. Light may be confined to the vicinity of a low-index region in photonic crystal fibers. Such a fiber can be engineered to support only the fundamental guided mode at all frequencies, to be used as a large-mode-area fiber for fiber amplifiers or high-intensity light transmission, etc. Figure 8 shows an example of a photonic crystal fiber [9].

Theoretical studies of guided modes in photonic crystal fibers employ a wide variety of techniques, including plane wave expansion method [41], effective-index approach [42], localized basis function method [43], full-vector biorthonormal-basis modal method [44], and finite element method [45]. In paper VIII, an FDTD method is proposed for the full-wave analysis of guided modes in photonic crystal fibers.
3. Finite-Difference Time-Domain method

The Finite-Difference Time-Domain (FDTD) method is a very often used approach to solve Maxwell’s equations [46]. It has been used to solve a wide variety of problems related to electromagnetic waves, such as wave propagation, scattering, electronic circuits, antenna analysis, etc. In the present section, some details about the FDTD method will be given, and it is also shown how to use it to study photonic crystals.

3.1. Three-dimensional FDTD time-stepping formulas

For a linear isotropic material in a source-free region, the time-dependent Maxwell's curl equations can be written in the following form,

\[ \frac{\partial \vec{H}}{\partial t} = -\frac{1}{\mu(\vec{r})} \nabla \times \vec{E} \quad (1) \]

\[ \frac{\partial \vec{E}}{\partial t} = \frac{1}{\varepsilon(\vec{r})} \nabla \times \vec{H} - \frac{\sigma(\vec{r})}{\varepsilon(\vec{r})} \vec{E} \quad (2) \]

where \( \varepsilon(\vec{r}) \), \( \mu(\vec{r}) \) and \( \sigma(\vec{r}) \) are the position dependent permittivity, permeability and conductivity of the material, respectively.

Maxwell's equations can be discretized in space and time by a so-called Yee-cell technique [47] on a discrete three-dimensional mesh. Figure 9 depicts the unit Yee cell (not to be confused with the photonic crystal unit cell) of the three-dimensional mesh. The following FDTD time stepping formulas constitute the discretization (in space and time) of Maxwell's equations on a discrete three-dimensional mesh in a Cartesian \( xyz \) coordinate system [46],

\[ H^t_{x,j,k} \quad (i,j,k) = H^{t-1/2}_{x,j,k} + \Delta \frac{E^t_{y,j,k+1} - E^t_{y,j,k}}{\Delta \varepsilon} \quad (3) \]

\[ H^t_{y,j,k} \quad (i,j,k) = H^{t-1/2}_{y,j,k} + \Delta \frac{E^t_{z,j,k+1} - E^t_{z,j,k}}{\Delta \varepsilon} \quad (4) \]
\[ H_y^{n+1/2}_{i,j,k} = H_y^{n+1/2}_{i,j,k} - \frac{\Delta t}{\mu_{i,j,k}} \left( \frac{E_y^{n+1}_{i+1,j,k} - E_y^{n}_{i,j,k}}{\Delta x} - \frac{E_y^{n}_{i,j,k+1} - E_y^{n}_{i,j,k}}{\Delta y} \right), \hspace{1cm} (5) \]

\[ E_x^{n+1}_{i,j,k} = \frac{\sigma_{i,j,k}}{\varepsilon_{i,j,k}} \frac{\Delta t}{2} E_y^{n+1}_{i+1,j,k} + \frac{\Delta t}{\varepsilon_{i,j,k} + \sigma_{i,j,k} \Delta t/2} \left( \frac{H_z^{n+1/2}_{i,j,k}}{\Delta x} - \frac{H_z^{n+1/2}_{i,j,k-1}}{\Delta z} \right), \hspace{1cm} (6) \]

\[ E_y^{n+1}_{i,j,k} = \frac{\sigma_{i,j,k}}{\varepsilon_{i,j,k}} \frac{\Delta t}{2} E_x^{n+1}_{i,j,k} + \frac{\Delta t}{\varepsilon_{i,j,k} + \sigma_{i,j,k} \Delta t/2} \left( \frac{H_z^{n+1/2}_{i,j,k}}{\Delta z} - \frac{H_z^{n+1/2}_{i,j-1,k}}{\Delta x} \right), \hspace{1cm} (7) \]

\[ E_z^{n+1}_{i,j,k} = \frac{\sigma_{i,j,k}}{\varepsilon_{i,j,k}} \frac{\Delta t}{2} E_y^{n+1}_{i,j,k} + \frac{\Delta t}{\varepsilon_{i,j,k} + \sigma_{i,j,k} \Delta t/2} \left( \frac{H_x^{n+1/2}_{i,j,k}}{\Delta y} - \frac{H_x^{n+1/2}_{i,j-1,k}}{\Delta x} \right), \hspace{1cm} (8) \]

where the superscript \( n \) indicates the discrete time step, the subscripts \( i, j \) and \( k \) indicate the position of a grid point in the \( x, y \) and \( z \) directions, respectively. \( \Delta t \) is the time...
increment, and $\Delta x$, $\Delta y$, and $\Delta z$ are the space increments between two neighboring grid points along the $x$, $y$ and $z$ directions, respectively.

One can easily see that for a fixed total number of time steps the computational time is proportional to the number of discretization points in the computation domain, i.e., the FDTD algorithm is of order $N$.

### 3.2. Compact FDTD time-stepping formulas

For a system which is homogeneous along the $z$ direction, (e.g., the direction of photonic crystal fibers), one can introduce the propagation constant along the $z$-direction (propagation direction) $\beta$. Thus, each field component has the form $\phi(x, y, z) = \phi(x, y)e^{ikz}$, where $\phi$ denotes any field component. In Maxwell's equations, therefore, the $z$ derivatives can be replaced with $j\beta$, to reduce them to a two-dimensional space [48]. Figure 10 gives the unit Yee cell of the two-dimensional mesh over the cross-section of the system. For example, the discrete form of the $x$ component of $H_x$ becomes,

$$H_x|^{n+1/2} = H_x|^{n-1/2} - \frac{\Delta t}{\mu_{i,j}} \left( \frac{E_z|_{i,j+1}^{n} - E_z|_{i,j}^{n}}{\Delta y} - j\beta E_y|_{i,j}^{n} \right)$$

(9)

The rest of the equations for other field components can be obtained in a similar manner.

**Figure 10.** The unit Yee cell of the two-dimensional hybrid FDTD mesh.
The above equation introduces complex number into the computation. It does not change the complexity of computations when calculating the off-plane band structures for two-dimensional photonic crystals, since the boundary conditions are the complex Bloch theory (see the paper IV). However, when computing guided modes in photonic crystal fibers, one wishes to refer only to real number. One way to eliminate the complex number is to assume that $E_z$, $H_x$, and $H_y$ have a component $\cos(\beta z + \psi)$, and $H_z$, $E_x$, and $E_y$ have a component $\sin(\beta z + \psi)$ [49], where $\psi$ is the phase factor. Then, equation (9) becomes,

$$
H_z^{n+1/2}|_{i,j} = H_z^{n-1/2}|_{i,j} - \frac{\Delta t}{\mu_{ij}} \left( E_z^n_{i,j+1} - E_z^n_{i,j} \right) - \beta E_y^n_{i,j}, (10)
$$

Only real variables remain. The other field components are given by the following equations,

$$
H_x^{n+1/2}|_{i,j} = H_x^{n-1/2}|_{i,j} - \frac{\Delta t}{\mu_{ij}} \left( \beta E_z^n_{i,j} - E_z^n_{i+1,j} \right), (11)
$$

$$
E_x^{n+1}|_{i,j} = \frac{E_x^n_{i,j} - \sigma_{ij} \Delta t / 2}{\epsilon_{ij} + \sigma_{ij} \Delta t / 2} E_x^n_{i,j} +
\frac{\Delta t}{\epsilon_{ij} + \sigma_{ij} \Delta t / 2} \left( H_z^{n+1/2}|_{i,j} - H_z^{n+1/2}|_{i,j-1} + \beta H_y^{n+1/2}|_{i,j} \right), (13)
$$

$$
E_y^{n+1}|_{i,j} = \frac{E_y^n_{i,j} - \sigma_{ij} \Delta t / 2}{\epsilon_{ij} + \sigma_{ij} \Delta t / 2} E_y^n_{i,j} +
\frac{\Delta t}{\epsilon_{ij} + \sigma_{ij} \Delta t / 2} \left( -\beta H_x^{n+1/2}|_{i,j} - H_x^{n+1/2}|_{i,j-1} \right), (14)
$$

$$
E_z^{n+1}|_{i,j} = \frac{E_z^n_{i,j} - \sigma_{ij} \Delta t / 2}{\epsilon_{ij} + \sigma_{ij} \Delta t / 2} E_z^n_{i,j} +
\frac{\Delta t}{\epsilon_{ij} + \sigma_{ij} \Delta t / 2} \left( H_x^{n+1/2}|_{i,j} - H_x^{n+1/2}|_{i,j-1} - H_z^{n+1/2}|_{i,j-1} \right), (15)
$$
3.3. Two-dimensional FDTD time-stepping formulas

In a two-dimensional case, the fields can be decoupled into two transversely polarized modes, namely the $E$ polarization ($E_z, H_x,$ and $H_y$) and the $H$ polarization ($H_z, E_x,$ and $E_y$). The FDTD time-stepping formulas can be easily obtained by simply letting $\beta=0$ in the equations 10-15 for the Cartesian coordinate system.

For triangular lattice photonic crystals or honeycomb photonic crystals, it is difficult to discretize the unit cell (not the Yee cell) using the orthogonal Cartesian coordinate. Therefore, it is convenient to use a nonorthogonal FDTD method to study such systems. Define a nonorthogonal coordinate ($\xi, \eta$) in accordance with the skew lattice of the photonic crystal (with an angle $\theta$ between the axis $\xi$ and the axis $\eta$). We discretize the entire plane with a mesh of uniform cells formed by lines of constant $\xi$ and $\eta$, and obtain a two-dimensional nonorthogonal mesh as shown in Fig. 11. Thus, the following FDTD time-stepping formulas for the $E$ polarization case are obtained,

$$
\begin{align*}
H^{n+1/2}_{\xi,i,j} &= H^{n-1/2}_{\xi,i,j} - \frac{\Delta}{\mu_{i,j}} E^n_{z,i,j+1} - E^n_{z,i,j} + \frac{\cos\theta\Delta}{\mu_{i,j}} \\
& \quad \times \left( \frac{E^n_{z,i+1,j} + E^n_{z,i,j+1} - E^n_{z,i-1,j} - E^n_{z,i,j-1}}{4\Delta^2 \xi \sin \theta} \right),
\end{align*}
$$

(16)

Figure 11. A nonorthogonal two-dimensional mesh for a skew lattice. The axes are labeled by $\xi$ and $\eta$, and the angle between them is $\theta$. 
\[ H_{\eta}^{n+1/2} = H_{\eta}^{n-1/2} + \frac{\Delta t}{\mu_{i,j}} \left( E_{z,j+i+1}^{n} - E_{z,j+i}^{n} \right) - \frac{\cos \theta \Delta t}{\mu_{i,j}} \left( \sin \xi \sin \theta \left( E_{z,j+i+1}^{n} + E_{z,j+i}^{n} \right) - E_{z,j+i-1}^{n} - E_{z,j+i-2}^{n} \right) \]  

\[ E_{z}^{n+1/2} = E_{z}^{n-1/2} + \frac{\Delta t}{\varepsilon_{i,j} + \sigma_{i,j} \Delta t/2} \left( \frac{H_{\eta,j+i+1}^{n} - H_{\eta,j+i}^{n}}{\Delta \xi \sin \theta} - \frac{H_{\eta,j+i-1}^{n} - H_{\eta,j+i-2}^{n}}{\Delta \eta \sin \theta} \right) \]  

We can also obtain the following FDTD time-stepping formulas for the \( H \) polarization case,

\[ E_{x}^{n+1/2} = E_{x}^{n-1/2} + \frac{\Delta t}{\varepsilon_{i,j} + \sigma_{i,j} \Delta t/2} \left( \frac{H_{\eta,j+i+1}^{n} - H_{\eta,j+i}^{n}}{\Delta \xi \sin \theta} - \frac{H_{\eta,j+i-1}^{n} - H_{\eta,j+i-2}^{n}}{\Delta \eta \sin \theta} \right) \]

\[ E_{y}^{n+1/2} = E_{y}^{n-1/2} + \frac{\Delta t}{\varepsilon_{i,j} + \sigma_{i,j} \Delta t/2} \left( \frac{H_{\eta,j+i+1}^{n} - H_{\eta,j+i}^{n}}{\Delta \xi \sin \theta} - \frac{H_{\eta,j+i-1}^{n} - H_{\eta,j+i-2}^{n}}{\Delta \eta \sin \theta} \right) \]

\[ H_{z}^{n+1/2} = H_{z}^{n-1/2} - \frac{\Delta t}{\mu_{i,j}} \left( \frac{E_{\eta,j+i+1}^{n} - E_{\eta,j+i}^{n}}{\Delta \xi \sin \theta} - \frac{E_{\xi,j+i+1}^{n} - E_{\xi,j+i}^{n}}{\Delta \eta \sin \theta} \right) \]

**3.4. Numerical stability**

The choice of the time step \( \Delta t \) is not arbitrary. The FDTD time-stepping formulas require that \( \Delta t \) has a specific bound relative to the space increments \( \Delta x, \Delta y, \) and \( \Delta z \). This bound is necessary to avoid numerical instability, an undesirable possibility with explicit differential equation solvers that can cause the computed results to spuriously increase without limit as time-marching continues [46].

The three-dimensional FDTD time-stepping formulas are stable numerically if the following condition is satisfied [46],
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\[ \Delta t \leq 1/c \sqrt{\Delta x^{-2} + \Delta y^{-2} + \Delta z^{-2}}, \tag{22} \]

where \( c \) is the speed of the light. For compact FDTD time-stepping formulas, the stability condition becomes \[50\]

\[ \Delta t \leq 1/c \sqrt{\Delta x^{-2} + \Delta y^{-2} + (\beta/2)^2}. \tag{23} \]

For two-dimensional FDTD time-stepping formulas, the stability conditions for orthogonal case is \[46\]

\[ \Delta t \leq 1/c \sqrt{\Delta x^{-2} + \Delta y^{-2}}, \tag{24} \]

and for nonorthogonal case \[51\]

\[ \Delta t \leq \sin \theta/c \sqrt{\Delta \xi^{-2} + \Delta \eta^{-2}}. \tag{25} \]

3.5. Boundary conditions

Special consideration should be given to the boundary of the finite computational domain, where the fields are updated using special boundary conditions since information outside the computational domain is not available.

When calculating the band structures of photonic crystals, one naturally chooses a unit cell of lattice as the finite computation domain, and uses the periodic boundary condition, which satisfies the Bloch theory. Therefore, we have the following simple boundary conditions for updating the fields,

\[ E(\vec{r} + \vec{L}) = e^{i\vec{k} \cdot \vec{L}} E(\vec{r}) \]
\[ H(\vec{r} + \vec{L}) = e^{i\vec{k} \cdot \vec{L}} H(\vec{r}), \tag{26} \]

where \( \vec{L} \) is the lattice vector.

When calculating defect modes (or guided modes in photonic crystal fibers), one can also use the perfectly matched layer (PML) method \[52\] for the boundary treatment. In the PML, the electric or magnetic field components are split into two subcomponents (e.g., \( E_z = E_{zx} + E_{zy} \)) with the possibility of assigning losses to the individual split field components. The net effect of this is to create an absorbing medium (which is nonphysical) adjacent to the outer FDTD mesh boundary such that the interface between the PML and the FDTD mesh is reflectionless for all frequencies, polarizations, and angles of incidence. The FDTD technique can be applied directly for the numerical
implementation of the fields inside the PML without any special treatment (the details can be found in e.g. Ref. [52]).

One may use a combination of the periodic boundary condition and the PML when calculating the guided modes or surface modes in photonic crystals (see the paper VI and the paper VII).

### 3.6. Initial field distributions

In a conventional FDTD method, which is developed for solving electromagnetic scattering problems, one uses a known pulsed incident field as the initial field distribution (before the incident pulse reaches the scatterer). In our computations, an artificial initial field distribution is used. The non-physical components in the initial field distribution will disappear in the time evolution, and only the physical components will remain if the evolution time is long enough. The initial fields are different for different situations. The details can be found in the paper III and the paper V.

### 3.7. Transformation to the frequency domain

With the FDTD method, all the fields are obtained in the time domain. However, the dispersion relation (the band structures, guided modes, etc) of a photonic crystal is a relation between the frequency $\omega$ and the wave vector. Therefore, we need to perform a Fourier transform,

$$\int_{-\infty}^{\infty} u(t)e^{i\omega t} dt,$$

where $u$ is one of the field components. Unfortunately, the exact Fourier transform cannot be obtained since the information about $u(t)$ for $t<0$ is not available in our computation. However, one is not interested in the exact spectral shape of Fourier transform but the peaks of the spectral distribution, which correspond to the locations of the eigen frequencies. Therefore, one can use the following transformation to obtain the spectrum,

$$u(\omega) = \int_{0}^{N_J} u(t)e^{i\omega t} dt \approx \sum_{n=0}^{N_J} u(n\Delta t)e^{i\omega n\Delta t} \Delta t,$$
where \( N_t \) is the total number of time steps. The peaks of the function \( u(\omega) \) are located at the same places as the peaks in the Fourier transform of \( u(t) \), and these peaks become higher (more obvious) as \( N_t \) increases.

One should eliminate the zero-frequency longitudinal mode in the calculation, i.e., one should subtract the static component from the fields so that their time average is zero [53]. Also, it is not always necessary to calculate the above transformation at all the discretization points in the unit cell of lattice (the computation domain). One may choose 100 points randomly and then sum up the spectral amplitudes at all these points, i.e.,

\[
U(\omega) = \sum_{i,j}^{N_t} \left[ u_{i,j}(n\Delta t) - \frac{1}{n} \sum_{m=0}^{n} u_{i,j}(m\Delta t) \right] e^{i\omega_n \Delta t},
\]

where \((i,j)\) indicates the 100 randomly chosen points. The peaks of the spectral function \( U(\omega) \) indicate the locations of the eigen frequencies \( \omega \).
4. Plane wave expansion method

The plane wave expansion method, which solves Maxwell’s equations in frequency domain, is one of the most widely used methods in the study of photonic crystals. There are many versions of the plane wave expansion method [11,54-58]. In the present section, we give a short introduction to the method proposed by Ho, Chan and Soukoulis [11].

4.1. Master equation

Assume that each field has a harmonic time dependence $e^{-i\omega t}$. Maxwell’s curl equations can be written as (provided that the material permeability is $\mu_0$)

$$\nabla \times \vec{E} = i\omega \mu_0 \vec{H},$$  
(30)

$$\nabla \times \vec{H} = -i\omega \varepsilon_0 \varepsilon_r(\vec{r})\varepsilon_0 \varepsilon_r(\vec{r}) \vec{E},$$  
(31)

where $\varepsilon_r(\vec{r})$ is the dielectric constant function of photonic crystals. The above equations can be further simplified to

$$\nabla \times \left( \frac{1}{\varepsilon_r(\vec{r})} \nabla \times \vec{H} \right) = \frac{\omega^2}{c^2} \vec{H},$$  
(32)

where the speed of light $c = 1/\sqrt{\varepsilon_0 \mu_0}$. This is the master equation.

4.2. Eigenvalue problem

Since $\varepsilon_r(\vec{r})$ is periodic, we can use Bloch’s theorem to expand the $\vec{H}$ field in plane waves,

$$\vec{H}(\vec{r}) = \sum_G \sum_{\lambda=1,2} h_{\lambda G} \hat{e}_\lambda e^{i(k+G)\vec{r}},$$  
(33)

and also for the dielectric constant $\varepsilon_r(\vec{r})$,

$$\frac{1}{\varepsilon_r(\vec{r})} = \sum_G \varepsilon_r^{-1}(\hat{G}) e^{i\hat{G} \vec{r}},$$  
(34)
where \( \mathbf{k} \) is a wave vector in the Brillouin zone of the lattice, \( \mathbf{G} \) is a reciprocal-lattice vector, and \( \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2 \) are unit vectors perpendicular to \( \mathbf{k} + \mathbf{G} \) because of the transverse nature of \( \mathbf{H} \) (i.e., \( \nabla \cdot \mathbf{H} = 0 \)). Substituting into the master equation we obtain the following matrix equations:

\[
\sum_{\mathbf{G}} \mathbf{G}(\mathbf{k} + \mathbf{G}) \mathbf{e}^{-1}(\mathbf{G} - \mathbf{G})(\hat{\mathbf{e}}_2 \cdot \hat{\mathbf{e}}_2 \quad -\hat{\mathbf{e}}_2 \cdot \hat{\mathbf{e}}_1) h_{\mathbf{G} \mathbf{k}} = \left(\frac{\omega}{c}\right)^2 h_{\mathbf{G} \mathbf{k}}. \tag{35}
\]

The above equation can be solved using standard matrix-diagonalization methods. For different wave vectors \( \mathbf{k} \), one can obtain a series of eigen-frequencies \( \omega \), which compose the band structures of photonic crystals.
5. Summary of papers

5.1. Paper I

Using the plane wave expansion method, we show that inclusions of elliptic air holes can be used effectively to obtain a larger complete band gap for 2D photonic crystals. For air holes in the gallium arsenide, we describe a two-step design using the rule of thumb for photonic band gaps to find quickly the optimal configuration, which gives the maximum complete band gap. The optimal complete band gaps for air holes in other dielectric medium are also studied. Such a 2D photonic crystal is very convenient for use as cladding for a photonic crystal fiber.

5.2. Paper II

In this paper, we consider an optimal design of a two-dimensional photonic crystal with a square lattice of air holes in gallium arsenide (GaAs) using the plane wave expansion method. Since $E$ polarization band gaps are favored in a lattice of isolated high-$\varepsilon$ regions, and $H$ polarization band gaps are favored in a connected lattice, a big complete two-dimensional band gap can be obtained by connecting dielectric rods with veins. The design has been improved further by using an optimization technique, namely, the conjugate gradient method. The complete two-dimensional band gap of our optimal design reaches $\Delta\omega=0.0762\ (\omega a/2\pi)$. To the best of our knowledge, our optimal design gives the largest complete two-dimensional band gap that has been reported so far in the literature for a square air/GaAs lattice.

5.3. Paper III

A FDTD scheme in a nonorthogonal coordinate system is presented in this paper to calculate the band structure of a two-dimensional photonic crystal consisting of a skew lattice. The present FDTD algorithm can easily be used for any complicated inclusion configuration, which can have both the dielectric and metallic inclusions. The method has been verified by comparing with the results obtained by other methods for some
special cases. The band structures for the square and triangular array of metallic columns in the air have been presented. The band structure of a photonic crystal with a dielectric layer coated on a metallic cylinder as an inclusion has also been studied, and it has been noticed that both the dielectric and metallic characteristics of the band structure are inherited. As one of the major advantages of the FDTD method, the computational time is proportional to the number of the discretization points in the computation domain (i.e., it is of order $N$).

5.4. Paper IV

An effective FDTD method to study the off-plane wave propagation in a two-dimensional photonic crystal is proposed in the present paper. The method requires only a two-dimensional mesh for a given off-plane wave number $k_z$. The CPU time and memory space have been reduced significantly. The method has been verified numerically by comparing with the conventional plane-wave expansion method. The numerical method can be used for a metallic photonic crystal without any extra effort. The off-plane band structures of a square lattice of metallic rods in air have been studied. It has been found that there exists a complete bandgap in such a metallic photonic crystal for nonzero $k_z$.

5.5. Paper V

A numerical method based on the finite-difference time-domain scheme for computing defect modes in two-dimensional photonic crystals (with dielectric or metallic inclusions) is presented. Our method can be used for any type of dielectric or metallic inclusions by utilizing an artificial initial field distribution. Compared to the FDTD transmission spectra method, the present method reduces the computation domain significantly. We demonstrate that, by means of this method, one can find defect modes, which are not activated by the incident plane wave in the FDTD transmission spectra method. The calculated eigen frequencies and field patterns for a defect in a square array of dielectric rods are consistent with those obtained by the plane wave expansion method. The defect modes for a metallic photonic crystal with a square array of copper
rods have also been studied, and our numerical results are consistent with experimental results.

5.6. Paper VI
Guided modes in a two-dimensional metallic photonic crystal waveguide are studied using a finite-difference time-domain method. A combination of the periodic boundary condition and the perfectly matched layer is used for the boundary treatment. The guided modes in the photonic crystal waveguide are related to those in a conventional metallic waveguide. There exists a cutoff frequency and consequently a mode gap at low frequencies (starting from zero frequency) in the photonic crystal metallic waveguide. Due to the loss of the translational symmetry in a metallic photonic bandgap waveguide, the band curves with the same symmetry may repel each other at a crossing point.

5.7. Paper VII
We have studied surface modes in two-dimensional dielectric and metallic photonic crystals using the FDTD method. Our computations show that surface metallic photonic crystals which are square lattice of metallic rods in air. However, the surface modes do not exist in a metallic photonic crystal, which is a square lattice of metallic rods in air. However, if we insert metallic rods in a dielectric medium (alumina), there are surface cavity modes in the (11) direction, since the metallic rods and the dielectric surface act as a cavity. The influence of the surface waves on the radiation pattern of a dielectric photonic crystal antenna has also been studied. The surface waves change the radiation pattern significantly. One should avoid those types of surfaces, which support surface modes, when constructing photonic crystal antennas.

5.8. Paper VIII
An efficient finite-difference time-domain method is proposed for the full-wave analysis of guided modes in photonic crystal fibers. The three-dimensional hybrid guided modes can be calculated by a two-dimensional mesh, if one assumes that the propagation
Summary of papers

constant along the $z$-direction (propagation direction) is $\beta$. Furthermore, only real variables are used in the present method. Therefore, computational time and computer memory are significantly reduced. The results for a honeycomb-based silica-air photonic crystal fiber are in very good agreement with the results from the plane expansion method.
6. References

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