ELSEVIER

Science and Technology of Advanced Materials 6 (2005) 837–841

SCIENCE AND TECHNOLOGY OF ADVANCED MATERIALS

www.elsevier.com/locate/stam

Principles of the plane-wave transfer-matrix method for photonic crystals

Zhi-Yuan Li*

Institute of Physics, Chinese Academy of Sciences, P. O. Box 603, Beijing 100080, China

Received 11 March 2005; revised 9 June 2005; accepted 9 June 2005
Available online 29 September 2005

Abstract

We introduce the principle of the plane-wave transfer-matrix method, a theoretical tool that we have recently developed systematically to solve optical problems of photonic crystals (PCs). In this formulation, the electromagnetic fields are expanded into superposition of plane waves associated with the crystal lattice, which facilitates access to many advanced Fourier analysis techniques. We briefly discuss the standard application of the TMM to solution of transmission, reflection and absorption spectra for a finite PC slab and photonic band structures for an infinite PC. Then we push the formulation further to handle wave propagation in semi-infinite PC crystal structures. The three-dimensional wood-pile PC is taken as an example to show the power of the theory.

Keywords: Photonic crystals; Plane waves; Transfer-matrix method; Functional elements

1. Introduction

Photonic crystals (PCs) are artificial materials made from periodic arrays of dielectric or metallic building blocks. The existence of photonic band gaps (PBGs) has brought about an unprecedented power to control and manipulate the propagation of electromagnetic (EM) waves [1–3]. The most promising and fundamental aspect of PCs is that they can serve as the physical platform of future ultra-small photonic integrated circuits, which involve a wide variety of functional elements and devices, such as waveguides, waveguide bends, cavities, beam splitters, modulators, optical switches, channel-drop filters, wave division multiplexers, and so on [4–8].

Many theoretical and numerical tools have been developed to understand and design PC structures, elements, and devices. Among them the popular ones are the plane-wave expansion method (PWEM) [9–11], finite-difference time-domain (FDTD) technique [12], and real-space transfer-matrix method [13]. These methods can study different aspects of the optical properties of PC structures. For instance, the PWEM can conveniently examine the photonic band diagram of an infinite PC, while the FDTD technique is the best weapon to govern the dynamics of wave transport in PC structures. Recently, we have systematically developed a plane-wave transfer-matrix method (PWTMM) and explored its power in application to a wide variety of problems involving PC structures, functional elements, and optical devices [14–20].

The PWTMM has several advantages. First, it can solve the standard problem of the photonic band structures [14] and the scattering (transmission, reflection, and absorption) spectrum [15,16]. As a frequency-domain technique, the PWTMM allows for accurate spectrum solution. When combined with a supercell technique, the approach can also handle PC waveguides and cavities [17–20]. Second, is exhibits excellent numerical convergency and accuracy due to the incorporation of many advanced Fourier-analysis skills [14,18,21,22], and the numerical burden is logarithmatically proportional to the sample length of a finite PC structure. Third, the approach can also handle metallic materials and PC structures that exhibit loss of power to the background [15,18]. Finally and most importantly, this approach can successfully handle wave propagation in semi-infinite PC structures, and efficiently explore the intrinsic optical properties of a variety of functional elements embedded in the PC background [17–20]. Armed with these powers, the PWTMM can deal with a large range

* Corresponding author. Tel.: +86 10 82648106; fax: +86 10 82649531.
E-mail address: lizy@aphy.iphy.ac.cn

1468-6996/$ - see front matter © 2005 Elsevier Ltd. All rights reserved.
doi:10.1016/j.stam.2005.06.013

of optical problems involving PC structures and devices. In the following sections we will briefly introduce the main principles of the PWTMM and its application to several typical problems. We will take the three-dimensional woodpile PC structure as an example to demonstrate the approach.

2. Principles of PWTMM

Like all other optical problems, the PMTMM also starts from Maxwell's equations. For a general PC structure Maxwell's equations read

$$\nabla \times \mathbf{E}(\mathbf{r}) = ik_0\mu(\mathbf{r})\mathbf{H}(\mathbf{r}),$$
$$\nabla \times \mathbf{H}(\mathbf{r}) = -ik_0\varepsilon(\mathbf{r})\mathbf{E}(\mathbf{r}). \tag{2.1}$$

Here $k_0=\omega/c$ is the wave number, c is the light speed in vacuum, and ω is the angular frequency of the EM wave. In usual photonic structures, the composite materials are nonmagnetic, and $\mu(\mathbf{r})=1$. But generally one can consider a general case where both $\varepsilon(\mathbf{r})$ and $\mu(\mathbf{r})$ are spatially periodic functions. For anisotropic composite materials, $\varepsilon(\mathbf{r})$ and $\mu(\mathbf{r})$ are even second-rank tensors.

Assume that the EM wave propagates along the z-axis direction. In the PWTMM, only the tangential components of EM fields, E_x, E_y, H_x, and H_y are considered. They satisfy four coupled differential equations that can be derived from Eq. (2.1) [14]. The PC can be looked upon as a stack of grating layers along the wave propagation direction. The grating is characterized by the primitive lattice $\mathbf{R}$(with basic vectors $\mathbf{a}_1$ and $\mathbf{a}_2$) and reciprocal lattice $\mathbf{G}$ (with basic vectors $\mathbf{b}_1$ and $\mathbf{b}_2$).

The EM fields at an arbitrary point $\mathbf{r}$ can be written into the superposition of Bragg waves (or plane waves).

$$\mathrm{E(r)} = \sum_{ij} \mathrm{E}_{ij}(z)\mathrm{e}^{i(k_{ij,x}x+k_{ij,y}y)},$$
$$\mathrm{H(r)} = \sum_{ij} \mathrm{H}_{ij}(z)\mathrm{e}^{i(k_{ij,x}x+k_{ij,y}y)}, \tag{2.2}$$

where the Bragg wave vector $\mathbf{k}_{ij}=(k_{ij},x,k_{ij},y)=(k_{0x},k_{0y})+ib_1+j\mathbf{b}_2=(k_{0x},k_{0y})+\mathbf{G}_{ij}$, with (k_{0x}, k_{0y}) being the incident wave vector. $\mathbf{E}_{ij}$ and $\mathbf{H}_{ij}$ are unknown expansion coefficients of the electric and magnetic fields. The permittivity and permeability functions are also expanded into plane-wave functions:

$$\varepsilon(\mathrm{r}) = \sum_{ij} \varepsilon_{ij}(z)\mathrm{e}^{i\mathrm{G}_{ij}\cdot\mathrm{r}}, \qquad \varepsilon^{-1}(\mathrm{r}) = \sum_{ij} \varepsilon_{ij}^{-1}(z)\mathrm{e}^{i\mathrm{G}_{ij}\cdot\mathrm{r}},$$
$$\mu(\mathrm{r}) = \sum_{ij} \mu_{ij}(z)\mathrm{e}^{i\mathrm{G}_{ij}\cdot\mathrm{r}}, \qquad \mu^{-1}(\mathrm{r}) = \sum_{ij} \mu_{ij}^{-1}(z)\mathrm{e}^{iG_{ij}\cdot\mathbf{r}}. \tag{2.3}$$

In the framework of the above basic mathematical formalisms, the overall working principles of the PWTMM can be well described by Fig. 1. First, as depicted in Fig. 1(a), the unit cell along the z-axis is divided into a number of thin slices, each of which is approximated as a lamellar grating with $\varepsilon_{ij}(z)$ etc. in Eq. (2.3) all being constants within the slice. Each thin slice is then surrounded by two infinitely thin air films that are artificially inserted in the two hand sides. The main advantage of this procedure is great simplicity and clarity: The solution to all different slices can be placed into a uniform free-space plane-wave space. Second, construct the transfer matrix for each slice, as depicted in Fig. 1(b). This requires the knowledge of EM fields in the two air films as well as within the slice. The field within the periodic slice can be solved by inserting the plane-wave expansion forms Eqs. (2.2) and (2.3) into Maxwell's equations Eq. (2.1), while the field in the air films has simple analytical solutions that are completely characterized by the plane-wave expansion coefficients [14]. The transfer matrix is defined to connect the column vectors consisting of plane wave coefficients in the right-hand air films (Ω_i^+, Ω_i^-) to those in the left-hand air films $(\Omega_{i-1}^+, \Omega_{i-1}^-)$. We can write down

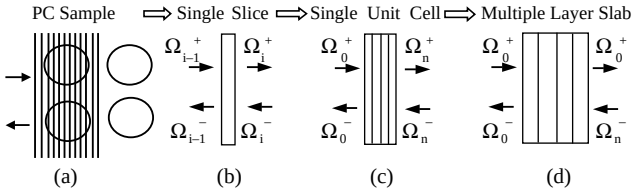

Fig. 1. Schematic picture showing how the PWTMM is applied to a photonic crystal.

$$\begin{pmatrix} \Omega_i^+ \\ \Omega_i^- \end{pmatrix} = t_i \begin{pmatrix} \Omega_{i-1}^+ \\ \Omega_{i-1}^- \end{pmatrix}, \qquad \begin{pmatrix} \Omega_i^+ \\ \Omega_{i-1}^- \end{pmatrix} = s^i \begin{pmatrix} \Omega_{i-1}^+ \\ \Omega_i^- \end{pmatrix}. \tag{2.4}$$

t_i and s^i are called T-matrix and S-matrix for the *ith* slice, respectively. General speaking, the T-matrix connects the fields at the right side of a slice to the fields at the left side, while the S-matrix connects the outgoing (scattering) fields to the ingoing (incident) fields for the slice.

With all the individual transfer matrices at hand, we can go to the third step as depicted in Fig. 1(c) to construct the unit-cell transfer matrix. This can be accomplished by using the recursion algorithms. The unit-cell T-matrix is simply given by $T=t_nt_{n-1}\ldots t_i\ldots t_2t_1$. This formulation is numerically unstable for thick samples because the exponentially growing and decaying terms involved in the slice T-matrix will accumulate simultaneously. In contrast, the S-matrix formulation is numerically stable as the formula only deals with exponentially decaying terms. The unit-cell S-matrix should be constructed as follows. Suppose the overall S matrix for the first $n-1$ slices and the S matrix for slice n have been calculated to be S^{n-1} and s^n, respectively,