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.

© 2005 Elsevier Ltd. All rights reserved.

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 logarithmically 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
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 wood-pile 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

\[ \nabla \times \mathbf{E}(r) = \text{i}k_0 \mu_0 \mathbf{H}(r), \]
\[ \nabla \times \mathbf{H}(r) = -\text{i}k_0 \varepsilon_0 \mathbf{E}(r). \]  \hspace{1cm} (2.1)

Here \( k_0 = \omega/c \) is the wave number, \( c \) is the light speed in vacuum, and \( \omega \) is the angular frequency of the EM wave. In usual photonic structures, the composite materials are nonmagnetic, and \( \mu(r) = 1 \). But generally one can consider a general case where both \( \varepsilon(r) \) and \( \mu(r) \) are spatially periodic functions. For anisotropic composite materials, \( \varepsilon(r) \) and \( \mu(r) \) 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 gratings 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 \( r \) can be written into the superposition of Bragg waves (or plane waves).

\[ \mathbf{E}(r) = \sum_{ij} \mathbf{E}_{ij}(z) e^{\text{i}(k_{ij,x}x + k_{ij,y}y)}, \]
\[ \mathbf{H}(r) = \sum_{ij} \mathbf{H}_{ij}(z) e^{\text{i}(k_{ij,x}x + k_{ij,y}y)}, \]  \hspace{1cm} (2.2)

where the Bragg wave vector \( \mathbf{k}_{ij} = (k_{ij,x}, k_{ij,y}) = (k_{0x}, k_{0y}) + \text{i}b_1 + \text{j}b_2 = (k_{0x}, k_{0y}) + \mathbf{G}_{ij} \), 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:

\[ \varepsilon(r) = \sum_{ij} \varepsilon_{ij}(z) e^{\text{i}(k_{ij,x}x + k_{ij,y}y)}, \]
\[ \varepsilon^{-1}(r) = \sum_{ij} \varepsilon^{-1}_{ij}(z) e^{\text{i}(k_{ij,x}x + k_{ij,y}y)}, \]  \hspace{1cm} (2.3)

\[ \mu(r) = \sum_{ij} \mu_{ij}(z) e^{\text{i}(k_{ij,x}x + k_{ij,y}y)}, \]
\[ \mu^{-1}(r) = \sum_{ij} \mu^{-1}_{ij}(z) e^{\text{i}(k_{ij,x}x + k_{ij,y}y)}. \]

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 \( k_{ij}(z) \) 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 problems 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 (\( \Omega_1^+, \Omega_1^- \)) to those in the left-hand air films (\( \Omega_{-1}^+, \Omega_{-1}^- \)). We can write down

\[ \begin{pmatrix} \Omega_i^+ \\ \Omega_i^- \end{pmatrix} = t_i \begin{pmatrix} \Omega_{i-1}^+ \\ \Omega_{i-1}^- \end{pmatrix}, \quad \begin{pmatrix} \Omega_i^+ \\ \Omega_i^- \end{pmatrix} = s^i \begin{pmatrix} \Omega_{i-1}^+ \\ \Omega_{i-1}^- \end{pmatrix}. \]  \hspace{1cm} (2.4)

\( t_i \) and \( s^i \) are called \( \text{T} \)-matrix and \( \text{S} \)-matrix for the \( i \)th slice, respectively. General speaking, the \( \text{T} \)-matrix connects the fields at the right side of a slice to the fields at the left side, while the \( \text{S} \)-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 \( \text{T} \)-matrix is simply given by \( T = t_i t_{i-1} \cdots t_{i-t} t_{i-t+1} \). This formulation is numerically unstable for thick samples because the exponentially growing and decaying terms involved in the slice \( \text{T} \)-matrix will accumulate simultaneously. In contrast, the \( \text{S} \)-matrix formulation is numerically stable as the formula only deals with exponentially decaying terms. The unit-cell \( \text{S} \)-matrix should be constructed as follows. Suppose the overall \( \text{S} \)-matrix for the first \( n-1 \) slices and the \( \text{S} \)-matrix for slice \( n \) have been calculated to be \( S^{n-1} \) and \( s^n \), respectively,
Involves metallic composite, the absorption spectra is waves with lateral wave vectors \( k \), where the summation is run over those homogeneous Bragg states, will not be scattered when propagating within the crystal. Then a natural boundary condition on the EM waves in a region very far from the PC surface can be found to completely overcome the obstacle towards this difficult problem [17].

The theory starts from the eigenequation for the PC:

\[
T \begin{pmatrix} \Omega^+ \\ \Omega^- \end{pmatrix} = \lambda \begin{pmatrix} \Omega^+ \\ \Omega^- \end{pmatrix},
\]

(3.6)

Solution of all the eigenvalues and eigenvectors of \( T \) leads to \( TS = \Lambda \Delta \), where \( \Lambda \) is a diagonal matrix composed of all eigenvalues \( \{ \lambda_i, i = 1, \ldots, N \} \), with \( N \) being the dimension of \( T \), \( S \) is a \( N \times N \) matrix with its \( ij \)th column being the eigenvector of \( T \) corresponding to the eigenvalue \( \lambda_i \). The Bloch states are among these eigenmodes for \( T \). \( T \) can be expressed into \( T = S \Lambda S^{-1} \). Let \( \Sigma = (\Sigma^+, \Sigma^-)^T = S^{-1}(\Omega^+, \Omega^-)^T \), Eq. (3.6) becomes \( \Delta \Sigma = \lambda \Sigma \). The unitary transformation \( S \) has served as a bridge to reflect the eigenmode in the original plane-wave basis to that in the new eigenstate basis. The column vector \( \Sigma \) has a very simple while elegant physical implication for the PC:

"every element \( \sigma_i \) in \( \Sigma = (\sigma_i, i = 1, \ldots, N) \) denotes an eigenmode of the transfer matrix \( T \), whose eigenvalue is \( \lambda_i \) and whose amplitude is \( \sigma_i \). The diagonal matrix \( \Lambda \) can be separated into two parts and rearranged into the following form

\[
A = \begin{pmatrix} \Lambda_+ & 0 \\ 0 & -\Lambda_- \end{pmatrix},
\]

(3.7)

where \( \Lambda_+ \) and \( \Lambda_- \) correspond to the positive and negative eigenmodes, respectively.

Now let us turn to the scattering problem by the semi-infinite PC structure. The fields after passing through \( n \) crystal layers are related with the fields at the air-crystal interface (with \( \Omega_0^+ \) and \( \Omega_0^- \) corresponding to the incident and reflection fields in air, respectively) via

\[
\begin{pmatrix} \Omega_n^+ \\ \Omega_n^- \end{pmatrix} = T^n \begin{pmatrix} \Omega_0^+ \\ \Omega_0^- \end{pmatrix},
\]

(3.8)
Projection into the eigenmode space yields
\[
\begin{pmatrix}
\Sigma_n^+ \\
\Sigma_n^-
\end{pmatrix} =
\begin{pmatrix}
\Lambda'^n & 0 \\
0 & \Lambda^n
\end{pmatrix}
\begin{pmatrix}
\Sigma_0^+ \\
\Sigma_0^-
\end{pmatrix},
\] (3.9)
which yields
\[
\Sigma_n^+ = \Lambda'^n \Sigma_0^+, \quad \Sigma_n^- = \Lambda^n \Sigma_0^-.
\] (3.10)

For a semi-infinite PC, there is no boundary to reflect the forward propagating eigenmodes into the backward propagating modes. This physical intuition imposes a natural boundary condition: All backwards propagating modes within the photonic crystal are exactly zero. Therefore, \(\Sigma_n^- = 0\) and \(\Sigma_0^- = 0\). Projection back to the plane-wave space leads to \(\Omega_0^+ = S_{11} \Sigma_0^+\) and \(\Omega_0^- = S_{21} \Sigma_0^-\), from which we get \(\Omega_0^+ = S_{11} \Sigma_0^+\) and \(\Omega_0^- = \Lambda'^n S_{11} \Omega_0^+\). The explicit form of the reflection and transmission fields in the plane-wave space are
\[
\Omega_0^- = S_{21} \Sigma_0^+ = S_{21} S_{11}^{-1} \Omega_0^+,
\] (3.11)
\[
(\Omega_n^+, \Omega_n^-) = (S_{11} \Sigma_n^+, S_{21} \Sigma_n^+).
\] (3.12)

The transmission field is consisting of both the Bloch’s mode and all other evanescent modes. At a plane very far away from the air-crystal interface, only the Bloch state survives. The transmission and reflection coefficients can be directly calculated from the plane-wave expansion coefficients.

Following the above physical concept of the eigenmode space, it is straightforward to solve other more complex problems. These include the problem of a Bloch-wave scattering by the air-crystal interface, scattering of both plane wave and Bloch wave by a coated semi-infinite PC structure, wave transport from one PC to another PC, and wave propagation through a slab sandwiched between two PC structures [17]. When the formulation is combined with a supercell technique, the PWTMM can efficiently handle optical problem of PC waveguides, for instance, their coupling with resonant cavities [17–20].

To demonstrate the power of the PWTMM, we consider the three-dimensional wood-pile PC structure, which exhibits a wide complete PBG and can be realized in the optical regime by means of advanced microfabrication technique [3]. The geometry of the crystal and the corresponding Brillouin zone is shown in Fig. 2(a) and (b). Due to the special geometrical configuration of the crystal, the PWTMM exhibits high performance in calculating the photonic band structures and transmission/reflection/absorption spectra. We have found that by using 121 plane waves the numerical convergency is better than 0.5%. An example of the simulation result is displayed in Fig. 3(a) and (b). The band structure and spectrum calculation well agree with each other in regard to the PBG position.

4. Summary

In conclusion, we have presented a brief review of the basic principle of the PWTMM and how it can be applied to
solve different problems for PC structures, elements, and devices. Armed with such a wide variety of powers, the PWTMM has become a good candidate to design high-performance PC functional elements that will finally lead to realization of PC integrated circuits. This work was supported by the National Key Basic Research Special Foundation of China No. 2004CB719804 and the National Natural Science Foundation of China No. 10404036.

References

[1] E. Yablonovitch, Inhibited spontaneous emission in solid-state physics and electronics, Phys. Rev. Lett. 58 (1987) 2059–2062.
[2] J.D. Joannopoulos, P.R. Villeneuve, S. Fan, Photonic crystals: putting a new twist on light, Nature 386 (1997) 143–149 London.
[3] S.Y. Lin, et al., A three-dimensional photonic crystal operating at infrared wavelengths, Nature 394 (1998) 251–253 London.
[4] A. Mekis, J.C. Chen, I. Kurland, S. Fan, P.R. Villeneuve, J.D. Joannopoulos, High transmission through sharp bends in photonic crystal waveguides, Phys. Rev. Lett. 77 (1996) 3787–3790.
[5] Z.Y. Li, K.M. Ho, Waveguides in three-dimensional photonic crystals, J. Opt. Soc. Am. B 20 (2003) 801–809.
[6] O. Painter, R.K. Lee, A. Scherer A, A. Yariv, J.D. O’Brien, P.D. Dapkus, I. Kim, Two-dimensional photonic band-gap defect mode laser, Science 284 (1999) 1819–1821.
[7] S.G. Johnson, P.R. Villeneuve, S. Fan, J.D. Joannopoulos, Linear waveguides in photonic-crystal slabs, Phys. Rev. B 62 (2000) 8212–8222.
[8] S. Fan, P.R. Villeneuve, J.D. Joannopoulos, H.A. Haus, Channel drop tunneling through localized states, Phys. Rev. Lett. 80 (1998) 960–963.
[9] K.M. Ho, C.T. Chan, C.M. Soukoulis, Existence of a photonic gap in periodic dielectric structures, Phys. Rev. Lett. 65 (1990) 3152–3155.
[10] Z.Y. Li, J. Wang, B.Y. Gu, Creation of partial band gaps in anisotropic photonic-band-gap structures, Phys. Rev. B 58 (1998) 3721–3729.
[11] S.G. Johnson, J.D. Joannopoulos, Block-iterative frequency-domain methods for Maxwell’s equations in a plane-wave basis, Opt. Express 8 (2001) 173–190.
[12] A. Taflove, Computational Electrodynamics: The Finite-Difference Time-Domain Method, Artech House INC, Norwood, 1995.
[13] J.B. Pendry, Photonic band structures, J. Mod. Opt. 41 (1994) 209–229.
[14] Z.Y. Li, L.L. Lin, Photonic band structures solved by a plane-wave-based transfer-matrix method, Phys. Rev. E 67 (2003) 046607.
[15] Z.Y. Li, K.M. Ho, Analytic modal solution to light propagation through layer-by-layer metallic photonic crystals, Phys. Rev. B 68 (2003) 165104.
[16] L.L. Lin, Z.Y. Li, K.M. Ho, Lattice symmetry applied in transfer-matrix methods for photonic crystals, J. Appl. Phys. 94 (2003) 811–821.
[17] Z.Y. Li, K.M. Ho, Light propagation in semi-infinite photonic crystals and related waveguide structures, Phys. Rev. B 68 (2003) 155101.
[18] Z.Y. Li, K.M. Ho, Application of structural symmetries in the plane-wave-based transfer-matrix method for three-dimensional photonic crystal waveguides, Phys. Rev. B 68 (2003) 245117.
[19] Z.Y. Li, K.M. Ho, Anomalous propagation loss in photonic crystal waveguides, Phys. Rev. Lett. 92 (2004) 063904.
[20] Z.Y. Li, L.L. Lin, K.M. Ho, Light coupling with multimode photonic crystal waveguides, Appl. Phys. Lett. 84 (2004) 4699–4701.
[21] L. Li, Use of Fourier series in the analysis of discontinuous periodic structures, J. Opt. Soc. Am. A 13 (1996) 1870–1876.
[22] L. Li, New formulation of the Fourier modal method for crossed surface-relief gratings, J. Opt. Soc. Am. A 14 (1997) 2758–2767.