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FDTD algorithm for computing the off-plane band structure in a two-dimensional photonic crystal with dielectric or metallic inclusions

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Abstract

An effective numerical method based on the finite-difference time-domain scheme for computing the off-plane band structure of a two-dimensional photonic crystal is presented. The method is an order N method, and requires only a two-dimensional discretization mesh for a given off-plane wave number k_z although the off-plane propagation is a three-dimensional problem. The computation time and memory required is thus reduced significantly. The present method can be used for any type of inclusions and no additional effort is needed for metallic inclusions. The off-plane band structures of a square lattice of metallic rods in the air are studied, and a complete bandgap for some nonzero off-plane wave number k_z is found.

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1. Introduction

Photonic crystals, which are periodic dielectric or metallic structures, can provide a possibility of eliminating electromagnetic wave propagation within a frequency band, i.e., a photonic band gap (PBG) [1–3]. Two-dimensional photonic crystals have attracted considerable attentions since they are easier to fabricate than three-dimensional ones (besides their particular usefulness in integrated optics). The propagation of electromagnetic waves in two-dimensional photonic crystals has been studied both theoretically and experimentally in the literature. Most of the studies have been focused on the wave propagation along the x–y plane (perpendicular to the axes of the inclusions) with the z component of the wave vector (i.e., the off-plane wave number) $k_z = 0$. Wave propagation out of this plane is very important for studies of photonic crystal-based antennas [4], photonic crystal lasers [5], photonic crystal optical fiber [6], etc.

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Using the plane wave expansion method, Maradudin et al. [7] and Feng et al. [8] have presented some results for the off-plane band structures of two-dimensional dielectric photonic crystals. The computational time growth is of order N^3 (N is the number of the plane waves) since the method involves the diagonalization of a matrix. In addition, the plane wave method can not be used directly for a metallic photonic crystal. Yang [9] has also studied the off-plane band structures of a two-dimensional photonic crystal by a finite-difference *frequency-domain* method. Although it is a finite difference method, the method is of order N^3 (here N is the number of spatial discretization points) since it also requires a matrix diagonalization.

In this Letter, we give simulation and analysis for the off-plane wave propagation in a two-dimensional photonic crystal by an effective finite-difference time-domain (FDTD) method, which reduces the computation time and memory space significantly.

2. Model and numerical algorithm

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

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu(\mathbf{r})}\nabla \times \mathbf{E}, \tag{1}$$

$$\frac{\partial \mathbf{E}}{\partial t} = \frac{1}{\varepsilon(\mathbf{r})}\nabla \times \mathbf{H} - \frac{\sigma(\mathbf{r})}{\varepsilon(\mathbf{r})}\mathbf{E}, \tag{2}$$

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

These equations can be discretized in space and time by a so-called Yee-cell technique [10,11]. The following FDTD time stepping formulas are the discretization (for space and time) of Maxwell's equations on a discrete three-dimensional mesh in a Cartesian x–y–z coordinate system [11]:

$$H_x|_{i,j,k}^{n+1/2} = H_x|_{i,j,k}^{n-1/2} + \frac{\Delta t}{\mu_{i,j,k}}\left(\frac{E_y|_{i,j,k+1/2}^{n} - E_y|_{i,j,k-1/2}^{n}}{\Delta z} - \frac{E_z|_{i,j+1/2,k}^{n} - E_z|_{i,j-1/2,k}^{n}}{\Delta y}\right), \tag{3}$$

$$H_y|_{i,j,k}^{n+1/2} = H_y|_{i,j,k}^{n-1/2} + \frac{\Delta t}{\mu_{i,j,k}}\left(\frac{E_z|_{i+1/2,j,k}^{n} - E_z|_{i-1/2,j,k}^{n}}{\Delta x} - \frac{E_x|_{i,j,k+1/2}^{n} - E_x|_{i,j,k-1/2}^{n}}{\Delta z}\right), \tag{4}$$

$$H_z|_{i,j,k}^{n+1/2} = H_z|_{i,j,k}^{n-1/2} + \frac{\Delta t}{\mu_{i,j,k}}\left(\frac{E_x|_{i,j+1/2,k}^{n} - E_x|_{i,j-1/2,k}^{n}}{\Delta y} - \frac{E_y|_{i+1/2,j,k}^{n} - E_y|_{i-1/2,j,k}^{n}}{\Delta x}\right), \tag{5}$$

$$\begin{aligned} E_x|_{i,j,k}^{n+1} = {} & \frac{\varepsilon_{i,j,k} - \sigma_{i,j,k}\Delta t/2}{\varepsilon_{i,j,k} + \sigma_{i,j,k}\Delta t/2} E_x|_{i,j,k}^{n} \\ & + \frac{\Delta t}{\varepsilon_{i,j,k} + \sigma_{i,j,k}\Delta t/2}\left(\frac{H_z|_{i,j+1/2,k}^{n+1/2} - H_z|_{i,j-1/2,k}^{n+1/2}}{\Delta y} - \frac{H_y|_{i,j,k+1/2}^{n+1/2} - H_y|_{i,j,k-1/2}^{n+1/2}}{\Delta z}\right), \end{aligned} \tag{6}$$

$$\begin{aligned} E_y|_{i,j,k}^{n+1} = {} & \frac{\varepsilon_{i,j,k} - \sigma_{i,j,k}\Delta t/2}{\varepsilon_{i,j,k} + \sigma_{i,j,k}\Delta t/2} E_y|_{i,j,k}^{n} \\ & + \frac{\Delta t}{\varepsilon_{i,j,k} + \sigma_{i,j,k}\Delta t/2}\left(\frac{H_x|_{i,j,k+1/2}^{n+1/2} - H_x|_{i,j,k-1/2}^{n+1/2}}{\Delta z} - \frac{H_z|_{i+1/2,j,k}^{n+1/2} - H_z|_{i-1/2,j,k}^{n+1/2}}{\Delta x}\right), \end{aligned} \tag{7}$$

$$E_z|_{i,j,k}^{n+1} = \frac{\varepsilon_{i,j,k} - \sigma_{i,j,k}\Delta t/2}{\varepsilon_{i,j,k} + \sigma_{i,j,k}\Delta t/2} E_z|_{i,j,k}^{n} + \frac{\Delta t}{\varepsilon_{i,j,k} + \sigma_{i,j,k}\Delta t/2}\left(\frac{H_y|_{i+1/2,j,k}^{n+1/2} - H_y|_{i-1/2,j,k}^{n+1/2}}{\Delta x} - \frac{H_x|_{i,j+1/2,k}^{n+1/2} - H_x|_{i,j-1/2,k}^{n+1/2}}{\Delta y}\right), \tag{8}$$

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, Δt is the time increment, and Δx, Δy, and Δz are the space increments between two neighboring grid points along the x, y, and z directions, respectively.

For the off-plane propagation, each field component has the form $\phi(x, y, z) = \phi(x, y)e^{ik_z z}$, where ϕ denotes any field component. Therefore, the fields at neighboring grid points along the z direction satisfy the following relations:

$$E_p|_{i,j,k\pm1}^{n} = E_p|_{i,j,k}^{n} e^{ik_z\Delta z}, \quad H_p|_{i,j,k\pm1}^{n} = H_p|_{i,j,k}^{n} e^{ik_z\Delta z}, \quad p = x, y. \tag{9}$$

Then Eqs. (3)–(8) can be written in the following forms if we let $\Delta z \to 0$ and omit the index k [12]:

$$E_z|_{i,j}^{n+1} = \frac{\varepsilon_{i,j} - \sigma_{i,j}\Delta t/2}{\varepsilon_{i,j} + \sigma_{i,j}\Delta t/2} E_z|_{i,j}^{n} + \frac{\Delta t}{\varepsilon_{i,j} + \sigma_{i,j}\Delta t/2}\left(\frac{H_y|_{i+1/2,j}^{n+1/2} - H_y|_{i-1/2,j}^{n+1/2}}{\Delta x} - \frac{H_x|_{i,j+1/2}^{n+1/2} - H_x|_{i,j-1/2}^{n+1/2}}{\Delta y}\right), \tag{10}$$

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

$$H_y|_{i,j}^{n+1/2} = H_y|_{i,j}^{n-1/2} + \frac{\Delta t}{\mu_{i,j}}\left(\frac{E_z|_{i+1/2,j}^{n} - E_z|_{i-1/2,j}^{n}}{\Delta x} - ik_z E_x|_{i,j}^{n}\right), \tag{12}$$

$$H_z|_{i,j}^{n+1/2} = H_z|_{i,j}^{n-1/2} + \frac{\Delta t}{\mu_{i,j}}\left(\frac{E_x|_{i,j+1/2}^{n} - E_x|_{i,j-1/2}^{n}}{\Delta y} - \frac{E_y|_{i+1/2,j}^{n} - E_y|_{i-1/2,j}^{n}}{\Delta x}\right), \tag{13}$$

$$E_x|_{i,j}^{n+1} = \frac{\varepsilon_{i,j} - \sigma_{i,j}\Delta t/2}{\varepsilon_{i,j} + \sigma_{i,j}\Delta t/2} E_x|_{i,j}^{n} + \frac{\Delta t}{\varepsilon_{i,j} + \sigma_{i,j}\Delta t/2}\left(\frac{H_z|_{i,j+1/2}^{n+1/2} - H_z|_{i,j-1/2}^{n+1/2}}{\Delta y} - ik_z H_y|_{i,j}^{n+1/2}\right), \tag{14}$$

$$E_y|_{i,j}^{n+1} = \frac{\varepsilon_{i,j} - \sigma_{i,j}\Delta t/2}{\varepsilon_{i,j} + \sigma_{i,j}\Delta t/2} E_y|_{i,j}^{n} - \frac{\Delta t}{\varepsilon_{i,j} + \sigma_{i,j}\Delta t/2}\left(\frac{H_z|_{i+1/2,j}^{n+1/2} - H_z|_{i-1/2,j}^{n+1/2}}{\Delta x} - ik_z H_x|_{i,j}^{n+1/2}\right). \tag{15}$$

From Eqs. (10)–(15) one sees that only a two-dimensional mesh in a x–y plane is used although the original off-plane propagation problem is a three-dimensional one. One can also see from the above equations 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 (note that the plane wave expansion method is of order N^3). Thus, the present method reduces significantly both the memory space and the CPU time.

The FDTD time-stepping formulas are stable numerically if the following condition is satisfied [13]:

$$\Delta t \leqslant \frac{1}{c\sqrt{\Delta x^{-2} + \Delta y^{-2} + (k_z/2)^2}}, \tag{16}$$

where c is the speed of the light.

If $k_z = 0$ (i.e., the case of in-plane propagation), the above equations can be decoupled into E-polarization equations (10)–(12) and H-polarization equations (13)–(15). The details of the algorithm for the in-plane propagation by the FDTD method can be found in our previous work [14], which has been used for computing defect modes [15] and guided modes [16] in two-dimensional photonic crystals.

Special consideration should be given to the boundary of the finite computational domain, where the fields are updated using special boundary conditions since information out of the computational domain is not available. Since the structure of the photonic crystal is periodic, one naturally uses the periodic boundary condition, which satisfies the Bloch theory. An artificial initial field distribution is introduced in the present FDTD algorithm. 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. All the fields are obtained in the time domain in the present method. In order to obtain the spectral information, one needs to transform the calculated fields from the time domain to the frequency domain by a Fourier transform. Details for the boundary condition, the initial field distribution, and the Fourier transform can be found in our previous work (for the case of in-plane propagation) [14].

3. Numerical results and discussion

First we verify our FDTD method numerically by comparing with the conventional plane wave expansion method. Consider a two-dimensional photonic crystal with a square lattice of dielectric rods in the air. The radius of the rods is $R = 0.2a$, where a is the lattice constant. The relative permittivity of the rods is $\varepsilon_r = 8.9$. In our FDTD computation, the unit lattice cell contains 3600 (60×60) grid points, and the total number of the time steps is 30,000 with each time step $\Delta t = 0.95/(c\sqrt{\Delta x^{-2} + \Delta y^{-2} + (k_z/2)^2})$, where c is the speed of the light. Fig. 1 shows the band structure of the photonic crystal when the off-plane wave number $k_z = 0.40(\pi/a)$. The solid curves are obtained by the plane wave expansion method, and the circles are obtained by our FDTD method. From this figure one sees that our FDTD results are in a good agreement with those obtained by the plane wave expansion method.

Next we study the off-plane band structures of a metallic photonic crystal. 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 ω^{-1}. For the plane wave method, such a metallic case is much more complicated than the case of purely dielectric materials, since it requires to solve a generalized nonlinear eigenvalue problem. One may use a perturbative plane wave approach [17] to solve this problem. However, such an approach requires the diagonalization of an equivalent, enlarged matrix, which increases the computational time and memory. In our FDTD method, we assume that the conductivity σ is a constant for the metal in the frequency range of interest, and

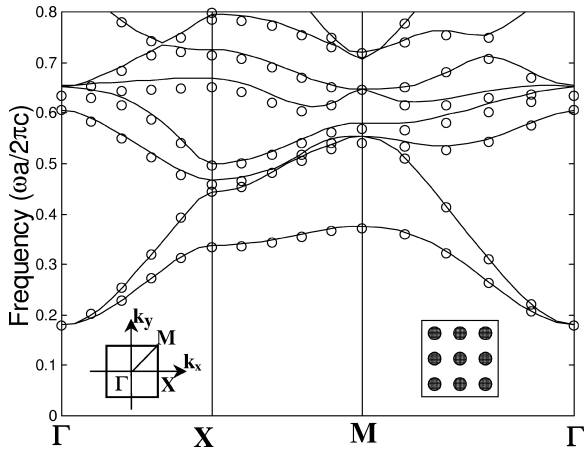

Fig. 1. Photonic band structures for a square lattice of dielectric rods ($\varepsilon_r = 8.9$) in air. The radius of the rods is $R = 0.2a$. The off-plane wave number is $k_z = 0.4(\pi/a)$. The solid curves are obtained by the plane wave expansion method, and the circles are obtained by the present FDTD method.

we simply substitute the value of the conductivity σ in the FDTD time stepping formulas (10)–(15) according to the specific conducting material that is used as inclusions.

Our previous in-plane studies [14] have shown that only an E-polarization bandgap exists in a metallic photonic crystal. However, there is no in-plane bandgap for the H-polarization since metallic rods are almost transparent for the H-polarization [18]. Therefore, there is no complete band gap for such a metallic photonic crystal when $k_z = 0$. However, Briks et al. [19] have shown that it is possible to find a complete bandgap in a *dielectric* photonic crystal with refractive index contrast as small as that of silica–air, for some nonzero k_z. They have also used this property to fabricate the first photonic fiber [6,20]. One may wonder whether it is possible to find a complete band gap for an off-plane propagation case in a *metallic* photonic crystal.

Consider a square array of metallic rods in air. The radius of the metallic rods is $R = 0.2a$. We use copper as the inclusion material and $\sigma = 5.80 \times 10^7$ S/m is used for the copper conductivity [21]. In our FDTD computation, the unit lattice cell contains 14,400 (120×120) grid points, and the total number of the time steps is 60,000 with each time step $\Delta t = 0.95/(c\sqrt{\Delta x^{-2} + \Delta y^{-2} + (k_z/2)^2})$. Fig. 2 shows the band structure of the photonic crystal when the off-plane wave number $k_z = 8.0(\pi/a)$. One can see from this figure that there exists a complete bandgap with central frequencies at $4.025(2\pi c/a)$. We also study the band strictures for other values of k_z. Our FDTD calculations show that the bandgap appears when k_z increases to about $6.0(\pi/a)$. The bandgap map is shown in Fig. 3, where the bandgap width varies as k_z varies. From Fig. 3 one sees that the bandgap exists for a very large range of k_z. The bandgap width reaches $0.0294(2\pi c/a)$ when $k_z = 9.0(\pi/a)$. Meanwhile, the bandgap width increases as k_z increases. For comparison, one may recall that the maximum width of the complete bandgap for a square lattice of air holes in gallium arsenide is only $0.0188(2\pi c/a)$ [22]. Thus, the off-plane complete bandgap for the *metallic* photonic crystal may be useful for constructing a photonic crystal fiber. Since the central frequency for the complete bandgap is larger than $3.0(2\pi c/a)$, the corresponding wavelength is less than $a/3$. Therefore, the metallic photonic crystal with a relatively larger lattice constant can operate at a relatively shorter wavelength. For example, if one wishes to operate the metallic photonic crystal at wavelength 1.5 μm (which is commonly used for optical communication), the lattice constant of the metallic photonic crystal can be larger than 4.5 μm, which makes the fabrication much easier.

A real metal may have a frequency dependent conductivity, and may have different values as the frequency varies throughout the range over which the band structures in Fig. 2 are calculated. The FDTD method is a time domain method, and a frequency-dependent conductivity in the time domain can be characterized by a susceptibility kernel (a function of time) in terms of time convolution (see, e.g., [23]). Therefore, the FDTD method can be applied to Maxwell's equations for frequency dependent media (see, e.g., [24]). One can use a so-called ODE (ordinary

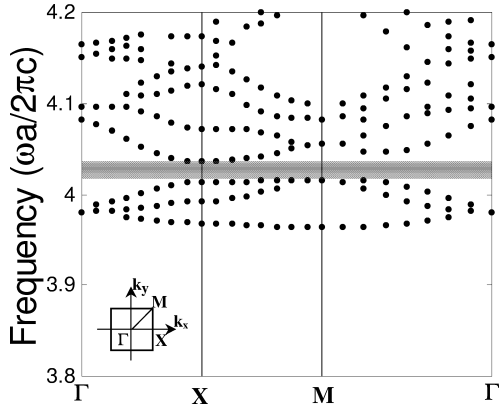

Fig. 2. Photonic band structures for a square lattice of copper rods in air. The radius of the rods is $R = 0.2a$. The off-plane wave number is $k_z = 8.0(\pi/a)$.

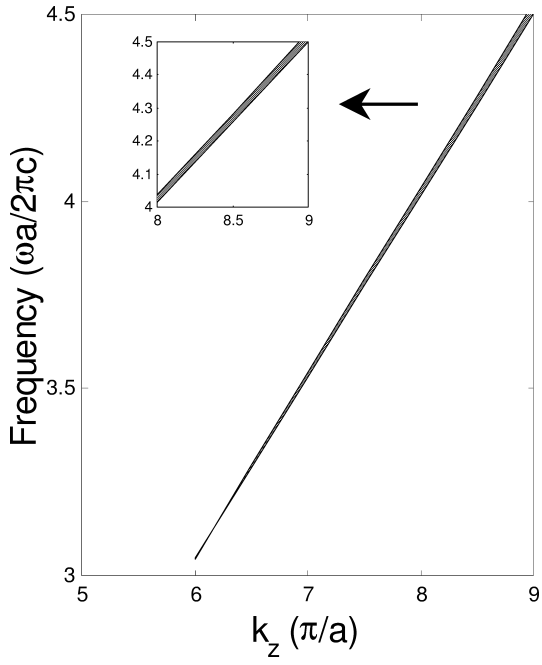

Fig. 3. Bandgap map as k_z varies for a square array of copper rods in the air. The radius of the rods is $R = 0.2a$.

differential equation) representation to improve greatly (by an order of N) the computational efficiency of the time convolution in the FDTD algorithm (see, e.g., [25]). Nevertheless, since the copper conductivity is so high one can treat it as a perfect conductor (i.e., with infinitely large conductivity). Our numerical results have indicated that the band structures remain virtually the same if one increases the value of the copper conductivity by 1 (or any) order. Therefore, the influence of the frequency-dependence of the *copper* conductivity to the band structures presented in Fig. 2 is negligible.

4. Conclusions

In conclusion, we have presented an effective FDTD method to study the off-plane wave propagation in a two-dimensional photonic crystal. The method requires only a two-dimensional mesh for a given off-plane wave number k_z, and is an order N method. 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 the air has been studied. It has been found that there exists a complete bandgap in such a metallic photonic crystal for nonzero k_z.

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