# OFF-PLANE PROPAGATION OF ELECTROMAGNETIC WAVES IN TWO-DIMENSIONAL ELECTROMAGNETIC BAND-GAP STRUCTURES

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### 1. Introduction

Photonic and electromagnetic 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 easy to fabricate. The propagation of electromagnetic waves in two-dimensional photonic crystals has been studied both theoretically and experimentally in the literature. Most of the studies focused on the wave propagation along the *x*-*y* plane perpendicular to the axes of the inclusions with the *z* component of wave vector  $k_z=0$ . However, the wave propagation out of this plane is very important for the studies of photonic crystal-based antennas [4-5], photonic crystal lasers [6], photonic crystal optical fiber [7], etc.

Using the plane wave expansion method, Maradudin *et al.* [8] and Feng *et al.* [9] have presented some results for the off-plane band structures of the two-dimensional photonic crystal. The computational time growth is of order  $N^3$  for the plane wave expansion method. Therefore, This method is time and memory consuming for a large system (for example, the defect modes of a two-dimensional photonic crystal). In this paper, we give simulation and analysis for off-plane wave propagation in a two-dimensional photonic crystal by the finite-difference time-domain (FDTD) method. For a given  $k_z$ , the simulation requires only a two-dimensional mesh [10]. It reduces the memory space and CPU time significantly. The off-plane defect modes, i.e., the guided modes in the *z* direction are also studied.

### 2. Method

It is well known that for the wave propagation in the *x-y* plane ( $k_z=0$ , in-plane propagation) in a two-dimensional photonic crystal, Maxwell's equations decouple into *E*-polarization equations and *H*-polarization equations. However, these two modes are hybrid for an off-plane propagation where  $k_z^1 0$ . For a linear isotropic material with permittivity *e*, permeability *m* and conductivity *s* in a source free region, one can use the following FDTD time stepping formulas for  $E_z$  and  $H_x$  [10],

$$E_{z}\Big|_{i,j}^{n} = \frac{\boldsymbol{e}_{i,j} - \boldsymbol{s}_{i,j}\Delta t/2}{\boldsymbol{e}_{i,j} + \boldsymbol{s}_{i,j}\Delta t/2} E_{z}\Big|_{i,j}^{n} + \frac{\Delta t}{\boldsymbol{e}_{i,j} + \boldsymbol{s}_{i,j}\Delta t/2} \left(\frac{H_{y}\Big|_{i+1/2,j}^{n+1/2} - H_{y}\Big|_{i-1/2,j}^{n+1/2}}{\Delta x} - \frac{H_{x}\Big|_{i,j+1/2}^{n+1/2} - H_{x}\Big|_{i,j-1/2}^{n+1/2}}{\Delta y}\right),$$
(1)

and,

$$H_{x}\Big|_{i,j}^{n+1/2} = H_{x}\Big|_{i,j}^{n-1/2} - \frac{\Delta t}{\mathbf{m}_{i,j}} \left( \frac{E_{z}\Big|_{i,j+1/2}^{n} - E_{z}\Big|_{i,j-1/2}^{n}}{\Delta y} - \frac{1 - e^{-ik_{z}\Delta z}}{\Delta z} E_{y}\Big|_{i,j}^{n} \right)$$
(2)

where the index *n* denotes the discrete time step, indices *i* and *j* denote the discretized grid point in the *x*-*y* plane, respectively.  $\Delta t$  is the time increment, and  $\Delta x$ ,  $\Delta y$ , and  $\Delta z$  are the intervals between neighboring grid points along the *x*, *y*, and *z* directions, respectively. (The similar formulas for  $H_y$ ,  $H_z$ ,  $E_x$ , and  $E_y$  can be obtained easily.)

One can easily see from the above equations that only a two-dimensional mesh is used in the algorithm although the computational problem is three-dimensional. Thus, the memory space and CPU time are significantly reduced. From the formulas one can also know 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  $N^3$ ).

Special consideration should be given at the boundary of the finite computational domain, where the fields are updated using special boundary conditions, for 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, which satisfies the Bloch theory, is introduced in the 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.

#### 3. Results and Discussion

The present method can be used to calculate band structures of two-dimensional photonic crystals when  $k_z$ <sup>1</sup> 0. 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 e=8.9. In our

FDTD computation, the unit lattice cell contains 1296 (36×36) grid points, and the total number of the time steps is 20000 with each time step  $\Delta t = 1/c\sqrt{\Delta x^2 + \Delta y^2}$ , where *c* is the speed of the light. Figure 1 shows the band structure of the photonic crystal for the wave vector  $k_z$ =0.4 (*p/a*). The solid curves are obtained by the plane wave expansion method, and circles are the results obtained by our FDTD method. The FDTD results are in good agreement with those obtained by the plane wave expansion method.

Now we consider a two-dimensional photonic crystal with a triangular lattice of air holes in a medium of relative permittivity e=13. The radius of the air holes is R=0.48a. The calculation shows that there is a complete band gap for both the *E*- and *H*-polarization between 0.448 and 0.524 ( $2\pi c/a$ ) for the propagation in the plane perpendicular to the air holes ( $k_z=0$ ). As shown in Fig. 2, the frequencies of the lower and upper band edges of this gap shift to higher values as the wave vector  $k_z$  increases. The width of the complete band gap initially increases, then decreases monotonically as  $k_z$  increases, and finally vanishes at  $k_z=1.72$  ( $\pi/a$ ) [8].

If we remove one air hole in the perfect photonic crystal, i.e., introduce a defect, the defect extends into the third dimension, and forms a line channel which can guide electromagnetic waves. This structure is in the form of an optical fiber [7]. The defect modes in this structure for  $k_z$ <sup>1</sup> 0 are the guided modes in the *z* direction. Therefore, it is very important to study these guided modes for the understanding of the properties of the photonic optical fibers.

The defect is studied using a supercell technique, in which the defect is placed in each repeated supercell of a sufficiently large size. In the present paper, we consider a 7x7 supercell, which contains 49 unit cells, and remove the center air hole. Each unit cell contains 1296 ( $36 \times 36$ ) grid points, and the total number of the time steps is 20000. The calculated guided modes in the z direction are shown in Fig. 2.



Figure 1. Photonic band structure for a square lattice of dielectric rods (e=8.9) in the air. The radius of the rods is R=0.2a. The offplane wave number  $k_z=0.4$  (p(a)). The solid curves are obtained by the plane wave expansion method, and circles are the results obtained by our FDTD method.

Figure 2. Guided modes in the *z* direction for a triangular lattice of air holes in a dielectric medium ( $\varepsilon = 13$ ). The defect is obtained by removing one air hole. The shaded regions indicate the edge of the complete band gap. The solid line is for the modes extended from the in-plane *E*-polarization defect modes, and the dash lines are the modes extended from the in-plane *H*-polarization defect modes.

For the in-plane propagation, i.e.,  $k_z=0$ , our calculation shows that there are three defect modes at the frequencies 0.471 ( $2\pi c/a$ ) for the *E*-polarization, and 0.4610 and 0.5080 ( $2\pi c/a$ ) for the *H*-polarization. As the wave vector  $k_z$  increases, the frequencies of these modes increase monotonically. All the modes finally vanish as  $k_z$  increases.

Since  $k_z^{1}$  0, these defect modes can propagate in the *z* direction. However, they are local modes, which are confined in the defect region, and can not propagate in the *x*-*y* plane freely. Therefore, they are guided modes inside the defect region along the *z* direction. In fact, such a line defect can be used to fabricate the photonic crystal optical fiber [7].

We also notice that all these guide modes are related to the original defect modes for the in-plane propagation. In particular, the field patterns of the guided modes are very similar to those of in-plane defect modes, and thus can be considered as continuous extensions of the in-plane *E*- or *H*-polarization defect modes.

The present method for off-plane wave propagation is also very important for studies of the photonic crystal antennas, which will also be presented in the talk.

### 4. Conclusions

In conclusions, we present a method based on FDTD scheme to study the off-plane electromagnetic waves propagation in two-dimensional photonic crystals by utilizing an artificial initial field distribution. Our results for the band structure of a square lattice of dielectric rod in the air are in good agreement with the results obtained by the plane wave expansion method. The defect modes for a two-dimensional photonic crystal with a triangular lattice of air holes in a dielectric medium are also studied. The defect is obtained by removing the center air hole, and the guided modes can be considered as the guide modes in the *z* direction since the wave vector  $k_z^1$  0. The studies show that these guided modes are extended from the in-plane defect modes.

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