FDFD and FDTD Analysis of Photonic Crystals and Loss Effect on Propagation Modes

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Abstract

A band diagram is the fundamental for investigation of the electromagnetic properties of periodic structures such as photonic crystals in optics or electromagnetic band gap structures in antenna engineering. In this paper, the two famous computational methods, finite difference frequency domain (FDFD) and finite difference time domain (FDTD) methods are applied for band diagram calculation of 2-D photonic crystals. Both of the methods are compared due to computational time and accuracy. Furthermore the loss effects on propagation modes of periodic structures have been investigated and the relationship between normalized frequency and changing the loss of the periodic structures has been found.

1. Introduction

In recent years, there has been a growing research activities related to the development of new artificial materials whose characteristics are useful for many disciplines such as optics, microwave engineering, antenna engineering, and electromagnetic compatibility. These materials are often called Metamaterials or particularly referred as photonic crystals [2, 4, 5] in optics, electromagnetic band gap (EBG) structures [1,3] in microwave and antenna engineering, and so forth. These materials are fabricated by periodic structures. In the development of these materials, it is necessary to know that how the wave behaves in these materials. The wave behavior is expressed by $k - w$ diagram, where k is wave number and w is angular frequency. Therefore, the $k - w$ diagram is important to understand the properties of periodic structures.

Numerical analysis is important in the design and applications of artificial materials. A variety of numerical methods have been utilized to calculate the propagation characteristics of 2-D periodic structures. The conventional plane wave expansion (PWE) method [4], although commonly employed in periodic structures research, suffers from slow convergence of the Fourier transform of the dielectric function. The finite element method (FEM) [6] is also a famous method in waveguide mode analysis with outstanding flexibility and accuracy, but its formulation is more difficult than the finite difference method (FDM) [7] and requires huge computer resources owing to its inherent methodology. On the other hand, the FDTD [8~10] and FDFD [13,14] methods have high capability of modeling the periodic structures. With concerning of these facts, FDFD and FDTD have been applied for periodic structures analysis including electromagnetic scattering and propagation modes analysis [5,11].

In the first half of this paper, FDFD and FDTD methods are applied for calculation of propagation modes in EBG structure as shown in Fig. 1. Both of the methods are compared due to calculation time and accuracy. In the last half of this paper, loss effects on propagation modes are investigated, because almost all of the materials have losses, so the loss effects are important for fabrication.

2. Formulation

FDTD and FDFD methods have high capability of electromagnetic calculation and propagation modes detection. FDTD and FDFD are applied for, TM case, mode propagation of the geometry shown in Fig.1. This figure shows a cross section of two-dimensional periodic structure in which the object is

placed in x-y plan and the unit cell is illustrated by dashed lines, where **r** is the radius of the rods and **a** is the periodic length. Here FDFD and FDTD methods are briefly summarized as follow.

2.1 FDFD and FDTD methods

FDFD Maxwell's equations are as follow.

$$\frac{\partial \breve{E}_z}{\partial x} = j\omega\mu_0\mu\breve{H}_y \quad (1a) \quad ; \quad \frac{\partial \breve{E}_z}{\partial y} = -j\omega\mu_0\mu\breve{H}_x \quad (1b) \quad ; \quad \frac{\partial H_y}{\partial x} - \frac{\partial \breve{H}_x}{\partial y} = j\omega\varepsilon_0\varepsilon\breve{E}_z \quad (1c)$$

After applying the central difference scheme, the term can be arranged in the following matrix equation.

$$j\omega \begin{bmatrix} \varepsilon_0\varepsilon_z & 0 & 0 \\ 0 & -\mu_0\mu_x & 0 \\ 0 & 0 & -\mu_0\mu_y \end{bmatrix} \begin{bmatrix} \mathbf{E_z} \\ \mathbf{H_x} \\ \mathbf{H_y} \end{bmatrix} = \begin{bmatrix} 0 & -\mathbf{V_y} & \mathbf{V_x} \\ \mathbf{U_y} & 0 & 0 \\ -\mathbf{U_x} & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{E_z} \\ \mathbf{H_x} \\ \mathbf{H_y} \end{bmatrix} \quad (2)$$

After some algebraic arrangements, we have

$$\{\mathbf{B} - k_0^2\mathbf{I}\} \cdot \mathbf{E_z} = \mathbf{0} \quad (3a) \quad ; \quad \mathbf{B} = -\varepsilon_z^{-1}\{\mathbf{V_y}\mu_x^{-1}\mathbf{U_y} + \mathbf{V_x}\mu_y^{-1}\mathbf{U_x}\} \quad (3b)$$

Where $\mathbf{V_x}$, $\mathbf{V_y}$, $\mathbf{U_x}$, and $\mathbf{U_y}$ are space differential operators [5] along x and y directions. Since eq.(3) is an eigenvalue problem, the QR method or the Implicitly Restarted Arnoldi (IRA) method [12] can be successfully applied to obtain the eigenvlaues.

In the FDTD calculation the field equations are solved in time domain under the periodic boundary condition. After that the fields are converted through Fourier transform to frequency domain, and then the band diagram is obtained by searching the peaks of the Fourier spectrum for the specific wave numbers K_x *and* K_y . The accuracy depends heavily on the resolution of the peak search.

2.2 Periodic Boundary Condition

Due to the periodic geometry, the field distribution in a periodic structure should satisfy the Bloch theorem. Bloch conditions for periodic structure are as

$$\mathbf{H}(\mathbf{r} + \mathbf{T}) = e^{-j\mathbf{k}\cdot\mathbf{T}}\mathbf{H}(\mathbf{r}) \quad (4a) \quad ; \quad \mathbf{E}(\mathbf{r} + \mathbf{T}) = e^{-j\mathbf{k}\cdot\mathbf{T}}\mathbf{E}(\mathbf{r}) \quad (4b)$$

where **T** is the lattice vector of the periodic structure. Therefore, in the analysis of periodic structure, we only need to consider the unit cell for our calculation along with the periodic boundary condition (PBC) [5, 15] resulting from the Bloch conditions. For the periodic structure with square lattice as shown in Fig. 1, the PBC can be expressed as

$$\boldsymbol{\psi}(x + a, y) = e^{-jk_x a}\,\boldsymbol{\psi}(x, y) \quad (5a) \quad ; \quad \boldsymbol{\psi}(x, y + a) = e^{-jk_y a}\,\boldsymbol{\psi}(x, y) \quad (5b)$$

Where $\boldsymbol{\psi}$ is either the electric or magnetic field in the unit cell and k_x and k_y are the wave numbers in x and y directions respectively.

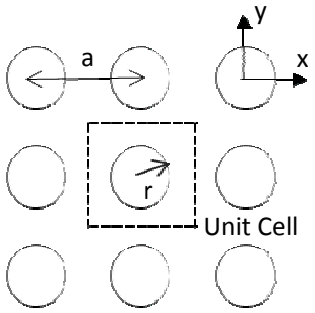

Fig. 1. The cross section of square lattice of 2-D periodic structure and its unit cell

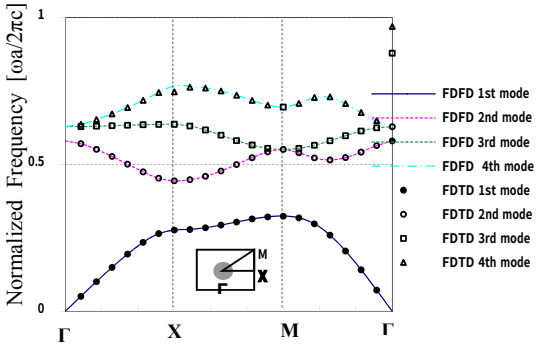

Fig. 2. Band diagram of first 4 Propagation modes

3. Numerical Results

3.1 Comparison of FDFD and FDTD for Band Diagram Calculation

Fig. 2 shows the band diagram for the first 4 propagation modes calculated by the FDFD and FDTD methods when the object of the Fig. 1 is composed of dielectric cylinders with relative permittivity and radius of 8.9 and $0.2\boldsymbol{a}$ respectively, where the computation region is 20×20 cells. Both of the methods indicate almost the same results, however FDTD disagree with FDFD when two modes degenerate. This is caused by the difference of the eigenvalue calculation and the peak search. We can identify and obtain multiple roots of the characteristic equation of the eigenvlaue problem in FDFD even if they are very close to each other, however in FDTD, there is only one peak appears in the Fourier spectrum when the modes are very close to each other or degenerating. Therefore, the higher eigenfrequency is recognized as the one belonging to the lower mode as shown at the point M in Fig. 2 and Fig. 3. For higher modes shown in Fig. 3, although the FDFD method seems to have no problem basically, however, the relatively large disagreement is observed as the modes become higher. This is for the reason that the sequential two modes reset in very close eigenfrewquencies, and these peaks given by the FDTD calculation are also very close to each other. Therefore, the positions of these peaks cannot be distinguished well depending on the resolution of the numerical Fourier transformation.

The calculation time required in above calculation is shown in Fig. 4. This time is normalized by that for the case of 400 cells ($NX = NY = 20$). It is found that the FDTD method requires shorter time than the FDFD method. It is also cleared that IRA method is effective for reducing the computational time than QR method in FDFD. Therefore the FDTD method is useful for reducing the computation time required for modes calculation; however the FDFD method should be sued when we need the accurate results especially for higher modes.

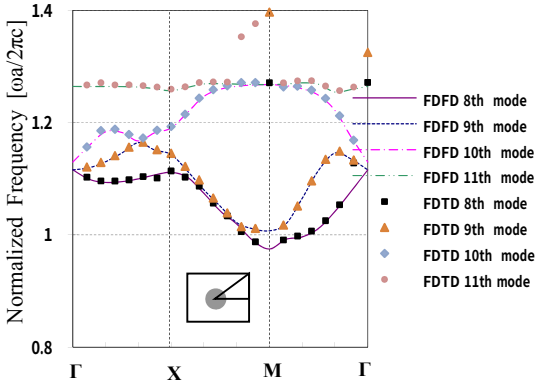

Fig. 3. Band diagram for first 8 to 11 Propagation modes

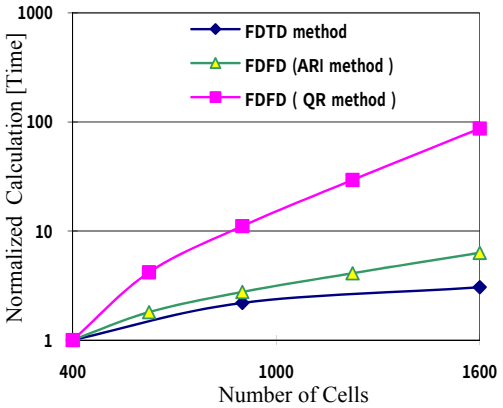

Fig. 4. Calculation Time of FDFD and FDTD methods

3.2 Loss Effects on Propagation Modes

Considering the periodic cylinders of Fig. 1 as lossy cylinders. The relative permittivity of the lossy periodic structure is

$$\varepsilon_r = \varepsilon' - j\epsilon'' = \varepsilon'(1 - j\varepsilon''/\varepsilon') \tag{6}$$

Where ε' is real part and $\epsilon''$is the imaginary part of the complex relative permittivity. The value of ε' is 8.9 and $\varepsilon''/\varepsilon'$ is changing here for investigating the loss effects of the material. Fig. 5 shows the band diagram of the first propagation mode in irreducible Brillouin zone. The results by FDFD and FDTD show that at every point of irreducible Brillouin zone, when $\varepsilon''/\varepsilon'$ increases the normalized frequency decreases.

Fig. 6 shows the relationship between the normalized imaginary part of the frequency and $\varepsilon''/\varepsilon'$. From Fig. 6, it can be seen that when $\varepsilon''/\varepsilon'$ approaches to 1, the normalized imaginary part of frequency also increases but when $\varepsilon''/\varepsilon'$increases further then the normalized imaginary part of the

frequency decreases. Fig. 6 shows the normalized imaginary part of the frequency of the first eight propagation modes for $K_x = \pi/3$ and $K_y = 0$ in irreducible Brillouin zone.

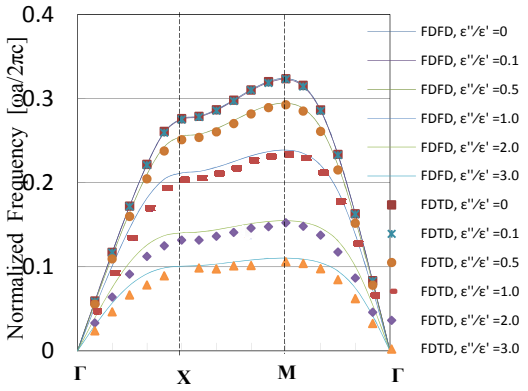

Fig. 5. Band structure for variation of $\varepsilon''/\varepsilon'$

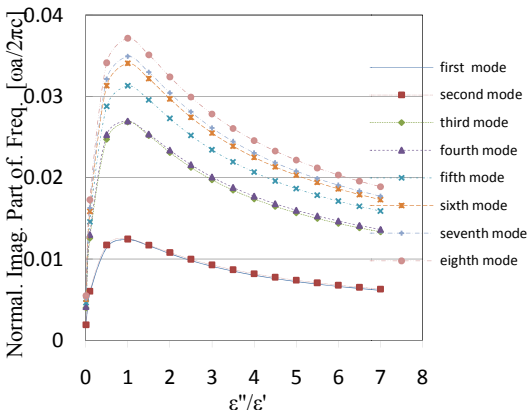

Fig. 6. Normal. Imag. part of Freq. versus $\varepsilon''/\varepsilon'$

4. Conclusion

This paper studied the computer resources and the accuracy for calculation of the band diagram of periodic structure using the FDFD and FDTD methods. As computation time is concerned, the FDTD method has a clear advantage over the FDFD method. However, the FDTD method issues unexpected values when two modes have very close characteristics. For high accuracy, especially for higher modes, the FDFD method should be used because the FDTD method has error in the resolution of peak search when the modes are very close to each other.

This paper also investigated the loss effects on propagation modes. It has been found that the normalized frequency decreases with increasing of $\varepsilon''/\varepsilon'$ of the relative permittivity. It is also investigated that the normalized imaginary part of the frequency increases when $\varepsilon''/\varepsilon'$ increases from 0 to 1, however, when this value increases further then the normalized imaginary part of the frequency decreases instead of increasing.

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