# Band Diagram Analysis of Frequency-Dependent Photonic Band-Gap Structures Using FDFD Method

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## Abstract

Recently, photonic band-gap (PBG) structures are under intense research due to their various applications in optics, microwave, and antenna engineering. Therefore, the accurate modelling of band diagram of frequency-dependent PBG structures is highly needed because the electric properties of all of the materials depend on frequency. In this paper, a new finite-difference frequency-domain (FDFD) algorithm is derived to calculate the propagation modes in frequency-dependent PBG structures. For validity of this method, the results are compared with the finite-difference time-domain (FDTD) method.

Keywords: PBG structure mode propagation FDFD FDTD

# **1. Introduction**

Photonic band-gap (PBG) structures or photonic crystals (PCs) [1] are artificial materials that consist of periodic structures with different refractive indices. Over the past more than 30 years, researchers have made remarkable achievements in this area. Recently, there has been considerable interest in analysis of band structure of frequency-dependent or linear dispersive PBG structures in which the relative permittivity of the material is frequency-dependent. Appropriate treatment of frequency-dependent materials is needed for accurate modelling of propagation modes over a wide range of frequencies in microwave and optical ranges. The finite-difference time-domain (FDTD) method is the famous computational electromagnetic technique for modelling of wave propagation [2][3]. In order to model frequency-dependent materials, the usual Yee FDTD time-stepping equations need to be modified. Modified FDTD algorithm have been introduced to deal with the frequency-dependent materials [4]-[6]. However, FDTD does not have enough accuracy in calculation of band structure for frequency-dependent PBG structures. FDTD first calculates the fields and then the eigenmodes can be obtained using these fields values. Therefore the accuracy is affected due to many reasons. Spurious eigenfrequencies will appear in addition to the desired solutions if the data is noisy or some eigenfrequencies may be missed if the excitation or monitor is not properly placed. FDTD cannot detect the eigenfrequencies when they are very close to each other or FDTD has limitation in resolution of degenerated modes.

On the other hand, the finite-difference frequency-domain (FDFD) method can analyze the band diagram of PBG structure accurately, because the FDFD algorithm is finalized with an eigenvalue matrix equation, and every eigen-mode can be found directly from the solution of this matrix equation and there is no need to use field values or to set observation and source points [7]-[11]. If we look back to the history of FDFD method, Yang [10] proposed a finite-difference frequency-domain based on directly discretizing the Helmholtz's equation in the homogeneous sub-regions and field matching at the central grid point. After that various FDFD algorithms have been introduced that are applicable for different applications and reducing the computational time.

In this paper, a new FDFD method is derived to calculate the band diagram of PBG structures built with frequency-dependent materials characterized by Debye model. The formulation of this method is summarized with eigenvlaue problem, from which one can find the eigenfrequencies easily. The eigenfrequencies, are calculated using the Implicitly Restarted Arnoldi (IRA) algorithm [12]. The normalized frequencies versus the wave numbers in irreducible Brillouin zone can be found from these eigenfrquencies

straight forward. As this method uses eigenvalue equation and there is no chance to lose the eigenfrequency for any of the band point, therefore it can compute the propagation modes in frequency-dependent PBG structures accurately. This FDFD method can lead to model other types of frequency-dependant or dispersive PBG structures. In order to validate this method, the results are compared with the FDTD method, that show a high accuracy and stability. In this paper, the TM case of 2-dimensional (2D) PBG structure for square lattice is analyzed, where the TE case is straight forward.

#### 2. Formulation

In order to develop the new FDFD algorithm for PBG structure composed of dispersive Debye medium, we start form the basics of traditional FDFD method [1]. The differential Maxwell's equations in frequency domain are

$$\nabla \times \mathbf{E} = -j\omega\mu_0\mu\mathbf{H} \tag{1}$$

$$\nabla \times \mathbf{H} = j\omega\varepsilon_0 \varepsilon \mathbf{E} \tag{2}$$

Where  $\mu$  and  $\varepsilon$  are relative permeability and permittivity respectively. In Eq.(2) we replace the relative permittivity  $\varepsilon$  by the single-pole Debye medium relative permittivity which has the following complex form

$$\varepsilon'(\omega) = \varepsilon_{\infty} + \frac{\varepsilon_s - \varepsilon_{\infty}}{1 + j\omega t_0} = \varepsilon_{\infty} + X(\omega)$$
(3)

Where  $\varepsilon_s$  is the static relative permittivity or the permittivity where the frequency is zero,  $\varepsilon_{\infty}$  is the relative permittivity at infinite frequency, and  $t_0$  is the relaxation time. Discretizing of (1) and (2), after replacing of relative permittivity of Debye medium, using Yee's mesh as shown in Fig. 1, and further arranging of the equations yield the following matrix equation.

$$j\omega \begin{bmatrix} \varepsilon_0 \varepsilon_z' & 0 & 0\\ 0 & -\mu_0 \mu_x & 0\\ 0 & 0 & -\mu_0 \mu_y \end{bmatrix} \begin{bmatrix} \mathbf{E}_z\\ \mathbf{H}_x\\ \mathbf{H}_y \end{bmatrix} = \begin{bmatrix} 0 & -\mathbf{V}_y & \mathbf{V}_x\\ \mathbf{U}_y & 0 & 0\\ -\mathbf{U}_x & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{E}_z\\ \mathbf{H}_x\\ \mathbf{H}_y \end{bmatrix}$$
(4)

Where  $V_x, V_y, U_x$ , and  $U_y$  are field coefficients square matrices formed according to the boundary condition [1].  $\mu_x$ ,  $\mu_y$ , and  $\varepsilon_z$  are diagonal matrices representing the permeability or permittivity values at the corresponding grid points.  $\mathbf{H}_x, \mathbf{H}_y$ , and  $\mathbf{E}_z$  are field vectors at the grid points. By eliminating of  $\mathbf{H}_x$  and  $\mathbf{H}_y$  from (4), we have the following matrix equation.

$$-\omega^2 \varepsilon_0 \varepsilon_z \mathbf{E}_z - \mathbf{A} \mathbf{E}_z = 0 \tag{5}$$

Where A is the characteristic matrix as

$$A = \frac{1}{\mu_0} (V_y * \mu_x^{-1} * U_y + V_x * \mu_y^{-1} * U_x)$$
(6)

After replacing the value of  $\varepsilon_z$  into equation (5) and further arrangements of the terms, we obtain the following equation.

$$-j\omega^{2}\varepsilon_{\infty}I_{1}\mathbf{E}_{z} + \omega^{3}\varepsilon_{\infty}t_{0}\mathbf{E}_{z} - j\omega^{2}(\varepsilon_{s} - \varepsilon_{\infty})\mathbf{E}_{z} - j(\frac{1}{\varepsilon_{0}})\mathbf{A}I_{1}\mathbf{E}_{z} + \omega(\frac{1}{\varepsilon_{0}})\mathbf{A}t_{0}\mathbf{E}_{z} = 0$$
(7)

Where  $I_1$  is the unit matrix;  $\varepsilon_s$ ,  $\varepsilon_{\infty}$ , and  $t_0$  are diagonal matrices composed of permittivity or relaxation time values at the grid points. With the substitutions of  $B = \varepsilon_{\infty} t_0$ ,  $C = j\varepsilon_{\infty} I_1$ ,  $D = j(\varepsilon_s - \varepsilon_{\infty})$ ,  $E = j\frac{A}{\varepsilon_0}I_1$ , and  $F = \frac{A}{\varepsilon_0}t_0$  into (7), and further algebraic arrangements of the terms, we can have as

$$-\omega^{2}(C+D)\mathbf{E}_{z} - \mathbf{E}\mathbf{E}_{z} + \omega \mathbf{F}\mathbf{E}_{z} = -\omega^{3}\mathbf{B}\mathbf{E}_{z}$$
(8)

$$-\omega^2 \mathbf{B}^{-1} (\mathbf{C} + \mathbf{D}) \mathbf{E}_{\mathbf{z}} - \mathbf{B}^{-1} \mathbf{E} \, \mathbf{E}_{\mathbf{z}} + \omega \mathbf{B}^{-1} \mathbf{F} \, \mathbf{E}_{\mathbf{z}} = -\omega^3 \, \mathbf{E}_{\mathbf{z}}$$
(9)

$$\omega^2 \mathbf{B}^{-1} (\mathbf{C} + \mathbf{D}) \mathbf{E}_{\mathbf{z}} + \mathbf{B}^{-1} \mathbf{E} \, \mathbf{E}_{\mathbf{z}} - \omega \mathbf{B}^{-1} \mathbf{F} \, \mathbf{E}_{\mathbf{z}} = \omega^3 \, \mathbf{E}_{\mathbf{z}}$$
(10)

We can solve (10) for  $\omega$  by using the following matrix equation.

$$\mathbf{G}\,\mathbf{Y} = \boldsymbol{\omega}\,\mathbf{Y} \tag{11}$$

Where

$$\mathbf{G} = \begin{bmatrix} \mathbf{B}^{-1}(\mathbf{C}+\mathbf{D}) & -\mathbf{B}^{-1}\mathbf{F} & \mathbf{B}^{-1}\mathbf{E} \\ \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} & \mathbf{0} \end{bmatrix} \quad \text{and} \quad \mathbf{Y} = \begin{bmatrix} \boldsymbol{\omega}^{2} \mathbf{E}_{z} \\ \boldsymbol{\omega} \mathbf{E}_{z} \\ \mathbf{E}_{z} \end{bmatrix}$$

Equation (11) is an ordinary eigenvalue equation in which G is the characteristic matrix and  $\omega$  is the eigenvalues of matrix G that corresponds to eigenfrequencies. From Eq. (11), one can find the normalized frequencies as  $\frac{\omega a}{2 \pi c}$ , where a is the length of the unit cell and c is the speed of light in free space.

**3. Numerical Results** 

For the validity of our method, the band diagram of 2-D PBG structure composed of dispersive Debye media, with square lattice, has been analyzed. Here, a is the length of unit cell and r is the radius of the dispersive cylinders. r/a=0.2,  $a=1\,\mathrm{mm}$ , and  $\Delta x = \Delta y = 0.025\,\mathrm{mm}$ . In this FDFD method, the IRA algorithm is used to obtain the eigenfrequencies and in the FDTD method, the Harminv program is used to detect eigenfrequencies from the fields values [13]. For Debye model,  $t_0=9.4$  E-12,  $\varepsilon_s=4.0$ , and  $\varepsilon_{\infty}$  is set as 3.0, and 2.0 for analysis and validation of the methods. In FDTD, Gaussian pulse is used as a point source.

First to confirm the validity of this FDFD method  $\mathcal{E}_{\infty}$  is set as 4.0, for this value the medium become pure dielectric for which we can use traditional FDFD straight forward, and the first eight propagation modes have been calculated and compared the results with the usual FDFD method [1] as shown in Fig. 2. The results of this FDFD algorithm are in excellent agreement with the usual FDFD method, which shows that the formulation of this algorithm is perfect. Fig. 3 shows the band diagram calculation of first eight propagation modes for which  $\mathcal{E}_{\infty}$  is set as 3.0 and 2.0 in both the FDFD and FDTD methods. The propagation modes calculated by this FDFD method are very clear, where the FDTD method has some irregularities in these modes calculations. In FDFD method the eigenfrequencies are obtained directly form eigenvalue equation and there is no field data needed, therefore every point of the band has its own value even if the two modes are placed very close or overlap to each other . However, in the FDTD method when two modes are very close or degenerated then both of them are difficult to detect and one of them will lose. This degeneration of mode values will increase in the higher modes, which can be count as one of the FDTD fault in band diagram calculation. The loosing of degenerated points of the modes in the FDTD method also can be seen in Fig. 4 for which  $\varepsilon_{\infty} = 2.0$ , where the FDFD values have high accuracy and there is no any value losing.

# 4. Conclusion

The new derived FDFD method is successfully applied for mode propagation in PBG structure built with dispersive Debye medium. The formulation of FDFD method is summarized with eigenvalue equation, therefore the eigenfrequencies for each point of the band can be obtained even if the two neighbour eigenfrequencies are very close or overlap to each other. The results of

band diagram calculations for dispersive PBG structure are compared with those calculated by FDTD method. The results show that the FDFD method is very stable and capable to model the band diagram of dispersive PBG structure efficiently and accurately.



**Fig. 1** Fields alignments for TM mode analysis of 2-D dispersive PBG structure.



**Fig. 3.** Comparison of FDFD and FDTD when the relative permittivity at infinite frequency is 3.0.

### References



**Fig. 2.** Comparison of conventional FDFD and this FDFD when the parameters in this FDFD are set the same as in conventional FDFD for dielectric case.



**Fig. 4.** Comparison of FDFD and FDTD when the relative permittivity at infinite frequency is 2.0.

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