New derived finite-difference frequency-domain method used for band structure analysis of 2-D EBG structure composed of Drude-type dispersive media

Amin Gul Hanif^{a)}, Takuji Arima^{b)}, and Toru Uno^{c)}

*Electronic and Information Department of Graduate School of Engineering,
Tokyo University of Agriculture and Technology
2–24–16 Naka-cho, Koganei-shi, Tokyo 184–0012, Japan*

a) 50012894005@st.tuat.ac.jp

b) t-arima@cc.tuat.ac.jp

c) uno@cc.tuat.ac.jp

Abstract: Electromagnetic wave properties in metamaterials including electromagnetic band gap (EBG) structures have been widely investigated due to their inherent capabilities for developing novel devices in the fields of optics, microwave and antenna engineering. In reality, most of the materials are dispersive or frequency-dependent, on the other hand, it is important to investigate how the performance of EBG structures depends on frequency. We propose herein a new finite-difference frequency-domain (FDFD) algorithm for band structure analysis of two-dimensional EBG materials composed of Drude-type dispersive media. This method is shown to lead to highly accurate and stable band structure calculation.

Keywords: band structure analysis, dispersive materials, EBG structure, FDFD, FDTD

Classification: Electromagnetic theory

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1 Introduction

Recently, remarkable progress has been made in the study of electromagnetic band gap (EBG) structures due to their various applications in optics, microwave, and antenna engineering [1, 2, 3]. The band structure of EBG structures, synonymous for photonic crystals in optics, has been researched for many years in frequency-independent materials. Recently, interest has grown in the analyzing dispersive or frequency-dependent EBG structures for novel applications. Therefore, accurate models of the band structure of EBG structures composed of dispersive materials is highly desirable for efficient analysis of wave propagation phenomena over a wide range of frequencies in microwave and optical fields.

Several numerical methods have been used to compute the band structure of two-dimensional (2-D) EBG structures. The most commonly used methods are the plane-wave expansion (PWE) method [3], the finite-difference time-

domain (FDTD) method [4, 5], and the finite-difference frequency-domain (FDFD) method [2, 6]. The PWE method is very simple and easy to apply. However, the resultant matrix of the PWE method is dense and large, thus making its computation heavy for large problems. The FDTD method is a widely-used electromagnetic computational method, which is also applicable for dispersive materials [7]. However, in some cases, the FDTD method does not provide accurate results for band structure calculation of EBG structures. To improve the accuracy of the conventional FDTD method, many FDTD algorithms have been proposed. Although the accuracy of the FDTD has been improved, it is still not sufficient. There is a chance of losing the resonant frequencies if the excitation and monitor points are not properly located in the calculation domain [4, 6]. In addition, spurious modes may appear in the band structure because of low spatial resolution [8]. Furthermore, the FDTD has limitations in resolving the degenerate eigenmodes [4].

Conversely, the FDFD method is highly accurate in band structure calculations of 2-D EBG structures [9, 10, 11, 12, 13, 14]. Because the FDFD method does not use spectral analysis, it does not have problems detecting spectral peaks. The FDFD method simply uses the eigenvalue equation (calculates the eigenvalues of the characteristic matrix composed of field coefficients) and is capable to obtain the eigenfrequencies clearly even if they are very close to each other or degenerate. Yang [9] proposed a FDFD method based on discretizing the Helmholtz equation in the homogeneous sub-regions and field matching at the central grid point. Following that work, various 2-D FDFD algorithms were developed for band structure calculations of EBG structures. Nevertheless, it has not been possible to calculate the band structure for lossy or any other type of dispersive materials with the FDFD method. Lately, we developed an improved 2-D FDFD algorithm that includes electrical conductivity in its formulation and that allows the calculation of the band structure of 2-D lossy EBG structures [13]. In addition, we have also proposed a new 2-D FDFD algorithm for band structures calculation of Debye-type dispersive EBG structures [14].

In this paper, we propose a new FDFD algorithm for band structure analysis of 2-D EBG structures composed of Drude-type dispersive materials. Because this algorithm uses only the eigenvalue equation, there is no chance to lose the eigenfrequency for any of the band points. This allows accurate computation of the propagation modes in Drude-type dispersive EBG structures. To validate this method, the results are compared with the FDTD method which shows high accuracy and stability.

2 Formulation

The formulation has been developed for TM_z mode, single-pole Drude-type dispersive materials. First, we start from Maxwell's equations in the frequency domain

$$\nabla \times \mathbf{E} = -j\omega\mu_0\mu_r \mathbf{H} \quad (1)$$

$$\nabla \times \mathbf{H} = j\omega\varepsilon_0\varepsilon_r \mathbf{E} \quad (2)$$

where μ_r and ε_r are the relative permeability and permittivity, respectively. Here, the relative permittivity ε_r is replaced with the single-pole Drude-type frequency-dependent relative permittivity ε'_r

$$\varepsilon'_r(\omega) = 1 + \frac{\omega_p^2}{-\omega^2 + j\omega v_c} \quad (3)$$

where ω_p is the Drude-pole frequency, v_c is the inverse of the Drude-pole relaxation time, and ω is the angular frequency. Discretizing Eqs. (1) and (2), with Yee's mesh as shown in Fig. 1 (a), and further arranging the equations yields the following matrix equation.

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

where ε'_z is a diagonal matrix composed of Drude relative permittivity at the grid points; $\mathbf{V}_x$, $\mathbf{V}_y$, $\mathbf{U}_x$, and $\mathbf{U}_y$ are square matrices containing space-differential operators along x and y directions; μ_x and μ_y are diagonal matrices of relative permeability at the grid points; $\mathbf{H}_x$, $\mathbf{H}_y$, and $\mathbf{E}_z$ are column matrices containing the field values. Periodic boundary conditions, on the square unit cell as shown in Fig. 1 (b), are placed in the space-differential operators [2]. For simplicity, we eliminate $\mathbf{H}_x$ and $\mathbf{H}_y$ from (4), which leads to

$$-\omega^2 \varepsilon_0 \varepsilon'_z \mathbf{E}_z - \mathbf{A} \mathbf{E}_z = 0 \quad (5)$$

Where $\mathbf{A}$ is a sparse matrix composed of space differential operators and the inverse of relative permeability matrices

$$\mathbf{A} = \frac{1}{\mu_0} (\mathbf{V}_y * \mu_x^{-1} * \mathbf{U}_y + \mathbf{V}_x * \mu_y^{-1} * \mathbf{U}_x) \quad (6)$$

we insert the value of ε'_z into Eq. (5) and can write

$$-\omega^2 \varepsilon_0 \left(\mathbf{I} + \frac{\omega_p^2}{-\omega^2 \mathbf{I} + j\omega \mathbf{v}_c} \right) \mathbf{E}_z = \mathbf{A} \mathbf{E}_z \quad (7)$$

where $\mathbf{I}$ is the identity matrix.

$$-\omega^2 \varepsilon_0 \mathbf{I} \mathbf{E}_z - \frac{\omega^2 \varepsilon_0 \omega_p^2}{-\omega^2 \mathbf{I} + j\omega \mathbf{v}_c} \mathbf{E}_z = \mathbf{A} \mathbf{E}_z \quad (8)$$

After substituting of $\omega_s = \omega_p^2$ and performing some algebraic manipulations we have

$$\omega^4 \varepsilon_0 \omega_s^{-1} \mathbf{E}_z - j\omega^3 \varepsilon_0 \mathbf{V}_c \omega_s^{-1} \mathbf{E}_z - \omega^2 \varepsilon_0 \mathbf{I} \mathbf{E}_z = -\omega^2 \omega_s^{-1} \mathbf{A} \mathbf{E}_z + j\omega \mathbf{V}_c \omega_s^{-1} \mathbf{A} \mathbf{E}_z \quad (9)$$

$$-j\omega^3 \varepsilon_0 \mathbf{V}_c \omega_s^{-1} \mathbf{E}_z - \omega^2 \varepsilon_0 \mathbf{I} \mathbf{E}_z + \omega^2 \omega_s^{-1} \mathbf{A} \mathbf{E}_z - j\omega \mathbf{V}_c \omega_s^{-1} \mathbf{A} \mathbf{E}_z = -\omega^4 \varepsilon_0 \omega_s^{-1} \mathbf{E}_z \quad (10)$$

$$-j\omega^3 \mathbf{V}_c \omega_s^{-1} \mathbf{E}_z - \omega^2 \mathbf{I} \mathbf{E}_z + \omega^2 \omega_s^{-1} \frac{\mathbf{A}}{\varepsilon_0} \mathbf{E}_z - j\omega \mathbf{V}_c \omega_s^{-1} \frac{\mathbf{A}}{\varepsilon_0} \mathbf{E}_z = -\omega^4 \omega_s^{-1} \mathbf{E}_z \quad (11)$$

Fig. 1. (a) Yee's mesh for TM mode analysis (b) The square unit cell

$$j\omega^2\omega_s\mathbf{V}_c\omega_s^{-1}\mathbf{E}_z + \omega\omega_s\mathbf{E}_z - \omega\frac{\mathbf{A}}{\varepsilon_0}\mathbf{E}_z + j\omega_s\mathbf{V}_c\omega_s^{-1}\frac{\mathbf{A}}{\varepsilon_0}\mathbf{E}_z = \omega^3\mathbf{E}_z \quad (12)$$

Substituting $\mathbf{B} = j\omega_s\mathbf{V}_c\omega_s^{-1}$, $\mathbf{C} = \omega_s - \frac{\mathbf{A}}{\varepsilon_0}$, and $\mathbf{D} = j\omega_s\mathbf{V}_c\omega_s^{-1}\frac{\mathbf{A}}{\varepsilon_0}$ into (12) yields

$$\omega^2\mathbf{B}\mathbf{E}_z + \omega\mathbf{C}\mathbf{E}_z + \mathbf{D}\mathbf{E}_z = \omega^3\mathbf{E}_z \quad (13)$$

We can reform (13) into eigenvalue equation

$$\mathbf{H}\mathbf{Z} = \omega\mathbf{Z} \quad (14)$$

where

$$\mathbf{H} = \begin{bmatrix} \mathbf{B} & \mathbf{C} & \mathbf{D} \\ \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} & \mathbf{0} \end{bmatrix} \quad \text{and} \quad \mathbf{Z} = \begin{bmatrix} \omega^2\mathbf{E}_z \\ \omega\mathbf{E}_z \\ \mathbf{E}_z \end{bmatrix} \quad (15)$$

The quantity ω is the eigenvalue of matrix $\mathbf{H}$, from which one finds the normalized eigenfrequency to be $\omega a/2\pi c$, where a is periodic length and c is the speed of light in vacuum.

3 Numerical results

The analysis model is a 2-D EBG structure composed of Drude-type dispersive periodic cylinders with square lattice. The unit cell contains only one cylinder with radius r and has periodic length a as shown in Fig. 1 (b). Other parameters are $r/a = 0.2$, $a = 1$ mm, and $\Delta x = \Delta y = 0.025$ mm. For the FDFD method, the Arnoldi algorithm [15] is used to compute the eigenvalues. In the FDTD calculation, the recursive-convolution (RC) approach is used to model the Drude dispersive materials [4]. In order to verify the validity of this new FDFD algorithm and also to analyze the dispersive properties of the material, different values of the frequency-dependent permittivity are used.

Fig. 2 shows normalized frequency of the first five (1st to 5th) eigenmodes of the band structure calculated by FDFD and FDTD methods. Fig. 2 (a)

Fig. 2. Band structure computation of the dispersive EBG using FDFD and FDTD methods. (a) Both methods give good agreement. (b) The methods do not agree sufficiently well because of an increase in the lossy term of the relative permittivity.

illustrates the band structure computation for $\omega_p = 1.0 \cdot 10^{14}$ and $V_c = 1.0 \cdot 10^{13}$. In this calculation, the band gap is created at the beginning of the range of frequencies. Both methods agree well in this computation, except that, because of degenerate modes, the FDTD method calculates some irregular values for Γ and M points in the irreducible Brillouin zone.

Fig. 2 (b) shows the band structure computation for $\omega_p = 1.0 \cdot 10^{14}$ and $V_c = 1.0 \cdot 10^{14}$. In this calculation, the FDTD method produces some errors, as seen in the Γ -M band and that are due to an increase in V_c of the relative permittivity because V_c is associated with the loss term of the relative permittivity, and the FDTD method has low accuracy for calculating the eigenfrequencies in the lossy case [13]. Fig. 3 (a) shows the band structure calculation for $\omega_p = 1.0 \cdot 10^{12}$ and $V_c = 1.0 \cdot 10^{13}$, for which we have low imaginary part of the relative permittivity. In this calculation there is no band gap and most of the mode values overlap each other or there are many degenerate modes, where the FDTD method has difficulties calculating the degenerate modes because they appear at the same frequency. However, the FDFD method is capable of calculating all the modes because it uses the eigenvalues and can compute the modes even if they are very close to each other. Fig. 3 (b) shows the band structure calculation using the FDFD method for $\omega_p = 1.0 \cdot 10^{14}$, where V_c has been set to $V_c = 1.0 \cdot 10^{12}$ and $V_c = 1.0 \cdot 10^{15}$. As the loss term or V_c increases the normalized frequency decreases, but this FDFD algorithm still calculates the eigenfrequencies of all of the eigenmodes accurately.

Fig. 3. (a) Band structure calculation using FDFD and FDTD methods for a low value of relative permittivity for which the modes are degenerate. (b) Band structure calculation for two different values of the lossy term of relative permittivity using the FDFD algorithm.

4 Conclusion

In this paper, a new FDFD algorithm is proposed to analyze the band structure of 2-D EBG structures composed of Drude-type dispersive materials. The simulation results are compared with the FDTD method, which show that the FDFD algorithm can accurately calculate the band structure. This algorithm successfully calculates the eigenfrequencies of the degenerate modes as seen at M point of irreducible Brillouin zone. Furthermore, this algorithm relies only on linear algebra and directly uses the eigenvalue equation; thus it enables the analysis of the band structure of different types of Drude dispersive materials.