Modified Yee's Cell for Finite-Difference Time-Domain Modeling of Periodic Boundary Guiding Structure

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***Abstract* - A modified Yee's Cell is proposed for the finite-difference time-domain (FDTD) modeling of the waveguide structure with the longitudinally periodic boundary condition. For the presented FDTD scheme based on the Floquet's theorem, an arrow representing a complex field component in the original Yee's cell is divided into two real-arrow and imaginary-arrow separated by a half of the longitudinal spatial-increment, $\Delta z/2$. By the proposed mesh scheme and the periodicity of the computational domain, the handling of the complex field function and the periodic boundary condition is streamlined, resulting in the reduction of the computation time and memory. To verify the proposed scheme, the dispersion diagram of a corrugated parallel-plate waveguide is obtained and compared with the transmission line analysis. Also, the numerical stability condition and the numerical dispersion relation are given.**

I. INTRODUCTION

Guided wave propagation through the periodic guiding structure (PGS) has been a subject of interest for a long time due to its slow-wave and stop-band characteristic. The application of the PGS covers the integrated optics area, including distributed feedback lasers, distributed Bragg reflection lasers, and quasiphase-matched second-harmonic generation, and microwave's area, including traveling-wave tube, filter, and delay line.[1][2] So far, based on the Floquet's theorem[2], the PGS has been mostly analyzed using mode-matching technique, method of moment, finite element method, transmission line matrix method, and finite-difference time-domain (FDTD) method.[3-8] Among these analysis methods, FDTD method is a strong candidate for the numerical analysis of anisotropic, inhomogeneous, and irregular-formed PGS.[6][7] Particularly, the recent introduction of photonic-bandgap (PBG) material technology[9] requires accurate and efficient analysis methods of arbitrary-shaped PGS.

Several attempts based on the Floquet's theorem, have been published related to the FDTD modeling of the PGS, where the periodic boundary condition (PBC) is imposed into the FDTD algorithm for the longitudinally periodic waveguide structure. Cangellaris et al introduced a hybrid spectral/FDTD method.[6] By the periodicity of the computational domain, their scheme computes the longitudinal-spatial-derivative spectrally using the discrete Fourier series representation, which satisfies the PBC and higher-order derivative at once. On the other hand, Celuch-Marcysiak and Gwarek suggested a spatially looped algorithm using the basic central-difference scheme for the FDTD modeling of the PGS.[7] To implement the PBC in their algorithm, the looping operator is adopted.

For the PGS analysis, we present a new FDTD scheme for the calculation of the periodic function in the same computational domain as [6]. In the presented FDTD algorithm, the PBC is directly implemented without any looping operator like [7]. However, the longitudinal spatial derivative using the fast Fourier transform (FFT) used in [6] requires additional time and memory resource compared to the basic central-difference scheme of the standard FDTD method. Therefore, in this paper, we propose a newly modified Yee's cell, by which the derivatives with respect to all of the temporal and spatial variables are approximated using the central-differences. Therefore, this paper with [6] makes it possible the trade-off between the numerical accuracy and the computational resources in the FDTD simulation for the periodic wave in the PGS. To our knowledge, since there has been not clearly explain about the physical meaning of the time-domain complex function used in FDTD simulation such as [6], the next section will open this issue by the time-domain representation of the wave function in the PGS.

II. FDTD SCHEME USING MODIFIED YEE'S CELL

While the Floquet's theorem is usually presented in frequency(ω)-domain, it can be used in time-domain to determine the propagation characteristic of a longitudinally periodic structure. When a wave is guided by an arbitrary waveguide structure periodic in z-direction with period d, the time-domain representation of the wave propagating with a propagation constant β parallel to z-axis is given by both positive-going and negative-going waves, as shown in Eq.(1). In general, it includes both cosine and sine harmonics.

$$
\begin{aligned}
&F(x,y,z,t)\Big|_{\text{propagating with the specified propagation constant }\beta} \\
&= \sum_{l=1}^{N} \begin{bmatrix} a_{\omega_l}^{+}(x,y,z)\cos(\beta z-\omega_l t) \\ + b_{\omega_l}^{+}(x,y,z)\sin(\beta z-\omega_l t) \\ + a_{\omega_l}^{-}(x,y,z)\cos(\beta z+\omega_l t) \\ + b_{\omega_l}^{-}(x,y,z)\sin(\beta z+\omega_l t) \end{bmatrix} \\
&= \mathrm{Re}\left[f(x,y,z,t)e^{j\beta z}\right] \qquad (1)
\end{aligned}
$$

(1) is the time-domain representation of the wave guided by the PGS based on the Floquet's theorem, where the wave function is represented by the real part of the complex function $f(x,y,z,t)e^{j\beta z}$. According to the Brillouin diagram for an arbitrary PGS[2], the wave function propagating with a propagation constant β is the superposition of the waves with discrete multiple frequencies. In (1), the superscript and the subscript of the coefficients ($a_{\omega_l}^{+}$, $b_{\omega_l}^{+}$, $a_{\omega_l}^{-}$ and $b_{\omega_l}^{-}$) denote the propagation direction and the corresponding frequency, respectively. Since these coefficients are varying with (x,y,z) and specified for each frequencies, these are longitudinally periodic with period L from the Floquet's theorem. Their periodicity gives (2) for $f(x,y,z,t)$, whose real part and imaginary part are given in (3).

$$f(x,y,z+d,t) = f(x,y,z,t) \qquad (2)$$

$$f(x,y,z,t) = f^{r}(x,y,z,t) + jf^{i}(x,y,z,t) \qquad (3a)$$

$$f^{r}(x,y,z,t) = \sum_{l=1}^{N}\begin{bmatrix}\{a_{\omega_l}^{+}(x,y,z)+a_{\omega_l}^{-}(x,y,z)\}\cos\omega_l t \\ +\{b_{\omega_l}^{+}(x,y,z)-b_{\omega_l}^{-}(x,y,z)\}\sin\omega_l t\end{bmatrix} \qquad (3b)$$

$$f^{i}(x,y,z,t) = -\sum_{l=1}^{N}\begin{bmatrix}\{a_{\omega_l}^{+}(x,y,z)-a_{\omega_l}^{-}(x,y,z)\}\sin\omega_l t \\ +\{b_{\omega_l}^{+}(x,y,z)+b_{\omega_l}^{-}(x,y,z)\}\cos\omega_l t\end{bmatrix} \qquad (3c)$$

When solving Maxwell's equation for the wave given by (1), the unknowns are the frequencies (ω_l), the number (N) of those frequencies, and the coefficients of the positive-going and negative-going waves. Consequently, for the convenience in the numerical computation, all of the unknowns can be obtained by solving the complex function, $f(x,y,z,t)$, defined in β-domain. Moreover, (3) tells the relation of $f(x,y,z,t)$ to the positive-going wave and the negative-going wave, by which the β-domain calculation of the periodic field in the PGS is physically meaningful.

To perform the FDTD simulation in the β-domain, the longitudinal spatial-derivative $\partial/\partial z$ should be replaced by $\partial/\partial z + j\beta$. If the original Yee's cell[10] is employed when constructing the finite-difference equations in β-domain, the positions of the field variables for the $j\beta$ operation are not assigned. To avoid the extra computation for these unassigned fields, the real-part and the imaginary-part of each field component should be properly located in the spatial mesh. For the efficient implementation of the central-difference leapfrog scheme, we modify Yee's cell in the following way; the real-part and imaginary-part of each field component are located separately, by a half of the longitudinal spatial-increment, $\Delta z/2$, as graphically described in Fig. 1. While six arrows in a unit spatial mesh represents six field components in the standard FDTD, an arrow in the original Yee's cell[10] is divided into two real-arrow and imaginary-arrow in the modified Yee's cell scheme. Then, the positions for the $j\beta$ operation are assigned spatially. By using the modified Yee's cell, the presented FDTD algorithm for the complex time-domain periodic function is streamlined to implement the central-difference approximation, also resulting in the reduction of the computation time and memory.

The presented FDTD method calculates the electric field $\vec{E}(x,y,z,t)$ and the magnetic field $\vec{H}(x,y,z,t)$ represented by the same way as (1) and (3) just in a single period ($0 \le z < d$) with the PBC given in (2). The Maxwell's curl equation is presented in (4).

$$\varepsilon\frac{\partial}{\partial t}\begin{bmatrix}E_x\\E_y\\E_z\end{bmatrix} = \begin{bmatrix}0 & -\frac{\partial}{\partial z}-j\beta & \frac{\partial}{\partial y}\\ \frac{\partial}{\partial z}+j\beta & 0 & -\frac{\partial}{\partial x}\\ -\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0\end{bmatrix}\times\begin{bmatrix}H_x\\H_y\\H_z\end{bmatrix} \qquad (4a)$$

$$-\mu\frac{\partial}{\partial t}\begin{bmatrix}H_x\\H_y\\H_z\end{bmatrix} = \begin{bmatrix}0 & -\frac{\partial}{\partial z}-j\beta & \frac{\partial}{\partial y}\\ \frac{\partial}{\partial z}+j\beta & 0 & -\frac{\partial}{\partial x}\\ -\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0\end{bmatrix}\times\begin{bmatrix}E_x\\E_y\\E_z\end{bmatrix} \qquad (4b)$$

All of the field variables in (4), where (x,y,z,t) dependence is omitted for simplicity, are periodic. Using this proposed spatial mesh scheme, the update equations are streamlined in (5), for the real-part of E_x component.

$$E^{r}_{x(i+0.5,j,k,n+1)} = \left(\frac{1-\dfrac{\sigma_{(i+0.5,j,k)}\Delta t}{2\varepsilon_{(i+0.5,j,k)}}}{1+\dfrac{\sigma_{(i+0.5,j,k)}\Delta t}{2\varepsilon_{(i+0.5,j,k)}}} \right) E^{r}_{x(i+0.5,j,k,n)}$$

$$+\left(\frac{\dfrac{\Delta t}{\varepsilon_{(i+0.5,j,k)}}}{1+\dfrac{\sigma_{(i+0.5,j,k)}}{2\varepsilon_{(i+0.5,j,k)}}} \right) \times \left(\begin{array}{l} \beta\left(H^{i}_{y(i+0.5,j,k,n+1/2)} \right) \\ + \dfrac{H^{r}_{z(i+0.5,j+0.5,k,n+1/2)} - H^{r}_{z(i+0.5,j-0.5,k,n+1/2)}}{\Delta y} \\ - \dfrac{H^{r}_{y(i+0.5,j,k+0.5,n+1/2)} - H^{r}_{y(i+0.5,j,k-0.5,n+1/2)}}{\Delta z} \end{array} \right) \quad (5)$$

In (5), Δx, Δy, and Δz are the spatial mesh sizes and Δt is the time step. $E^{r}_{x(i,j,k,n)}$ represents the real-part of E_x(iΔx,jΔy,kΔz,nΔt). The update equations for the remained 11 components can be derived in the same manner. In the presented FDTD method, the PBC is directly implemented by (2).

Since the original Yee's cell is modified, the usual Courant stability criterion and the numerical grid dispersion relation must be modified. The presented FDTD algorithm for the PGS is completed by (6) and (7) with the modified Yee's cell and the simple PBC. (6) and (7) are the numerical stability criterion and the numerical dispersion relation for the presented FDTD scheme, respectively.

$$c_0 \Delta t \sqrt{\left(\frac{1}{\Delta x}\right)^2 + \left(\frac{1}{\Delta y}\right)^2 + \left(\frac{1}{\Delta z} + \frac{\beta}{2}\right)^2} \le 1 \quad (6)$$

In (6), c_0 is the maximum speed of light in the computational domain.

$$\left\{ \frac{1}{c_0 \Delta t} \sin\left(\frac{\omega \Delta t}{2}\right) \right\}^2 = \left(\begin{array}{l} \left\{ \dfrac{1}{\Delta x} \sin\left(\dfrac{\tilde{k}_x \Delta x}{2}\right) \right\}^2 \\ + \left\{ \dfrac{1}{\Delta y} \sin\left(\dfrac{\tilde{k}_y \Delta y}{2}\right) \right\}^2 \\ + \left\{ \dfrac{1}{\Delta z} \sin\left(\dfrac{\tilde{k}_z \Delta z}{2}\right) + \dfrac{\beta}{2} \right\}^2 \end{array} \right) \quad (7)$$

(7) is derived assuming the plane monochromatic traveling-wave trial solution with wave number vector $(\tilde{k}_x, \tilde{k}_y, \tilde{k}_z)$ and frequency ω.

III. NUMERICAL RESULT

To demonstrate the validity of the modified Yee's cell, a periodically corrugated parallel-plate waveguide, as shown in Fig. 2, is analyzed. The ω-β dispersion relation of a TM mode are computed and compared to that obtained by the transmission line analysis [2]. The dispersion equation given by the simple transmission line analysis is known quite accurate as long as s is much smaller than d and wavelength. In the FDTD simulation, the spatial mesh size was taken as Δx = Δz = 0.5 mm. From the numerical stability criterion (6), the time step was chosen to be 1ps. Each simulation is executed with the predetermined propagation constant (β). The peak frequencies of the modes for the β used in each FDTD run is obtained by the FFT of the calculated transient waveform, as predicted by (1). The FDTD simulation and the followed FFT for each β give the dispersion diagram, which is shown in Fig.3. The continuous curve is calculated by the transmission line analysis[2] and the circles are obtained by the presented FDTD scheme with the modified Yee's cell. By observing that the two dispersion diagrams are quite well matched, it can be said that the validity of the suggested Yee's cell is demonstrated.

IV. CONCLUSION

In this paper, the modification of the original Yee's cell is presented for the FDTD modeling of the PGS. Using the modified Yee's cell, the efficient handling of the complex field function is enabled in the implementation of the FDTD code with the central-difference scheme. In other words, the presented Yee's cell saves the computing time and the memory resource by the proper allocations of the real and the imaginary parts of each field components. The validity of the modified Yee's cell is also successfully demonstrated. For the presented scheme, the numerical stability condition and the numerical dispersion relation are also given. Although the proposed scheme is demonstrated by the 2-dimensional PGS analysis, the applications to the 3-dimensional PGS are straightforward.

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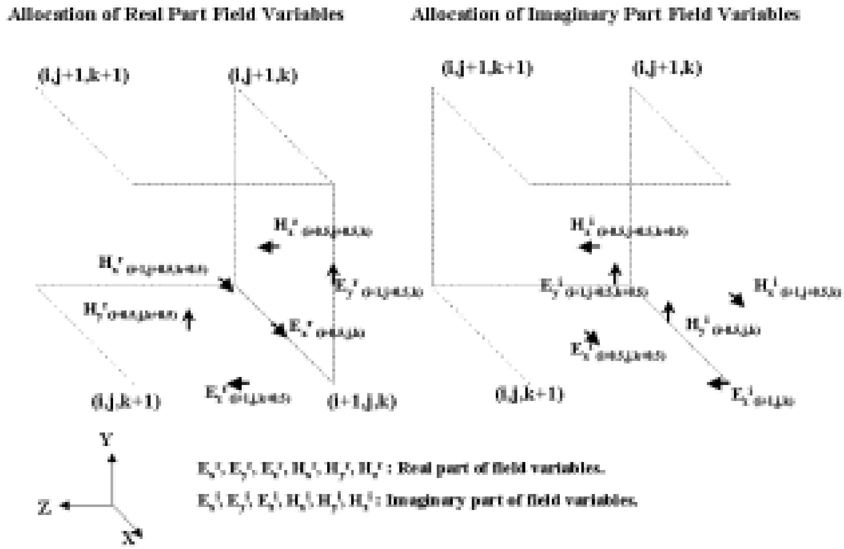

Fig.1 Proposed modified Yee's cell for the FDTD modeling of the PGS. To avoid the confusion of the location of each field component in this mesh, the real parts and the imaginary parts are separately described. Although the real mesh and the imaginary mesh are separately given, they are computed simultaneously, as shown in (5).

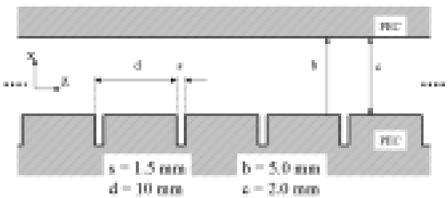

Fig.2 Periodically corrugated parallel-plate waveguide (period *d*) to compare the proposed FDTD simulation with the transmission line analysis[2].

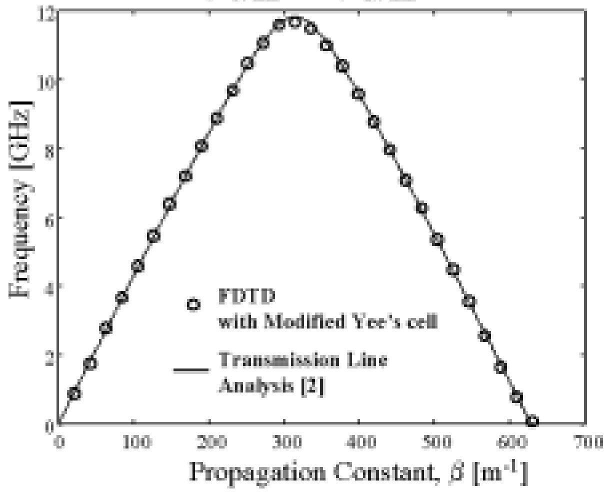

Fig.3 The first branch of ω–β dispersion diagram of the corrugated parallel plate waveguide shown in Fig.2. The solid line represents the calculation based on the transmission line analysis[2] and the circles represent the calculation by the proposed FDTD simulation using the modified Yee's cell. As can be seen from the graph, the two calculation results agree pretty well, demonstrating the validity of the proposed FDTD simulation for the PGS modeling.