A Hybrid Spectral/FDTD Method for the Electromagnetic Analysis of Guided Waves in Periodic Structures

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Abstract— **A hybrid spectral/FDTD (finite-difference time-domain) method is introduced for the analysis of electromagnetic wave propagation in anisotropic, inhomogeneous periodic structures. Discrete Fourier series representations for the field components are used for the spectral calculation of spatial derivatives along the axes of periodicity. Thus, the computational domain is restricted to a single period. Maxwell's system is then solved as an initial value problem on a slightly modified FDTD grid for the prediction of the (eigen)frequencies of the propagating modes for a given value of the propagation constant. Numerical results for two-dimensional periodic structures are in excellent agreement with results obtained using other numerical methods.**

I. Introduction

THIS letter presents a hybrid spectral/FDTD method developed for the efficient electromagnetic analysis of periodic structures of high complexity. More specifically, the proposed method is aimed at the computationally efficient extraction of the propagation characteristics of electromagnetic waves in two- and three-dimensional, inhomogeneous, anisotropic geometries which are periodic in one or two dimensions. In addition to their slow-wave and filter characteristics, recent applications of periodic dielectric structures for integrated optics purposes include, distributed feedback lasers, distributed Bragg reflection lasers, and quasiphase-matched second-harmonic generation.

The inclusion of a spectral technique into an FDTD formulation maintains favorable qualities of each method. FDTD is well known for its simplicity in analyzing complicated geometries which include inhomogeneities and anisotropies, while spectral techniques are best known for their accuracy [1]. Specifically, the employment of the Fourier transform in the direction of periodicity garners two desirable advantages. First, using the properties of the Fourier transform to calculate derivatives insures higher accuracy. Second, the Fourier transform automatically enforces periodic boundary conditions which restricts the computational domain to a single period.

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II. The Spectral/FDTD Method

For the sake of simplicity, the formulation of the hybrid spectral/FDTD method is presented for the case of a two-dimensional periodic structure. Without loss of generality, the media are assumed to be nonmagnetic with permeability $\mu_0 = 4\pi \times 10^{-7}$ H/m. As far as their dielectric properties are concerned, the media are characterized by the electric permittivity tensor

$$\bar{\bar{\epsilon}} = \begin{bmatrix} \epsilon_{xx}(x,z) & 0 & 0 \\ 0 & \epsilon_{yy}(x,z) & 0 \\ 0 & 0 & \epsilon_{zz}(x,z) \end{bmatrix},$$

where $\epsilon_{ii}(x,z)$, $i = x,y,z$, are periodic functions of z with period d, $\epsilon_{ii}(x, z+d) = \epsilon_{ii}(x,z)$, and their independence of y reflects the fact that the periodic structure under study is two-dimensional.

From the two possible types of wave propagation in the z direction, transverse magnetic (TM_z) and transverse electric (TE_z), the TM_z type is used for the presentation of the proposed spectral/FDTD method. Let β_0 be the unknown propagation constant. Then the electric and magnetic fields for the TM_z guided waves are of the form

$$\begin{aligned}\mathcal{E}_x(x,z,t) &= E_x(x,z,t)e^{-j\beta_0 z} \\ &= \left(\sum_{n=-\infty}^{\infty} \hat{e}_x^{(n)}(x,t)e^{jn(2\pi z/d)}\right)e^{-j\beta_0 z} \qquad (1)\end{aligned}$$

$$\begin{aligned}\mathcal{E}_z(x,z,t) &= E_z(x,z,t)e^{-j\beta_0 z} \\ &= \left(\sum_{n=-\infty}^{\infty} \hat{e}_z^{(n)}(x,t)e^{jn(2\pi z/d)}\right)e^{-j\beta_0 z} \qquad (2)\end{aligned}$$

$$\begin{aligned}\mathcal{H}_y(x,z,t) &= H_y(x,z,t)e^{-j\beta_0 z} \\ &= \left(\sum_{n=-\infty}^{\infty} \hat{h}_y^{(n)}(x,t)e^{jn(2\pi z/d)}\right)e^{-j\beta_0 z}, \qquad (3)\end{aligned}$$

where the Fourier series representations are a direct consequence of the periodicity of the functions E_x, E_z, and H_y according to Floquet's theorem for periodic structures [2]. Maxwell's curl equations can be written in the following form

$$\mu_0 \frac{\partial H_y}{\partial t} = \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} + j\beta_0 E_x \qquad (4)$$

$$\epsilon_{xx}\frac{\partial E_x}{\partial t} = -\frac{\partial H_y}{\partial z} + j\beta_0 H_y \qquad (5)$$

$$\epsilon_{zz}\frac{\partial E_z}{\partial t} = \frac{\partial H_y}{\partial x}, \qquad (6)$$

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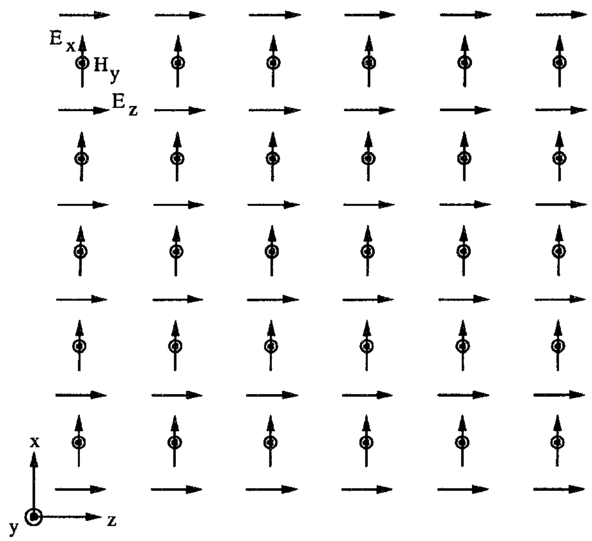

Fig. 1. Mesh for TM mode in hybrid spectral/FDTD method.

where the dependence of the periodic functions E_x, E_z, and H_y on x, z, t has been omitted for simplicity.

The numerical solution of (4)–(6) is based on a hybrid spectral/FDTD approximation of the spatial derivatives. The approximation utilizes the grid shown in Fig. 1. The grid extends over a single period of the structure. Derivatives with respect to x are approximated using central differences. As far as the derivatives with respect to z (direction of periodicity) are concerned, they are computed spectrally as follows.

The values of the periodic function E_x at the grid points $z_i = (i/N)d$, $i = 0, 1, 2, \cdots, N-1$, where N is the number of grid points along z, are used to calculate its discrete Fourier coefficients for a given (x, t)

$$\tilde{e}_x^{(n)}(x,t) = \frac{1}{N}\sum_{i=0}^{N-1} E_x(x, z_i, t)e^{-j(2\pi n z_i/d)}, \quad -N/2 \le n \le N/2-1. \quad (7)$$

The derivative $\partial E_x/\partial z$ is then approximated as

$$\frac{\partial E_x(x, z_i, t)}{\partial z} \simeq \sum_{-N/2}^{N/2-1}\left(j\frac{2\pi n}{d}\right)\tilde{e}_x^{(n)}(x,t)e^{j(2\pi n z_i/d)}, \quad i = 0, 1, \cdots, N-1. \quad (8)$$

The derivative $\partial H_y/\partial z$ is computed in a similar fashion.

Clearly, the aforementioned spectral computation of derivatives along z facilitates the exact enforcement of the periodic boundary conditions, and is responsible for the restriction of the computational domain to a single cell of the periodic structure. The discrete Fourier transforms in (7) and (8) are computed efficiently using standard FFT routines.

In a manner similar to the standard FDTD method, electric and magnetic fields are staggered in time so that central-difference approximations to the time derivatives can be used. Given the value of the propagation constant β_0, as well as initial conditions for the fields over the unit cell of the structure, the discrete system of Maxwell's equations is integrated in time using a leap-frog scheme. The eigenfrequencies of the system, i.e., the frequencies at which the various propagating modes in the periodic structure exhibit the selected propagation constant β_0, are computed from the Fourier transforms of the time histories of the fields. More specifically, these eigenfrequencies correspond to the peaks in the Fourier spectra.

TABLE I
PARAMETERS FOR FIG. 1

ϵ_{r_I}	1.0
$\epsilon_{r_{II}}$	$(1.875)^2$
$\epsilon_{r_{III}}$	$(1.85)^2$
h	$4.0\mu m$
w	$2.5\mu m$
d	$5.0\mu m$

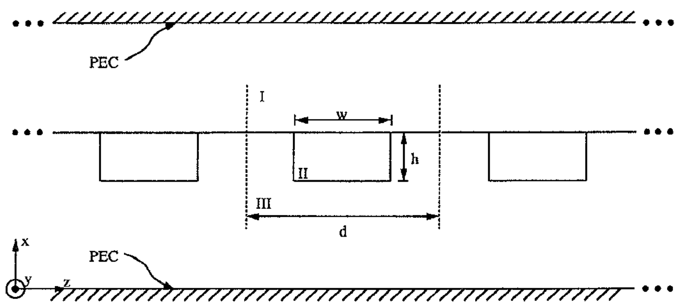

Fig. 2. Periodically segmented dielectric waveguide structure.

The details of numerical stability of this hybrid spectral/FDTD scheme will be discussed in a later article. It can be shown that, for the two-dimensional case considered here, the scheme is stable provided that

$$v(\Delta t) \le (\Delta x)\left[1 + \left(\frac{\Delta x}{\Delta z}\right)^2\left(\frac{\beta_0(\Delta z)}{2} + \frac{\pi}{2}\right)^2\right]^{-\frac{1}{2}}, \quad (9)$$

where v is the maximum value of the speed of light in the computational domain, Δt is the time step used in the numerical integration, and Δx, Δz are the grid sizes along x and z, respectively.

III. RESULTS

To demonstrate the validity of the proposed method, the periodically segmented waveguide shown in Fig. 2 was analyzed. The pertinent values for the structure are listed in Table I. Such waveguides are recently used for the quasiphase-matched second harmonic generation of blue light [3]. The structure shown in Fig. 2 was analyzed in [4] using a mode-matching approach. It was noted in [4] that the dispersion curve for the fundamental mode of the segmented waveguide agrees "to at least six significant digits of accuracy with those obtained by using a regular slab waveguide model, provided that the index of the slab [is] taken to be the weighted average of [n_{II}] and [n_{III}]," where $n_{\text{II}} = \sqrt{\epsilon_{r_{\text{II}}}}$ and $n_{\text{III}} = \sqrt{\epsilon_{r_{\text{III}}}}$. The transcendental equation for the TM modes of the slab waveguide is well known, giving a convenient model for comparison.

TABLE II
COMPARISON BETWEEN SLAB MODEL AND THIS METHOD

$\beta(\times 10^6 m^{-1})$	Mode	Slab Model f (THz)	This Method f (THz)	% Difference
6.75	TM_0	173.518	173.308	−0.121
13.71	TM_0	351.633	351.627	−0.002
	TM_1	352.805	352.839	+0.010
20.815	TM_0	533.540	533.680	+0.064
	TM_1	534.437	534.655	+0.041
	TM_2	535.868	536.045	+0.033
26.405	TM_0	676.692	676.966	+0.040
	TM_1	677.437	677.740	+0.045
	TM_2	678.658	678.986	+0.048
	TM_3	680.287	680.601	+0.046

For the hybrid technique described in this paper, choice of the initial condition is critical for speeding-up its convergence. For the specific structure, the mode profiles of the slab waveguide formed by a cross section across regions I, II, and III in Fig. 2 were used for the transverse representation of the initial field distribution. As far as the spectral estimation process is concerned, the scheme used was prompted by an approach found in [5]. At the conclusion of each time step the correlation of the field in the guide to the initial condition is performed,

$$f(t) = \int dz \int dx H_y^*(x, z, t = 0) H_y(x, z, t). \qquad (10)$$

At the end of the computation, the FFT of $f(t)$ is found and analyzed for the peaks which give the frequencies of the modes for the particular β_0 used.

In the analysis, perfect electric conductors were used 1.4 μm above the air/substrate interface and 7.0 μm below the interface for simple grid truncation. The discretization in the transverse direction was taken as $dx = 21.0$ nm. In the direction of periodicity, the discretization was $dz = 78.1245$ nm, which corresponds to the period divided by 64. Each simulation was run for 4096 time steps.

Table II shows a comparison of the values found using the slab waveguide model and this method. The agreement between the two methods is seen to be excellent. As a matter of fact, the conclusion in [4] that the dispersion properties of the segemented guide can be deduced from the analysis of a regular slab guide with index refraction equal to the weighted averages of $n_{\rm II}$ and $n_{\rm III}$, seems to be valid for higher order modes as well. The accuracy is maintained even when multiple modes are present in the structure.

IV. CONCLUSION

In this letter, we showed that inclusion of a spectral technique in an FDTD formulation eases the analysis of periodic structures. By using FDTD, inhomogenities and anisotropies are easily modeled. By using spectral, only a single period needs to be modeled and accuracy is increased.

The approach presented is an eigenvalue solver. By specifying the value of the phase constant, the frequency values of the corresponding modes are found. This is a reversal of the method used in frequency domain techniques, where the frequency is specified and the corresponding phase constants of the guided modes are found. However, in a frequency domain technique, the solution of a matrix eigenvalue problem is required which can be very expensive computationally for electrically large periodic structures. For example, for a three-dimensional grid of $5\lambda \times 5\lambda \times 5\lambda$ with a modest discretization of $\lambda/10$, taking into account the three components of one of the fields, there are 375 000 unknowns in the finite element matrix for a frequency domain technique. By extending the present method to three dimensions, the authors feel a great reduction in computational effort can be achieved.

In the last section, the accuracy obtainable was demonstrated. That accuracy can be further increased by iterative means. By using the field distribution found at the end of a run as the excitation for a new run at the same β_0, improvement and convergence of the results should be seen. By such iterative refinement, answers within computational accuracy should be achievable.

This method's greatest usefulness lies in its capability to model periodic structures that have complex geometries and anisotropy. Open structures can be easily handled by applying the analysis used to modify Maxwell's equations to obtain Mur's second-order radiation boundary conditions. In future publications, applications of the method to such structures are sure to be presented as well as extension of the method to three-dimensional structures.

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