Generalized Finite-Difference Time-Domain Method Utilizing Auxiliary Differential Equations for the Full-Vectorial Analysis of Photonic Crystal Fibers

Juan Juan Hu, Ping Shum, *Senior Member, IEEE*, Chao Lu, *Member, IEEE*, and Guobin Ren

***Abstract*—We present the generalized finite-difference time-domain full-vectorial method by reformulating the time-dependent Maxwell's curl equations with electric flux density and magnetic field intensity, with auxiliary differential equations using complex-conjugate pole-residue pairs. The model is generic and robust to treat general frequency-dependent material and nonlinear material. The Sellmeier equation is implicitly incorporated as a special case of the general formulation to account for material dispersion of fused silica. The results are in good agreement with the results from the multipole method. Kerr nonlinearity is also incorporated in the model and demonstrated. Nonlinear solutions are provided for a one ring photonic crystal fiber as an example.**

***Index Terms*—Auxiliary differential equation (ADE), finite-difference time-domain (FDTD), Kerr nonlinearity, material dispersion, photonic crystal fibers (PCF).**

I. INTRODUCTION

PHOTONIC crystal fibers (PCFs) have attracted a great deal of attention in optics research domain since its introduction in 1996 [1]. PCFs, generally classified in two classes, i.e., index-guiding PCF and photonic bandgap PCF, can offer many superior properties over conventional step-index fibers, such as endlessly single-mode operation, high birefringence, high/low nonlinearity, tailorable dispersion, or even guidance in a hollow core [2]. With the growing interest in PCFs, effective numerical modeling is an indispensable tool as mathematical analyses are difficult for PCF. Several modeling methods have been proposed to study the modal properties of PCFs, including the multipole method [3], [4], the beam propagation method [5], the finite-element method [6], and the finite-difference method in time-domain (FDTD) [7] or frequency-domain [8]. Among all these methods, the FDTD method has been recognized as a powerful technique since it offers several advantages, such as its ablity to treat frequency-dependent, nonlinear, or anisotropic material; generality, i.e., arbitrary shapes can be easily calculated; robustness, as numerous systems have been accurately modeled; easy implementation, as it is formulated directly from Maxwell's equations; and it allows parallel computing which greatly reduces computation time.

A compact two-dimensional FDTD (C2D-FDTD) approach is proposed to solve guided modes in PCF by assuming the propagation constant real and constant along the fiber axis [9]. Recently Jiang *et al.* [10] proposed that by implicitly including the Sellmeier formula in the formulation by introducing an auxiliary polarization current density, material dispersion of fused silica can be processed. However, for other frequency-dependent material, which the Sellmeier formula may not provide accurate estimation of the material permittivity, their formulation is no longer sufficient. Furthermore, the current model is not able to treat nonlinearities. To give a general and comprehensive modeling for material dispersion and nonlinearity in PCF, we use a generalized formulation of Maxwell's curl equations by flux density and magnetic field with complex-conjugate pole-residue pairs, and we demonstrate our approach is more general and robust to treat complicated material in PCF. The effective indexes of guided modes calculated by our FDTD model are found to be within 0.02% relative error compared to the multipole method. The Kerr nonlinearity is incorporated and a one ring PCF is used to demonstrate nonlinear solutions by our generalized model.

II. FORMULATION

For an isotropic material in a source-free region, the time-dependent Maxwell's curls equations for electric flux density $\mathbf{D}$, electric and magnetic field intensities $\mathbf{E}$ and $\mathbf{H}$ are arranged in a form

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu_0}\nabla \times \mathbf{E} \tag{1}$$

$$\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} \tag{2}$$

$$\mathbf{D}(\omega) = \varepsilon_0 \varepsilon_r(\omega)\cdot \mathbf{E}(\omega) \tag{3}$$

where μ_0 and ε_0 are vacuum permeability and permittivity. $\varepsilon_r(\omega)$ characterizes the material constitution between electric field intensity and electric flux density. As given in (4), ε_∞ is the linear index of the system, the second term is material dispersion described by the sum of complex-conjugate pole-residue pairs [11], and the third term is Kerr nonlinearity as a function of intensity, where $\rho = 2n_{\text{silica}}n_2$, and n_2 is Kerr

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nonlinearity coefficient of the material, therefore, $\rho = 0$ if it is air

$$\varepsilon_r(\omega) = \varepsilon_\infty + \sum_{k=1}^{K} c_k/(j\omega - \alpha_k) + c_k^*/\left(j\omega - \alpha_k^*\right) + \rho|\mathbf{E}|^2. \quad (4)$$

Here we define the auxiliary parameter S_k and S_k^* pairs to describe material dispersion. Since S_k and S_k^* are complex conjugates, we only need to store and update either $S_k(t)$ or $S_k^*(t)$ instead of both. Taking S_k for example

$$S_k = \varepsilon_0 c_k/(j\omega - \alpha_k)\mathbf{E}. \quad (5)$$

The parameters S_k in the time domain are expressed as

$$\frac{\partial S_k}{\partial t} - \alpha_k S_k = \varepsilon_0 c_k \mathbf{E}. \quad (6)$$

Therefore at every time step n in the sampled time domain

$$S_k^{n+1} = \frac{\varepsilon_0 \Delta t c_k}{1 - \Delta t \alpha_k/2}\mathbf{E}^{n+1} + \frac{1 + \Delta t \alpha_k/2}{1 - \Delta t \alpha_k/2} S_k^n. \quad (7)$$

Combining the auxiliary differential equation (ADE) (6) and the Maxwell curl equations [(1), (2)], we arrive at the corresponding ADE-FDTD implementation

$$\mathbf{E}^{\langle m+1\rangle} = \frac{\mathbf{D}^{n+1} - 2\sum\limits_{k=1}^{K} \mathrm{Re}\left(\kappa_k S_k^n\right)}{\varepsilon_0\varepsilon_\infty + 2\sum\limits_{k=1}^{K} \mathrm{Re}(\upsilon_k) + \varepsilon_0 \rho \left|\mathbf{E}^{\langle m\rangle}\right|^2} \quad (8)$$

where

$$\kappa_k = \frac{1 + \alpha_k \Delta t/2}{1 - \alpha_k \Delta t/2}, \quad \upsilon_k = \frac{\varepsilon_0 c_k \Delta t}{1 - \alpha_k \Delta t/2} \quad (9)$$

for $m = 0, 1, 2, \ldots$. Here the Kerr polarization term in (4) is updated with Newton iteration. $E^{\langle m\rangle}$ denotes the approximation of E^{n+1} at mth iteration of the Newton procedure and the initial estimate of E^{n+1} is E^n, i.e., $E^{\langle 0\rangle} = E^n$. Therefore, at each time step n, the electric field is obtained by the iterative calculations with the stored field value at time step $n - 1$, and each iteration gives an estimate of the field value until the iterative process completes. The index n denotes the discrete time step, Δt is the time increment. The parameters κ_k and υ_k are calculated using (9) and they are generally complex numbers, α_k and c_k are position dependent parameters. Updated E can be used in another updating of H. The above presented formulation using complex-conjugate pole-residue pairs is able to treat Debye media and Lorentz media in a unified manner [11], which definitely reduces implementation cost when dealing with different frequency-dependent materials. The advantage of our model, which is based on electric flux density and magnetic field intensity, is the robustness to treat complicated material while maintaining most of the formulation equations unchanged, i.e., for other materials in PCF, such as nonlinear dispersive materials, or gain mediums, only the constitutive material equation which relates the electric field and flux density needs corresponding modifications. The curl equations concerning flux density and magnetic field are unchanged. The Sellmeier formula is a special case of this model.

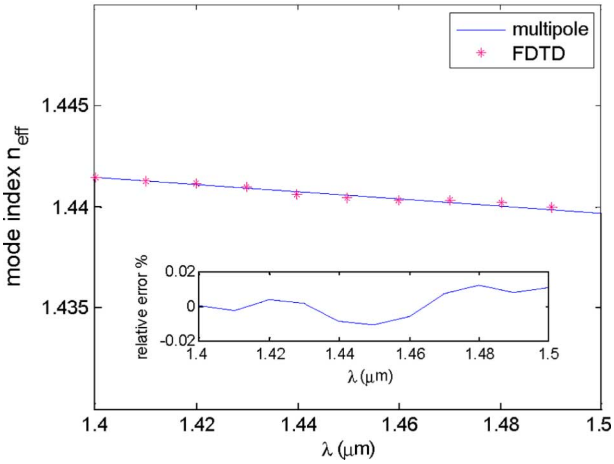

Fig. 1. Mode indexes of guided modes of the six-hole PCF. The stars are obtained by current FDTD model; the dotted line is obtained by multipole method. The largest relative error in effective index is less than 0.02%.

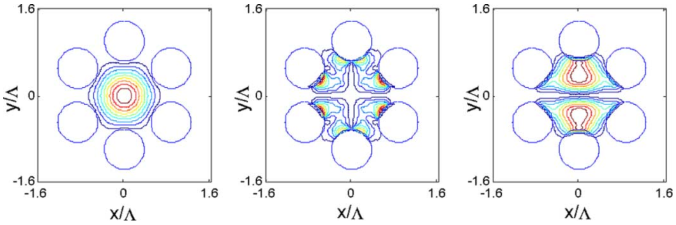

Fig. 2. Contour plots of the normalized fields $|E_x|$, $|E_y|$, and $|E_z|$ for an x-polarized fundamental mode for a six-hole PCF, with effective mode index $n_{\text{eff}} = 1.441469$.

In particular, let $\varepsilon_\infty = 1$, $c_k = -jb_k\omega_k/2$, and $\alpha_k = j\omega_k$, the above formulation is exactly the same as ADE formulation for a medium modeled by Sellmeier equation.

III. NUMERICAL RESULTS

Consider a structure with a single ring of six equally spaced air holes with $d = 5$ μm, $\Lambda = 6.75$ μm, $\lambda = 1.4$ μm, the background material is silica. The dielectric constant is described by Sellmeier formula, and the Kerr nonlinearity is zero. d denotes the air hole diameter; Λ is the hole to hole distance. The computation domain is shown in Fig. 1 with six holes in the cladding, fiber core is solid. The space increment of $\Delta x = \Delta y = \Lambda/50$. A total of 19 600 (140 × 140) mesh points are in the computation domain with ten PML cells on each side of the boundary and the total number of the time steps is 100 000, with each time step smaller than the Courant limit. In our work, $\Delta t = 0.1/c\sqrt{\Delta x^{-2} + \Delta y^{-2} + (\beta/2)^2}$, which depends on the input propagation constant β values. The calculated fields in time domain are transformed into frequency domain using fast Fourier transform techniques to extract spectral information [12]. The effective index for an x-polarized fundamental mode calculated by the current FDTD program is 1.441469, compared to the multipole method [4] which is 1.441465, we see a very good agreement. We further investigate the mode profile of electric field intensities at this wavelength as shown in Fig. 2, which are normalized electric fields and they correlate with the multipole method very well.

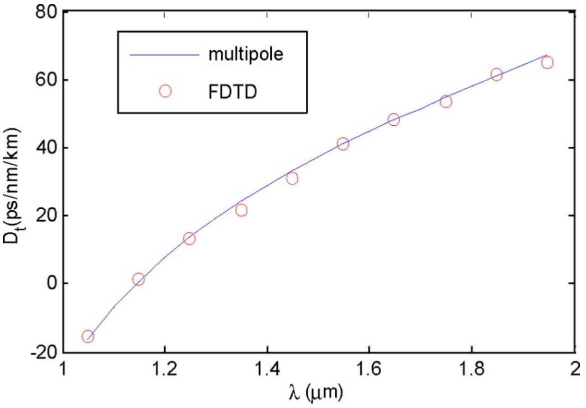

Fig. 3. Total chromatic dispersion of the six-hole PCF. The circles are obtained by current FDTD model; the solid line is obtained by multipole method.

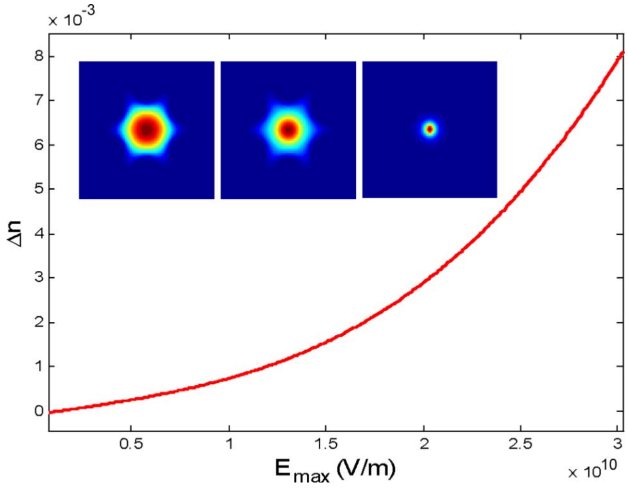

Fig. 4. Dependence of effective indexes difference on the input intensity. Three inset plots show intensity distribution of different solutions, i.e., linear mode, nonlinear modes with $E_{\max} = 0.5e10$ V/m, and $E_{\max} = 2.5e10$ V/m.

The calculated effective indexes of guided modes in the fiber are shown in Fig. 1, which includes the material dispersion. The wavelength spans from 1.4 to 1.5 μm. We see that they agree well; the largest relative discrepancy is less than 0.02% from multipole method. The total chromatic dispersion is also calculated and shown in Fig. 3. We could see the results obtained by our FDTD model match well with multipole method.

Next we present the nonlinearity analysis for the same fiber structure, without considering material dispersion for simplicity. A Gaussian profile with $E_{\max}$ in the center is launched as the initial field. The Kerr nonlinearity coefficient of silica, i.e., $n_2 = 2.7e - 20\ \mathrm{m}^2/\mathrm{W}$ is used. The nonlinear solutions have slight difference with linear solution, defined as $\Delta n = \beta/k_{\mathrm{sol}} - \beta/k_{\mathrm{fund}}$ in Fig. 4. In our model β is used as a user defined parameter to search for resonance frequency, corresponding to wavevector k_{sol}, and k_{fund} is the linear solution. The difference Δn shows a strong dependence on the initial field amplitude $E_{\max}$. Mode profiles at three typical amplitudes are shown as insets, which are linear mode, nonlinear modes with $E_{\max} = 0.5e10$ V/m and $E_{\max} = 2.5e10$ V/m, respectively. It agrees with [13] that the PCF structure is able to support stable solutions as the nonlinear fundamental mode. It is also clear that as field intensity increases, the mode self-focusing effect can be observed.

IV. CONCLUSION

We have given the basic formulation of our FDTD method based on flux density and magnetic field. And we have shown this method is a general approach to calculate the modal properties in PCFs with different frequency-dependent and nonlinear material. With appropriate parameters defined in the complex-conjugate pole-residue poles, general dispersive media can be processed. Fused silica is a special case and the Sellmeier formula can be treated as a particular case in the formulation as well. The results are in good correlation with multipole methods. We also demonstrate nonlinear analysis of a one-ring PCF assuming instantaneous response of Kerr type material by our generalized FDTD model.

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