FDTD ANALYSIS OF CHIRAL DISCONTINUITIES IN WAVEGUIDES

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Abstract—A simple finite difference time domain (FDTD) scheme is proposed for modeling three-dimensional (3D) nondispersive chiral media. Based on the recently reported new BI-FDTD mesh method and rearranged curl equations, this scheme implements a simple leapfrog algorithm. By adding the mirror layer, the perfect electric conductor (PEC) condition is implemented in the BI-FDTD mesh method of 3D problem. Results of this scheme are presented for the scattering coefficients of discontinuity in waveguides, which are partially filled with chiral or achiral media. The validation is performed by comparing the results with those obtained from the literature and software simulation.

1. INTRODUCTION

In contrast to isotropic media characterized by permittivity and permeability, chiral media contain an additional parameter in their constitutive equations, namely, the chirality parameter, which relates the electric field E with magnetic flux density B, and the magnetic field H with the electric displacement D [1–6]. Just because of the magnetoelectric coupling term in the constitutive equations the standard FDTD method cannot be directly applied to chiral materials. In recent years, many attempts have been made to model chiral media by using the FDTD method. These approaches include the wavefield decomposition in bi-isotropic media [7, 8], the second-order backward finite difference method [9], the BI-FDTD mesh method [10–14] and some other techniques [15–17]. In this paper, a simple FDTD scheme is proposed to model 3D nondispersive chiral media. The mesh division in this approach employs the same technique as in [10]. By

discretizing the rearranged curl equations [12], which is different from literature [13], a leapfrog algorithm for chiral media is achieved. To validate this method, we have calculated the scattering coefficients of waveguides, which are partially filled with chiral or achiral media. By comparing the results of [9] and Ansoft HFSS simulation, the accuracy of this method is demonstrated.

2. FORMULATION

The constitutive relations for chiral media can be written as [1]

$$\vec{D} = \varepsilon\vec{E} + \xi\vec{H} \tag{1a}$$

$$\vec{B} = \mu\vec{H} + \varsigma\vec{E} \tag{1b}$$

The electromagnetic coupling coefficients ξ, ς are expressed as

$$\xi = -j\kappa_r\sqrt{\mu\varepsilon}$$
$$\varsigma = j\kappa_r\sqrt{\mu\varepsilon}$$

where $j^2 = -1$, κ_r is normalized chirality parameter. Substituting (1a) and (1b) into the Maxwell's curl equations, we have [12]

$$\varepsilon_c\frac{\partial\vec{E}}{\partial t} = \nabla \times \vec{H} + \frac{\xi}{\mu}\nabla \times \vec{E} \tag{2a}$$

$$\mu_c\frac{\partial\vec{H}}{\partial t} = -\nabla \times \vec{E} - \frac{\varsigma}{\varepsilon}\nabla \times \vec{H} \tag{2b}$$

where

$$\varepsilon_c = \varepsilon(1 - \kappa_r^2), \quad \mu_c = \mu(1 - \kappa_r^2)$$

To implement a simple leapfrog algorithm for Equations (2a) and (2b), the BI-FDTD mesh method proposed in [10], which is shown in Figure 1, is used. The discretization forms of the above formulae are:

$$\vec{E}_1^{n+1} = \vec{E}_1^n + \frac{\Delta t}{\varepsilon_c}\left(\nabla \times \vec{H}_1^{n+1/2}\right) + \frac{\xi\Delta t}{\mu\varepsilon_c}\left(\nabla \times \vec{E}_2^{n+1/2}\right)$$

$$\vec{H}_2^{n+1} = \vec{H}_2^n - \frac{\Delta t}{\mu_c}\left(\nabla \times \vec{E}_2^{n+1/2}\right) - \frac{\varsigma\Delta t}{\varepsilon\mu_c}\left(\nabla \times \vec{H}_1^{n+1/2}\right)$$

$$\vec{H}_1^{n+1/2} = \vec{H}_1^{n-1/2} - \frac{\Delta t}{\mu_c}(\nabla \times \vec{E}_1^n) - \frac{\varsigma\Delta t}{\varepsilon\mu_c}(\nabla \times \vec{H}_2^n)$$

$$\vec{E}_2^{n+1/2} = \vec{E}_2^{n-1/2} + \frac{\Delta t}{\varepsilon_c}(\nabla \times \vec{H}_2^n) + \frac{\xi\Delta t}{\mu\varepsilon_c}(\nabla \times \vec{E}_1^n)$$

$$\tag{3}$$
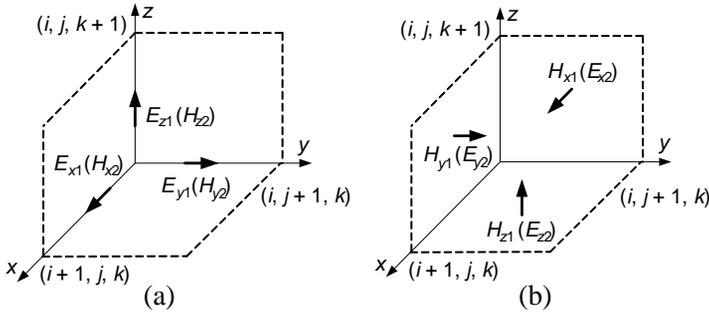
Figure 1. BI-FDTD mesh for 3D chiral media. (a) Field components sampled at integer time step. (b) Field components sampled at half-integer time step.

Take E_{x1} for example, the update formula is the following:

$$
E_{x1}^{n+1}\left(i+\frac{1}{2},j,k\right)
$$

$$
= E_{x1}^{n}\left(i+\frac{1}{2},j,k\right)
$$

$$
+\frac{\Delta t}{\varepsilon_c \Delta y}\left[H_{z1}^{n+\frac{1}{2}}\left(i+\frac{1}{2},j+\frac{1}{2},k\right)-H_{z1}^{n+\frac{1}{2}}\left(i+\frac{1}{2},j-\frac{1}{2},k\right)\right]
$$

$$
-\frac{\Delta t}{\varepsilon_c \Delta z}\left[H_{y1}^{n+\frac{1}{2}}\left(i+\frac{1}{2},j,k+\frac{1}{2}\right)-H_{y1}^{n+\frac{1}{2}}\left(i+\frac{1}{2},j,k-\frac{1}{2}\right)\right]
$$

$$
+\frac{\xi \Delta t}{\mu\varepsilon_c \Delta y}\left[E_{z2}^{n+\frac{1}{2}}\left(i+\frac{1}{2},j+\frac{1}{2},k\right)-E_{z2}^{n+\frac{1}{2}}\left(i+\frac{1}{2},j-\frac{1}{2},k\right)\right]
$$

$$
-\frac{\xi \Delta t}{\mu\varepsilon_c \Delta z}\left[E_{y2}^{n+\frac{1}{2}}\left(i+\frac{1}{2},j,k+\frac{1}{2}\right)-E_{y2}^{n+\frac{1}{2}}\left(i+\frac{1}{2},j,k-\frac{1}{2}\right)\right] \quad (4)
$$

In (3) and (4), Δt is the time step, Δx, Δy, Δz are the cell size, i, j, k are the indexes along the three dimensions ($x = i\Delta x$, $y = j\Delta y$, $z = k\Delta z$), and n is the time index ($t = n\Delta t$).

Since ξ and ς are both complex numbers in the above equations, and the source is real, it is obvious that the computed E_{x1}, E_{y1}, E_{z1}, H_{x1}, H_{y1}, H_{z1} are real, while E_{x2}, E_{y2}, E_{z2}, H_{x2}, H_{y2}, H_{z2} are imaginary. In fact, we regard the real part of E_{x1} as E_x in the conventional FDTD algorithm to calculate the reflection coefficient. The correctness of this method is demonstrated by the simulation results.

3. NUMERICAL RESULTS

To validate the proposed scheme, we calculate the scattering coefficients of WR 75 waveguides partially filled with chiral or achiral media as shown in Figure 2.
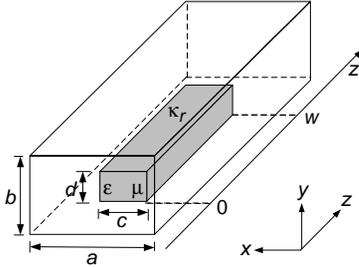
Figure 2. Configuration of a chiral media partially filled rectangular waveguide.
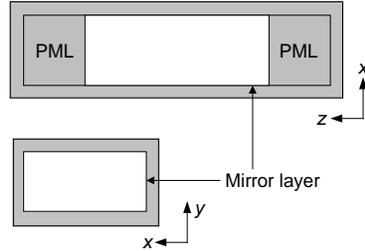
Figure 3. Mirror layer for the BI-FDTD mesh method.

To implement the effect of PEC boundary, we only have to set the tangential electric field values to zero in traditional Yee cell method. However, in the BI-FDTD mesh method, that is not enough. In fact, we add an additional layer to implement the effect of PEC. We called this layer a mirror layer, which is one cell thick in three dimensions as shown in Figure 3. Except setting the electric field value, on the PEC surface, to zero, we also have to set the mirror electric or magnetic field component's value according to the character of PEC. As to the tangential magnetic field and normal electric of the PEC surface, just only update according to formulae (3).

When the WR 75 waveguide, with a width of $a = 22.86$ mm and a height of $b = 10.16$ mm, is operated in the 8–12 GHz frequency range, only the dominant H_{10} mode can propagate [3, 4, 9]. The x and y directions cell size are as follows: $\Delta x = 0.5443$ mm, $\Delta y = 0.3378$ mm. Considering the mirror layer, the cell numbers of x and y directions are 44 and 32, respectively. As to the z direction, the cell size Δz and whole cell number $kmax$ are shown in Figures 4–7. The filled chiral or achiral media are surrounded by free space terminated by uniaxial perfectly matched layer absorbing boundary conditions (UPML ABC) in z direction. Each UPML ABC has 8 cells with polynomial grading $m = 4$. A sinusoidally modulated Gaussian pulse with $T = 250$ ps and $f_0 = 10$ GHz is used as the excitation source. The time-step size is $\Delta t = 0.5$ ps, and the iteration number is 10000.

In the first simulation, we take $d = b$, $w = 6$ mm, $\varepsilon = 8.2\varepsilon_0$,

$\mu = \mu_0$, and normalized chirality parameter $\kappa_r = 0$. In the next simulations, we take $d = 0.5b$, $\varepsilon = 2.56\varepsilon_0$, $\mu = \mu_0$. The values of long w and normalized chirality parameter κ_r are shown in Figures 5–7.

Figures 4–7 show the simulated results of reflection coefficients $|S_{11}|$ verse frequency by the proposed method and HFSS software,
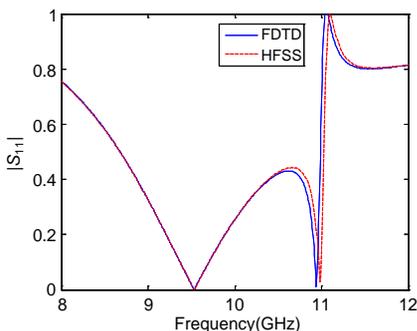
Figure 4. Amplitude of reflection coefficients $|S_{11}|$ versus frequency for a dielectric partially filled rectangular waveguide. Here, we take $d = b$, $w = 6\,\text{mm}$, $\Delta z = 0.3333\,\text{mm}$ and $kmax = 134$.
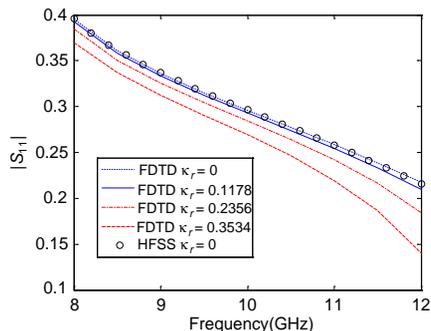
Figure 5. Amplitude of reflection coefficients $|S_{11}|$ versus frequency for a chiral partially filled rectangular waveguide. Here, we take $d = 0.5b$, $w = 7.62\,\text{mm}$, $\Delta z = 0.3464\,\text{mm}$ and $kmax = 136$.
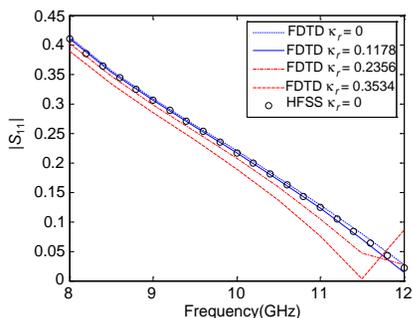
Figure 6. Amplitude of reflection coefficients $|S_{11}|$ versus frequency for a chiral partially filled rectangular waveguide. Here, we take $d = 0.5b$, $w = 10.16\,\text{mm}$, $\Delta z = 0.3464\,\text{mm}$ and $kmax = 146$.
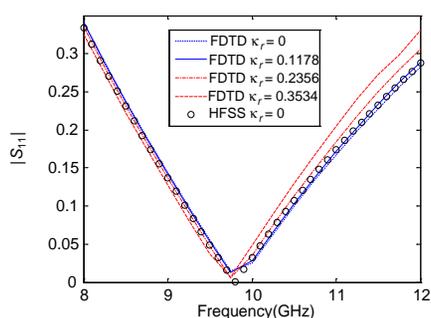
Figure 7. Amplitude of reflection coefficients $|S_{11}|$ versus frequency for a chiral partially filled rectangular waveguide. Here, we take $d = 0.5b$, $w = 14\,\text{mm}$, $\Delta z = 0.3464\,\text{mm}$ and $kmax = 160$.

Table 1. The reflection coefficients at the frequency of 10 GHz.

$|S_{11}|$	$\kappa_r = 0$			$\kappa_r = 0.1178$	
	This work	[9]	HFSS	This work	[9]
$W = 7.62\,\text{mm}$	0.296	0.305	0.296	0.293	0.305
$W = 10.16\,\text{mm}$	0.220	0.222	0.218	0.217	0.218
$W = 14\,\text{mm}$	0.025	0.040	0.033	0.028	0.045
$|S_{11}|$	$\kappa_r = 0.2356$			$\kappa_r = 0.3534$	
	This work	[9]		This work	[9]
$W = 7.62\,\text{mm}$	0.285	0.305		0.269	0.302
$W = 10.16\,\text{mm}$	0.207	0.204		0.190	0.173
$W = 14\,\text{mm}$	0.036	0.081		0.049	0.150

and excellent agreement is found. Table 1 presents the comparison of reflection coefficients between our calculated results and those from literature [9] and HFSS software simulations at the frequency of 10 GHz. These results provide the validation of our method.

4. CONCLUSION

This work has proposed a simple leapfrog algorithm for 3D nondispersive chiral media. The scattering coefficients of waveguides partially filled with chiral or achiral media have been computed. The validity and accuracy of the proposed approach have been tested through the comparison between the results of our method and those of others.

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