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Implementation of the FDTD method in cylindrical coordinates for dispersive materials: Modal study of C-shaped nano-waveguides

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ABSTRACT

The objective of this work is to develop a code based on the finite difference time domain method in cylindrical coordinates (CC-FDTD) that integrates the Drude Critical Points model (DCP) and to apply it in the study of a metallic C-shaped waveguide (CSWG). The integrated dispersion model allows an accurate description of noble metals in the optical range and working in cylindrical coordinates is necessary to bypass the staircase effect induced by a Cartesian mesh especially in the case of curved geometrical forms. The CC-FDTD code developed as a part of this work is more general than the Body-Of-Revolution-FDTD algorithm that can only handle structures exhibiting a complete cylindrical symmetry. A N-order CC-FDTD code is then derived and used to perform a parametric study of an infinitly-long CSWG for nano-optic applications. Propagation losses and dispersion diagrams are given for different geometrical parameters.

1. Introduction

Today, the race to miniaturize optical components requires the design of new and more complex structures requiring more elaborate simulation and manufacturing tools. For this, modeling and simulation tools in nano-photonics remain a challenging field of research. They are needed to explain complex physical phenomena and to optimize the geometrical and physical parameters of a given optical component in addition to its experimental design often very expensive. One of the useful methods in this field is the finite difference time domain (FDTD) [1,2]. This method, generally developed in Cartesian coordinates and based on the Yee scheme [2,3], can be implemented in cylindrical coordinates to accurately describe structures having a curved geometry. The modeling of these structures by classical Cartesian FDTD requires a very fine spatial discretization leading to a huge computation time together with a large memory space. In the case of revolution symmetrical structures, the azimuthal angle dependence of the electromagnetic field can be developed analytically in Fourier series. This leads to the well-known BOR-FDTD (Body Of Revolution-FDTD) algorithm where no discretization along the azimuthal angle is required [1,4].

In this work we extend the BOR-FDTD code to the case of structures having a partial cylindrical symmetry. For this purpose, a CC-FDTD (Cylindrical Coordinates-FDTD) algorithm [5–8] is developed for dispersive materials where the azimuthal angle derivative appearing in Maxwell's equations is discretized through a centered finite difference scheme as for the two other coordinates (radial and axial coordinates). Compared to the BOR-FDTD algorithm, the CC-FDTD addresses the case of any polarization state while one numerical simulation per azimuthal mode number (m with a field dependence $\exp(im\phi)$) is required within the BOR-FDTD. In addition, we incorporate the Drude critical points model (DCP) [9–11] that allows a very good description of the dispersion properties of noble metals over a large spectral range in view of modeling propagation inside metallic nano-waveguides.

An order-N FDTD code [4,12,13] is then derived in cylindrical coordinates to study the propagation properties of infinitly-long waveguides. The principle of the order-N algorithm is very simple and consists on exciting the structure by an initial field that verifies Maxwell's equations in addition to exhibit a broad spectrum covering all the possible eigenfrequencies of the structure. Then the code processes the field variations versus time. After the transient regime, only the eigenmodes of the structure remain and can be determined by calculating the spectral energy density $W(\lambda) = \frac{1}{2}(\vec{E}.\vec{D} + \vec{B}.\vec{H})$. To validate our code, several tests and convergence studies are achieved by comparing with other numerical simulations (BOR and Cartesian FDTD). After that, we applied this

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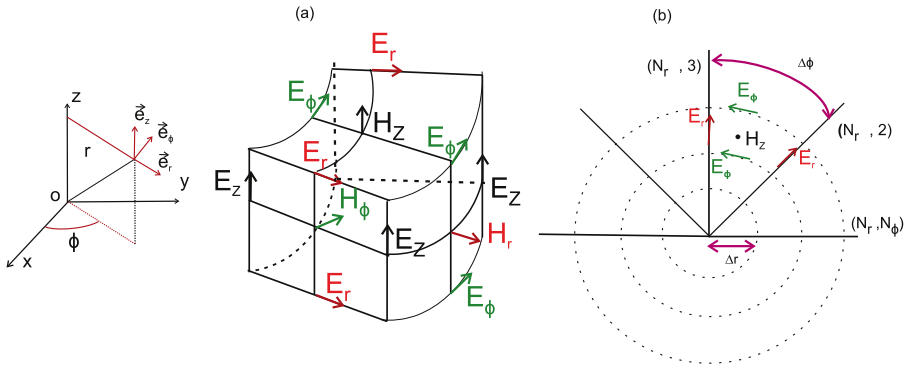

Fig. 1. Positions of the electric and magnetic field components according to the cylindrical Yee scheme in a) 3D case and b) 2D case.

code to the modal study of a metallic CSWG for nano-optical applications.

2. Theoretical developments

The CC-FDTD method is based on the numerical resolution of Maxwell's equations expressed in cylindrical coordinates (system of Eq. (1)) by following the adapted Yee scheme [1,3], shown on Fig. 1.

The CC-FDTD method is based on the numerical resolution of Maxwell's equations expressed in cylindrical coordinates:

$$\frac{\partial D_r}{\partial t} = \frac{1}{r}\frac{\partial H_z}{\partial \phi} - \frac{\partial H_\phi}{\partial z} \tag{1.a}$$

$$\frac{\partial D_\phi}{\partial t} = \frac{\partial H_r}{\partial z} - \frac{\partial H_z}{\partial r} \tag{1.b}$$

$$\frac{\partial D_z}{\partial t} = \frac{1}{r}\left(\frac{\partial (rH_\phi)}{\partial r} - \frac{\partial H_r}{\partial \phi}\right) \tag{1.c}$$

$$-\frac{\partial B_r}{\partial t} = \frac{1}{r}\frac{\partial E_z}{\partial \phi} - \frac{\partial E_\phi}{\partial z} \tag{1.d}$$

$$-\frac{\partial B_\phi}{\partial t} = \frac{\partial E_r}{\partial z} - \frac{\partial E_z}{\partial r} \tag{1.e}$$

$$-\frac{\partial B_z}{\partial t} = \frac{1}{r}\left(\frac{\partial (rE_\phi)}{\partial r} - \frac{\partial E_r}{\partial \phi}\right) \tag{1.f}$$

$\vec{D}$ and $\vec{B}$ are respectively the electric displacement and the magnetic fields. To determine the electromagnetic field $(\vec{E}, \vec{H})$ constitutive relations are needed. In the case of linear, isotropic, homogeneous and non-magnetic medium, these relations can be expressed as:

$$\vec{D}(\omega) = \varepsilon_0 \varepsilon_r(\omega)\vec{E}(\omega) \tag{2.a}$$

$$\vec{B}(\omega) = \mu_0 \vec{H}(\omega) \tag{2.b}$$

Where ω is the angular frequency of the electromagnetic field, ε_0 is the dielectric permittivity of vacuum and $\varepsilon_r(\omega)$ is the dielectric function of the considered medium. μ_0 is the magnetic permeability of vacuum ($\mu_0 \varepsilon_0 c^2 = 1$, with c is the light celerity).

In the scope of the paper, we are only dealing with the determination of the eigenmode properties of an infinite waveguide along the Oz direction.

$$\overrightarrow{\psi}(r, \phi, z, t) = \overrightarrow{\psi_0}(r, \phi, t)\exp(ik_z z) \tag{3}$$

where $\overrightarrow{\psi}$ is any electromagnetic field $(\vec{E}, \vec{D}, \vec{H}, \vec{B})$.

In this case, all the z−derivatives of Eq. (1) can be calculated analytically as a function of the wavevector component along the propagation direction through $\frac{\partial \overrightarrow{\psi}(r,\phi,z,t)}{\partial z} = ik_z \overrightarrow{\psi}(r, \phi, z, t)$ while r−, ϕ−, and t− derivatives are approximated by centered finite differences as in the classical case of Cartesian coordinates. The r coordinate is discretized as $i\Delta r$, the ϕ one by $j\Delta\phi$ and time by $n\Delta t$ with i, j, n are natural integers and Δr, $\Delta\phi$ and Δt are the step size along each variable. By using the electric constitutive relation Eq. (2.a) and applying the spatial and temporal discretizations, the system of Eq. (1) leads to express the $\vec{D}$ components as:

$$D_r^{n+1}(i,j) = D_r^n(i,j) + \triangle t\left[\frac{1}{\left(i+\frac{1}{2}\right)\Delta r}\frac{H_z^{n+\frac{1}{2}}(i,j) - H_z^{n+\frac{1}{2}}(i,j-1)}{\Delta\phi} - ik_z H_\phi^{n+\frac{1}{2}}(i,j)\right] \tag{4.a}$$

$$D_\phi^{n+1}(i,j) = D_\phi^n(i,j) + \triangle t\left[ik_z H_r^{n+\frac{1}{2}}(i,j) - \frac{H_z^{n+\frac{1}{2}}(i,j) - H_z^{n+\frac{1}{2}}(i-1,j)}{\Delta r}\right] \tag{4.b}$$

$$D_z^{n+1}(i,j) = D_z^n(i,j) + \frac{\triangle t}{(i-1)\Delta r} \times \left[\frac{\left((i)\Delta r H_\phi^{n+\frac{1}{2}}(i,j) - ((i-1)\Delta r)H_\phi^{n+\frac{1}{2}}(i-1,j)\right)}{\Delta r} - \frac{H_r^{n+\frac{1}{2}}(i,j) - H_r^{n+\frac{1}{2}}(i-1,j)}{\Delta\phi}\right] \tag{4.c}$$

The magnetic field components can be obtained similarly.

These equations remain valid for dispersive or non-dispersive dielectric materials. In this last case, the electric field $\vec{E}$ can be instantaneously calculated by dividing the $\vec{D}$ field by $\varepsilon_0\varepsilon_r$.

The stability condition of the CC-FDTD algorithm is given by the Courant-Friedrich-Levy (CFL) criterion [6] as follows:

$$\Delta t = \frac{\alpha}{c}\left(\left(\frac{1}{\triangle r}\right)^2 + \left(\frac{2}{\triangle r \triangle \phi}\right)^2 + \left(\frac{k_z}{2}\right)^2\right)^{-1/2} \tag{5}$$

where α is a less-dimensional coefficient $\in [0, 1]$. To avoid the numerical dispersion, the discretization step along the radial direction must verify this condition:

$$\Delta r \leq \frac{\lambda_{\min}}{n} \tag{6}$$

where $\lambda_{\min}$ is the minimum wavelength that propagates in the CC-FDTD grid and n is in the range of 15 to 20.