FULL-WAVE MODELING AND ANALYSIS OF DISPERSION-ENGINEERED MATERIALS AND PLASMON WAVEGUIDES

DISSERTATION

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ABSTRACT

The main focus of this dissertation is the development of full-wave modeling and the analysis of dispersion-engineered materials and plasmon waveguides. Among dispersion-engineered structures, we in particular focus on slow-wave photonic crystals (PhCs) where the dispersion curve $\omega(k)$ is approximated as a cubic polynomial, a quartic polynomial, or a linear combination of a quadratic polynomial and a quartic polynomial. We propose and investigate new compact plasmon waveguides operating at optical communication band ($\lambda_0 \sim 1550$ nm).

Slow-wave PhCs may consist of periodic arrangements of complex media such as ferromagnetic materials and anisotropic dielectrics. The dispersion curve is tailored by the choice of geometries and materials for each unit cell. We develop finite-difference time-domain (FDTD) algorithms suitable for the analysis of slow-wave PhCs. This will be performed by decoupling the time-marching update equations into two steps, viz. one associated with Maxwell’s equations and the other associated with the constitutive relations. The complex-frequency-shifted (CFS)-perfectly matched layer (PML) is employed to minimize spurious reflections from the outer boundary of the computational domain. We further extend the complex-envelope (CE)-alternating-direction-implicit (ADI)-FDTD algorithm to anisotropic media, in order to lift the Courant stability limit with no loss of accuracy.
Plasmon structures are based on metallic nanostructures and they are of great interest due to their extraordinary properties such as subwavelength guiding and highly localized field phenomena. By harnessing the extraordinary optical properties of plasmon structures, we propose two types of compact plasmon waveguides operating at optical communication band. The first plasmon waveguide is based on an ordered array of gold nanorings. Electromagnetic fields are guided along this nanoparticle-based plasmon waveguide by near-field coupling between closely spaced nanoparticles. The second plasmon waveguide is based on a surface plasmon (SP)-coplanar waveguide (CPW). The SP-CPW yields compact mode confinement and moderate propagation loss. The analysis and design of these two types of plasmon waveguides will be performed using the 3-D CFS-PML-FDTD algorithm extended for the Drude dispersion model.

Further algorithm improvements are described. We propose an efficient time-domain modeling for plasmon structures in the visible spectrum, based on the extension of the ADI-FDTD algorithm to the multispecies Drude-Lorentz dispersion model. We also introduce a novel locally-one-dimensional (LOD)-FDTD algorithm based on an iterative fixed-point correction to reduce the splitting error. Lastly, we investigate numerical artifacts of the CE-ADI-FDTD algorithm and discuss the way to reduce these numerical artifacts.
This work is dedicated to my family.
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CHAPTER 1

INTRODUCTION

Electromagnetic (EM) wave phenomena are governed by Maxwell’s equations and by materials through which EM waves propagate. The control of EM waves is of great interest for a myriad of applications in radio frequency (RF) and optical frequency ranges, including wireless communication, global positioning system (GPS), military defense, and integrated optics. Previously, the ability to control EM waves was limited because only naturally existing bulk materials were exploited. Bulk materials yield limited EM responses (speed, intensity, and confinement of fields) and thus their applications are also restricted. Recently, artificially structured media, referred to as metamaterials, have attracted much attention due to their unusual EM responses not found in nature [1,2]. Metamaterials increase degrees of freedom (DoF) for controlling EM waves and thus they can provide new applications at RF and optical frequency ranges [3–5].

We in particular focus on two types of metamaterials: dispersion-engineered materials and plasmon structures. Photonic crystals (PhCs) are dispersion-engineered materials and they have the ability to selectively allow propagating waves in a prescribed frequency range and the ability to control the speed of EM wave propagation [6–8]. Plasmon structures are based on metallic nanostructures and they have the ability
to confine EM fields in subwavelength dimensions, much beyond the diffraction limit \((\lambda/2)\) [9–11].

This dissertation is contributed to the development of full-wave modeling and the analysis of dispersion-engineered materials and plasmon structures. The computational algorithms are based on the finite-difference time-domain (FDTD) paradigm, which is famous for high geometrical flexibility, robustness, visualization capabilities, and \(O(N)\) computational complexity [12].

This dissertation is categorized into three parts. The first part focuses on dispersion-engineered materials supporting slow-wave propagation (Chapters 2, 3, 4), the second part concentrates on subwavelength plasmon waveguides (Chapters 5, 6), and in the last part, further algorithm improvement will be addressed (Chapters 7, 8, 9).

In Chapter 2, we study on magnetic photonic crystals (MPhCs). MPhCs are period arrangements of one ferromagnetic layer and two anisotropic dielectric layers and under proper design they can yield a cubic dispersion curve with a stationary inflection point (SIP) on the band diagram. We develop late-time stable FDTD algorithms to investigate exotic properties of MPhCs, such as wave slowdown, amplitude increase (via pulse compression), and EM unidirectionality. Additionally, we perform a sensitivity analysis of MPhC responses against excitation, ferromagnetic losses, and geometric parameter variations.

Nonmagnetic PhCs, made up of one isotropic layer and two misaligned anisotropic dielectric layers in each period, can also yield slow-wave propagation. In Chapter 3, we analyze PhCs with a degenerate band edge (DBE). DBE PhCs yield a quartic dispersion relation just below the DBE frequency rather than the conventional quadratic
dispersion relation present below a regular band edge (RBE). We investigate the gigantic field intensity enhancement at Fabry-Perot resonances associated with finite-stack DBE PhCs. This will be performed by extending the complex-envelope (CE) alternating-direction-implicit (ADI)-FDTD algorithm to anisotropic media. Also, we present a sensitivity analysis of the performance of DBE PhCs under various perturbations such as grounding, layer thickness perturbations, and anisotropic dielectric losses.

In Chapter 4, we turn our attention to PhCs with a split band edge (SBE). The dispersion curve $\omega(k)$ of SBE PhCs can be approximated as a linear combination of a quadratic term and a quartic term. One of the most significant differences between the DBE and the SBE is that the transmittance of the former depends on the incident wave polarization whereas in the latter it does not. We investigate the transmission behavior of SBE PhCs and perform a sensitivity analysis of their responses against geometrical and material perturbations. A comparison is also made between the sensitivity of SBE PhC responses versus that of DBE PhC responses. This study will be performed by employing the CE-ADI-FDTD algorithm presented in Chapter 3.

We propose novel compact optical waveguides operating at optical communication band ($\lambda_0 \sim 1550$ nm) by harnessing extraordinary EM responses of plasmon structures. We employ a 3-D CFS-PML-FDTD algorithm which accounts for the Drude dispersion model, to analyze and design these plasmon waveguides. In Chapter 5, we show how an ordered array of Au nanorings guides EM fields in subwavelength dimensions. Also, we provide main characteristics of this nanoring-based plasmon waveguide and illustrate its potential for subwavelength routing and switching functions.
In Chapter 6, we study a surface plasmon (SP)-coplanar waveguide (CPW). We investigate mode confinement and propagation length of the SP-CPW. We also investigate bending losses in 90° bends (zero radius of curvature) and suggest the way to reduce bending losses with less mode conversion loss.

In Chapter 7, we develop efficient time-domain algorithms for three-dimensional (3-D) plasmon structures in the visible spectrum. This can be done by extending the ADI-FDTD method towards the multispecies Drude-Lorentz dispersion model in a systematic fashion via auxiliary differential equations (ADEs) for equivalent current and polarization terms. We calculate localized plasmon resonances in Au nanoparticles described by a Drude-Lorentz dispersion model, providing improved computational performance of the proposed algorithm versus the standard FDTD algorithm.

In Chapter 8, we present an iterative, unconditionally stable locally-one-dimensional (LOD)-FDTD method. It is based on the use of an iterative fixed-point correction to reduce the splitting error. We illustrate the gain in accuracy of the proposed method versus the conventional LOD-FDTD method and the improved computational efficiency versus the iterative ADI-FDTD method.

In Chapter 9, we investigate in detail two spurious numerical artifacts of the CE-ADI-FDTD algorithm, viz. spurious charges and anomalous wave propagation (modes with positive phase velocity and negative group velocity). We illustrate particularly detrimental effects of spurious charges to CE-ADI-FDTD simulations and also show that spurious charges can be reduced by employing a fixed-point iterative correction.

In Chapter 10, the highlights of this dissertation are summarized.
CHAPTER 2

MAGNETIC PHOTONIC CRYSTALS

2.1 Introduction

Magnetic photonic crystals (MPhCs) are dispersion-engineered periodic materials and under proper design they can yield a cubic dispersion curve with a stationary inflection point (SIP) in a forward direction (from left to right) and no SIP in a backward direction (from right to left) [13, 14]. Fig. 2.1 shows a $\omega-k$ band diagram for a MPhC, where the asymmetry between positive and negative Bloch wavenumbers is evident, and the slope of the dispersion curve (and hence the group velocity) near the SIP is extremely small. Due to this extraordinary dispersion relation, MPhCs yield striking EM properties, such as wave slowdown (frozen modes), amplitude increase (pulse compression), and unidirectional characteristics [13, 14]. Since group velocities are extremely low near the SIP, EM pulses seem to be “frozen” inside MPhCs when propagating in the forward direction. At the same time, these forward propagating EM pulses can exhibit a dramatic growth in amplitude inside MPhCs. In the backward direction, EM waves inside MPhCs propagate in an ordinary fashion.

The simplest way to achieve a MPhC is through a periodic structure whose unit cell is composed of two $A$-layers (misaligned anisotropic dielectrics) with different
orientations and one $F$-layer (ferrite) [13], as depicted in Fig. 2.2. Spectral asymmetry is related to time reversal asymmetry and space inversion asymmetry. Magnetically polarized media must be used to achieve time reversal asymmetry and at least three layers in a unit cell must be employed to achieve space inversion asymmetry [13]. It should be noted that although MPhCs were first proposed for (semi-) infinite periodic structures, finite-size MPhCs also display similar properties and thus support frozen modes [15, 16].

Two main challenges exist for the FDTD analysis of MPhCs: (1) accurate treatment of both anisotropic dielectric and ferromagnetic responses simultaneously in both perfectly matched layer (PML) [17] and non-PML regions, and (2) late-time time-domain stability to simulate extremely slow-moving EM waves. In addition, because frozen modes exist in the very narrow bandwidth, a narrowband incident pulse should be employed in FDTD simulations. These two features — slow-wave propagation and a narrowband pulse — require accurate late-time FDTD algorithms.

Figure 2.1: Band diagram of a magnetic photonic crystal (MPhC).
With the above in mind, we utilize the *material-independent* PML formulation (D-H/B-E approach) [18]. The key feature of the D-H and B-E PML formulation is that the equations involving the (anisotropic and dispersive) material parameters are naturally decoupled from the PML-FDTD equations involving finite difference approximations to spatial derivatives in a complex coordinate space (to incorporate the PML implementations) [19,20]. Moreover, in this work, complex-frequency shifted (CFS) stretching [21, 22] is incorporated into PML in order not to admit spurious late time linear growth of axial fields [23].

The relationship between D and E (B and H) is completed by means of the constitutive relations. For non-dispersive anisotropic dielectric media, the FDTD equations can be formulated without much difficulties. However, for *lossy* ferromagnetic media, the FDTD equations should be carefully formulated. Two modelings of ferromagnetic media have been reported in the FDTD algorithm. The first approach uses the equation of motion of the magnetization vector [24, 25]. In this approach, however, the
FDTD Yee mesh should be modified. The second approach uses frequency-dependent permeability tensors and the resulting FDTD equations are obtained by transforming them into the time domain through recursive convolution (RC) [26–28]. To be compatible with the D-H and B-E PML formulation associated with the constitutive relations, permeability tensors (instead of equations of motion) are preferred for the ferromagnetic media. However, our extensive numerical experiments have indicated that the RC approach suffers from late-time instabilities in this case. In this work, the PML-FDTD formulation for ferromagnetic media is directly derived from the permeability tensors without RC. This derivation is similar to the procedure in deriving the ADE method for dispersive dielectric media [12].

2.2 Late-time Stable CFS-PML-FDTD Algorithm

We consider A-layers with with anisotropy in the $xy$ plane and $F$-layer with a $z$-directed DC magnetic bias field, under a plane wave propagating along $z$. Since the transverse fields ($x$ and $y$ components) are of interests and there is no coupling between transverse fields and axial fields, we need only $x$ and $y$ field components. The derived algorithm consists of two parts: Maxwell’s curl equations and the constitutive relations [29].

2.2.1 Maxwell’s Curl Equations

For arbitrary materials, Maxwell’s curl equations can be written as

$$\frac{\partial \mathbf{D}}{\partial t} = \mathbf{\nabla} \times \mathbf{H}, \quad (2.1a)$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\mathbf{\nabla} \times \mathbf{E}. \quad (2.1b)$$
Here, we use a modified nabla operator with complex stretching variables \([19, 20]\) for the PML implementation:

\[
\tilde{\nabla} = \hat{x} \frac{1}{s_x} \frac{\partial}{\partial x} + \hat{y} \frac{1}{s_y} \frac{\partial}{\partial y} + \hat{z} \frac{1}{s_z} \frac{\partial}{\partial z},
\]

(2.2)

where a CFS stretching \([21–23]\) is utilized so that

\[
s_{\xi} = \kappa_{\xi} + \frac{\sigma_{\xi}}{\nu_{\xi} + j\omega\epsilon_0},
\]

(2.3)

where \(\xi = x, y, z\). In the above, \(\sigma_{\xi}\) is the conductivity profile along the \(\xi\)-direction, \(\sigma_{\xi} \geq 0\). In practice, \(\kappa_{\xi} \geq 1\) and \(\nu_{\xi} \geq 0\). The standard PML stretching \([19]\) can be recovered by \(\nu_{\xi} = 0\). The CFS stretching \((\nu_{\xi} \neq 0)\) leads to a slightly more costly time-domain implementation than the standard PML stretching \((\nu_{\xi} = 0)\), but the former is more effective at absorbing evanescent waves and low-frequency fields (since it correctly recovers the elliptic equation regime for \(\omega \to 0\)). Moreover, it does not admit spurious late time linear growth of axial fields that otherwise may appear in some problems \([23]\). We have found that the relative difference between the PML implementations based on these two (standard and CFS) stretching functions is consistently below 0.1% and that both implementations yield stable results even for 160 million time steps in 1-D MPbCs (no axial fields involved in this case).

### 2.2.2 Constitutive Relations

Because frozen modes in MPbCs exist in a very narrow bandwidth, it is often not of fundamental importance to consider dispersion in \(A\)-layers. However, off-diagonal terms in the permeability tensor model of lossless \(F\)-layers exhibit a 90° phase difference to diagonal terms [see Eq. (2.6)]. Moreover, it is important to study the effect of ferromagnetic losses. Hence, it is highly desirable to model \(F\)-layers consistently by considering full dispersive models.
We assume the \( e^{j\omega t} \) time convention. The constitutive tensor of \( A \)-layers with anisotropy in the \( xy \) plane can be expressed as [13]

\[
\overline{\epsilon}_A(\omega) = \epsilon_0 \begin{bmatrix}
\epsilon_{xx} & \epsilon_{xy} & 0 \\
\epsilon_{xy} & \epsilon_{yy} & 0 \\
0 & 0 & \epsilon_{zz}
\end{bmatrix} \\
= \epsilon_0 \begin{bmatrix}
\epsilon_A + \delta_A \cos(2\varphi_A) & \delta_A \sin(2\varphi_A) & 0 \\
\delta_A \sin(2\varphi_A) & \epsilon_A - \delta_A \cos(2\varphi_A) & 0 \\
0 & 0 & \epsilon_{zz}
\end{bmatrix},
\]

(2.4a)

\[
\overline{\mu}_A(\omega) = \mu_0 \mu_r \overline{I},
\]

(2.4b)

where \( \overline{I} \) is the identity matrix. The parameter \( \delta_A \) is the magnitude of in-plane anisotropy, and \( \varphi_A \) is the orientation angle of the principle axis of the permittivity tensor in the \( xy \) plane.

For a saturated ferrite with a \( z \)-directed DC biasing magnetic field, the constitutive tensor is expressed as [30]

\[
\overline{\epsilon}_F(\omega) = \epsilon_0 \epsilon_r \overline{I},
\]

(2.5a)

\[
\overline{\mu}_F(\omega) = \mu_0 \left[
\begin{array}{ccc}
1 + \chi_{xx}(\omega) & \chi_{xy}(\omega) & 0 \\
\chi_{yx}(\omega) & 1 + \chi_{yy}(\omega) & 0 \\
0 & 0 & 1
\end{array}
\right],
\]

(2.5b)

where

\[
\chi_{xx}(\omega) = \chi_{yy}(\omega) = \frac{(\omega_0 + j\omega\alpha)\omega_m}{(\omega_0 + j\omega\alpha)^2 + (j\omega)^2},
\]

(2.6a)

\[
\chi_{xy}(\omega) = -\chi_{yx}(\omega) = \frac{j\omega_m}{(\omega_0 + j\omega\alpha)^2 + (j\omega)^2}.
\]

(2.6b)

In the above, \( \alpha \) is the damping (loss) constant, \( \omega_0 = \gamma H_0 \), and \( \omega_m = \gamma 4\pi M_s \), where \( \gamma \) is the gyromagnetic ratio, \( H_0 \) is the DC biasing magnetic field magnitude, and \( M_s \) is the DC saturation magnetization.
Now, we derive FDTD update equations for the constitutive relations. For A-layers [see Eq. (2.4a)], FDTD update equations for \( E \) fields can be obtained as

\[
E^n_x = \frac{\varepsilon_{yy}}{\varepsilon_0 \Lambda_e} D^n_x - \frac{\varepsilon_{xy}}{\varepsilon_0 \Lambda_e} D^n_y, \quad (2.7a)
\]
\[
E^n_y = \frac{\varepsilon_{xx}}{\varepsilon_0 \Lambda_e} D^n_y - \frac{\varepsilon_{xy}}{\varepsilon_0 \Lambda_e} D^n_x, \quad (2.7b)
\]

where \( \Lambda_e = \varepsilon_{xx}\varepsilon_{yy} - \varepsilon_{xy}^2 \). The superscript \( n \) indicates that the field is calculated at \( t = n \Delta t \). Note that \( E_x \) field depends on both \( D_x \) and \( D_y \), and, similarly, the \( E_y \) field depends on both \( D_x \) and \( D_y \).

For the \( F \)-layers [see Eq. (2.5b)], \( H \) fields are related to \( B \) fields in the frequency domain as follows

\[
B_x(\omega) = \mu_0 H_x(\omega) + \mu_0 \frac{(\omega_0 + j \omega \alpha) \omega_m}{(\omega_0 + j \omega \alpha)^2 + (j \omega)^2} H_x(\omega)
\]
\[
+ \mu_0 \frac{j \omega \omega_m}{(\omega_0 + j \omega \alpha)^2 + (j \omega)^2} H_y(\omega), \quad (2.8a)
\]
\[
B_y(\omega) = \mu_0 H_y(\omega) + \mu_0 \frac{(\omega_0 + j \omega \alpha) \omega_m}{(\omega_0 + j \omega \alpha)^2 + (j \omega)^2} H_y(\omega)
\]
\[
- \mu_0 \frac{j \omega \omega_m}{(\omega_0 + j \omega \alpha)^2 + (j \omega)^2} H_x(\omega). \quad (2.8b)
\]

After manipulating the above and using the inverse Fourier transform, time-domain differential equations can be obtained:

\[
(1 + \alpha^2) \frac{\partial^2 B_x}{\partial t^2} + 2 \omega_0 \alpha \frac{\partial B_x}{\partial t} + \omega_0^2 B_x = \mu_0 (1 + \alpha^2) \frac{\partial^2 H_x}{\partial t^2} + \mu_0 \alpha (2 \omega_0 + \omega_m) \frac{\partial H_x}{\partial t} + \mu_0 \omega_0 (\omega_0 + \omega_m) H_x + \mu_0 \omega_m \frac{\partial H_y}{\partial t}, \quad (2.9a)
\]
\[
(1 + \alpha^2) \frac{\partial^2 B_y}{\partial t^2} + 2 \omega_0 \alpha \frac{\partial B_y}{\partial t} + \omega_0^2 B_y = \mu_0 (1 + \alpha^2) \frac{\partial^2 H_y}{\partial t^2} + \mu_0 \alpha (2 \omega_0 + \omega_m) \frac{\partial H_y}{\partial t} + \mu_0 \omega_0 (\omega_0 + \omega_m) H_y - \mu_0 \omega_m \frac{\partial H_x}{\partial t}. \quad (2.9b)
\]
Utilizing the central differencing for first and second order derivatives, and double averaging over $\Delta t$ for zeroth-order derivatives, we obtain:

\[
a_1 B_x^{n+1/2} + a_2 B_x^{n-1/2} + a_3 B_x^{n-3/2} \\
= b_1 H_x^{n+1/2} + b_2 H_x^{n-1/2} + b_3 H_x^{n-3/2} \\
+ b_4 H_y^{n+1/2} - b_4 H_y^{n-3/2},
\]

(2.10a)

\[
a_1 B_y^{n+1/2} + a_2 B_y^{n-1/2} + a_3 B_y^{n-3/2} \\
= b_1 H_y^{n+1/2} + b_2 H_y^{n-1/2} + b_3 H_y^{n-3/2} \\
- b_4 H_x^{n+1/2} + b_4 H_x^{n-3/2},
\]

(2.10b)

where

\[
a_1 = \omega_0^2 \Delta t^2 + 4 \omega_0 \alpha \Delta t + 4 \alpha^2 + 4,
\]

\[
a_2 = 2 \omega_0^2 \Delta t^2 - 8 \alpha^2 - 8,
\]

\[
a_3 = \omega_0^2 \Delta t^2 - 4 \omega_0 \alpha \Delta t + 4 \alpha^2 + 4,
\]

\[
b_1 = \mu_0 \left[ \omega_0 (\omega_0 + \omega_m) \Delta t^2 + 2 \alpha (2 \omega_0 + \omega_m) \Delta t + 4 \alpha^2 + 4 \right],
\]

\[
b_2 = \mu_0 \left[ 2 \omega_0 (\omega_0 + \omega_m) \Delta t^2 - 8 \alpha^2 - 8 \right],
\]

\[
b_3 = \mu_0 \left[ \omega_0 (\omega_0 + \omega_m) \Delta t^2 - 2 \alpha (2 \omega_0 + \omega_m) \Delta t + 4 \alpha^2 + 4 \right],
\]

\[
b_4 = 2 \mu_0 \omega_m \Delta t.
\]
By solving Eqs. (2.10a) and (2.10b) simultaneously, FDTD update equations for $H_x$ and $H_y$ can be finally obtained

\[
H_x^{n+1/2} = -\frac{b_1 b_2}{b_1^2 + b_4^2} H_x^n - \frac{b_1 b_3 - b_4^2}{b_1^2 + b_4^2} H_x^{n-3/2} + \frac{b_2 b_4}{b_1^2 + b_4^2} H_y^n + \frac{b_1 b_4 + b_3 b_4}{b_1^2 + b_4^2} H_y^{n-3/2} + \frac{b_1 a_1}{b_1^2 + b_4^2} B_x^n + \frac{b_1 a_3}{b_1^2 + b_4^2} B_x^{n-3/2} - \frac{b_4 a_1}{b_1^2 + b_4^2} B_y^n - \frac{b_4 a_3}{b_1^2 + b_4^2} B_y^{n-3/2}, \tag{2.11a}
\]

\[
H_y^{n+1/2} = -\frac{b_1 b_2}{b_1^2 + b_4^2} H_y^n - \frac{b_1 b_3 - b_4^2}{b_1^2 + b_4^2} H_y^{n-3/2} - \frac{b_2 b_4}{b_1^2 + b_4^2} H_x^n - \frac{b_1 b_4 + b_3 b_4}{b_1^2 + b_4^2} H_x^{n-3/2} + \frac{b_1 a_1}{b_1^2 + b_4^2} B_y^n + \frac{b_1 a_3}{b_1^2 + b_4^2} B_y^{n-3/2} + \frac{b_4 a_1}{b_1^2 + b_4^2} B_x^n + \frac{b_4 a_3}{b_1^2 + b_4^2} B_x^{n-3/2}. \tag{2.11b}
\]

We note here that it is possible to derive alternative $H$ field FDTD update equations for ferrite media. For instance, the $H_x$ and $H_y$ fields can be first decoupled in the frequency domain (unlike the above), by solving Eqs. (2.8a) and (2.8b) simultaneously, and later inverse Fourier transformed. However, we found that the resulting FDTD formulation suffers from late-time instabilities. Therefore, we employ Eqs. (2.11a) and (2.11b) for MPhC simulations that follow.
2.3 MPhC Properties

We assume that the DC biasing magnetic field is $-z$-directed in $F$-layers, as depicted in Fig. 2.2. The geometrical dimensions are as follows

$$L_{A1} = L_{A2} = 5 \text{ mm},$$
$$L_F = 1 \text{ mm}.$$

For $A$-layers, the constitutive tensor (relative) parameters are as follows

$$\epsilon_{A1} = \epsilon_{A2} = 7,$$
$$\delta_{A1} = \delta_{A2} = 6,$$
$$\varphi_{A1} = 0^\circ,$$
$$\varphi_{A2} = 36.0963^\circ,$$
$$\epsilon_{zz,A1} = \epsilon_{zz,A2} = 1,$$
$$\mu_{r,A1} = \mu_{r,A2} = 1.$$

For $F$-layers, the constitutive tensor (relative) parameters are as follows

$$\epsilon_r = 5,$$
$$\omega_0 = 36.503 \times 10^9 \text{ rad/s},$$
$$\omega_m = 73.006 \times 10^9 \text{ rad/s}.$$

The total-field/scattered-field (TF/SF) formulation was used as a source condition [12]. The excitation pulse ($E_x$) is a sine wave modulated by a Gaussian pulse with unit peak amplitude. The operating angular frequency is $24.565 \times 10^9 \text{ rad/s}$ and the 5% fractional bandwidth (FBW) is 0.01%. Space step $\Delta z = 0.08333 \text{ mm}$ and Courant factor of 0.98 were used.
Figure 2.3: Snapshots of $|E_x|$ due to a narrowband, unit amplitude pulse incident on a lossless MPhC along the forward MPhC direction.

Fig. 2.3 shows snapshots of $|E_x|$ in the presence of a lossless MPhC with 500 unit cells for the forward propagating pulse. The results show that the peak value of the electric field increases by about eight times inside this MPhC (seventy times in terms of the peak value of field intensity). While the incident pulse spans about $10,000\lambda_0$ in air, the spatial span of the pulse inside the MPhC is extremely narrowed. In other words, when the incident pulse enters the MPhC in the forward direction, the EM wave is drastically slowed down (“frozen”), the pulse is compressed, and the amplitude increases dramatically. However, because the (relative) group velocity changes drastically near a SIP, the pulse propagation is highly dispersive, as can be seen from the pulse spread out in Fig. 2.3.
Figure 2.4: Snapshots of $|E_x|$ due to a narrowband, unit amplitude pulse incident on a lossless MPhC along the backward MPhC direction (i.e., the MPhC is reversed with respect to Fig. 2.3).

To illustrate the unidirectional property of MPhCs, the spatial order of layers is reversed ($F - A2 - A1$ layer arrangement) with respect to the previous one. Fig. 2.4 shows snapshots of $|E_x|$ in the presence of this lossless MPhC for “backward” propagation pulse. The pulse propagates at much faster speed in this case, and no growth in amplitude is observed in this “backward” propagation. As seen from Fig. 2.4, the “backward” propagating pulse reaches the far end of the MPhC at a much earlier time, and then it is reflected toward the near end of the MPhC. The direction of reflected pulse is now “forward” and hence the reflected pulse shows the amplitude increase and wave slowdown.

Because the group velocity for a finite bandwidth pulse including the SIP is spread around zero value, it is not meaningful to try to determine an effective or average
Figure 2.5: Normalized energy to calculate a (half-time, non-characteristic) effective rate of energy transport.

group velocity for the pulse in this highly dispersive regime. Instead, we adopt here the approach described in Ref. [31] to obtain an “effective rate” of (half-time) energy transport. This is determined by calculating the times at which half of the electromagnetic energy has been collected at two observation points. We note that this is a position dependent and not a characteristic quantity of the MPhC. To avoid reflections at the interface of the MPhC and air at the far end of the MPhC, 2,000 unit cells are employed. Fig. 2.5 shows the instantaneous (integrated) collected energy, which is normalized at the center of the 150th unit cell. By dividing the distance between the two observation points ($\Delta z = 1.1$ m) by the difference of times to collect half of the energy at these two points ($\Delta t = 2.274 \mu s$), the effective rate of energy transport for the forward propagating pulse is found to be about $0.0016c_0$. A similar
procedure is carried out for the backward direction. The time difference to collect half the energy at the two observation points is now \( \Delta t = 9 \text{ ps} \), which implies an effective rate of energy transport equal to \( 0.4074c_0 \). Hence, the effective half-time energy transfer slowdown is equal to about 250 times.

2.4 Sensitivity Analysis

Next, we illustrate the sensitivity of the MPhC response for five different scenarios:

i.) a lossless MPhC with frequency mismatched incident pulses, ii.) a lossless MPhC with wider band incident pulses, iii.) a lossy MPhC with different number of unit cells, iv.) a lossless MPhC with random variations on A-layer misalignments, and v.) a lossless MPhC with random variations on A- and F-layer thickness.

2.4.1 Frequency Sensitivity

To illustrate the impact of frequency deviations on the pulse propagation inside the MPhC, we change the center frequency of the incident pulse from \( \delta \omega = 0.01\% \) and from \( \delta \omega = 0.1\% \). Fig. 2.6 shows snapshots of \( |E_x| \) in the presence of the lossless MPhC for the frequency-shifted incident pulse with \( \delta \omega = 0.01\% \). The peak value of \( |E_x| \) inside the MPhC is decreased, and the average group velocity is increased, as compared to the matched frequency case (Fig. 2.3). Fig. 2.7 shows snapshots of \( |E_x| \) in the presence of the lossless MPhC for the frequency-shifted incident pulse with \( \delta \omega = 0.1\% \). As expected, the increase in the group velocity and the decrease in \( |E_x| \) is considerably more pronounced with a larger frequency mismatch.

It is also interesting to examine the sensitivity to the pulse center frequency versus the slope of dispersion curve. It is expected that the MPhC response becomes
Figure 2.6: Snapshots of $|E_x|$ in a lossless MPPhC. The narrowband, unit amplitude incident pulse is shifted in frequency, with $\delta \omega = 0.01\%$.

Figure 2.7: Snapshots of $|E_x|$ in a lossless MPPhC. The narrowband, unit amplitude incident pulse is shifted in frequency, with $\delta \omega = 0.1\%$. 
less sensitive to the center frequency for a (quasi-) MPhC, where the slope of dispersion curve (and hence group velocity) becomes small but not zero (i.e., no true SIP present). Fig. 2.8 shows dispersion relations for the original MPhC and two modified quasi-MPhC designs where group velocities are very small but not zero over a frequency range near the SIP frequency. These new quasi-MPhC designs are obtained by changing the thickness of $F$-layer. Snapshots of $|E_x|$ at time step twelve million are shown in Fig. 2.9 for the MPhC with $L_F = 1.0833$ mm and Fig. 2.10 for the MPhC with $L_F = 1.1667$ mm. Compared to the results shown in Fig. 2.3, Fig. 2.6, and Fig. 2.7, although the amplitude growth and pulse compression effects are diminished as expected, the frequency sensitivity becomes less critical for the quasi-MPhC designs [cf. Fig. 2.9 and Fig. 2.10]. Table 2.1 provides a comparison for a quantitative measure of the frequency sensitivity against the slope of dispersion curve. This measure is defined by the normalized difference between the $|E_x|$ envelopes, $\mathcal{E}_x$, for matched frequency ($\delta \omega = 0$) and frequency-shifted cases ($\delta \omega \neq 0$), and integrated along the MPhC length:

$$FS = \int dz \frac{\mathcal{E}_x(z, \delta \omega \neq 0) - \mathcal{E}_x(z, \delta \omega = 0)}{\mathcal{E}_x(z, \delta \omega = 0)}.$$  

(2.12)

### 2.4.2 Wideband Pulse Response

In order to compare the relative wideband pulse response against the narrowband response, we change the FBW of the excitation pulse from 0.01% to 0.1%. Fig. 2.11 shows snapshots of $|E_x|$ in the presence of the lossless MPhC for FBW = 0.1%. The peak field amplitude is reduced compared to the 0.01% case. Because the group velocity in the frequency range for FBW = 0.1% near the SIP is considerably spread
Figure 2.8: Dispersion curves of MPhCs with zero group velocity (SIP) and non-zero (but small) group velocities, with nearly linear slopes around the SIP frequency.

Figure 2.9: Snapshots of $|E_x|$ inside the MPhC at time step twelve million, with $L_F=1.0833\text{mm}$. 

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Figure 2.10: Snapshots of $|E_x|$ inside the MPhC at time step twelve million, with $L_F=1.1667\text{mm}$.

<table>
<thead>
<tr>
<th>MPhC</th>
<th>$FS(\delta\omega = 0.01%)$</th>
<th>$FS(\delta\omega = 0.1%)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_F=1\text{mm}$</td>
<td>0.782</td>
<td>2.561</td>
</tr>
<tr>
<td>$L_F=1.0833\text{mm}$</td>
<td>0.448</td>
<td>0.710</td>
</tr>
<tr>
<td>$L_F=1.1667\text{mm}$</td>
<td>0.445</td>
<td>0.456</td>
</tr>
</tbody>
</table>

Table 2.1: Comparison of frequency sensitivity ($FS$).

out, dispersion is increased, as seen from Fig. 2.11. The “effective” group velocity is also increased compared to the 0.01% case, as expected.

2.4.3 Ferromagnetic Losses

Next, we assess the sensitivity of the MPhC response to different ferromagnetic loss coefficients $\alpha$ [Eq. 2.6]. The EM pulse (not shown here) inside a MPhC with
\( \alpha = 10^{-5} \) is nearly identical to the lossless MPhC case \( \alpha = 0 \), with relative \( |E_x| \) peak amplitude ratio equal to 0.982. Fig. 2.12 shows snapshots of \( |E_x| \) for a MPhC with \( \alpha = 10^{-4} \). The decrease on the pulse amplification, compared to the lossless case in Fig. 2.3, is apparent here. The peak \( |E_x| \) ratio of this lossy MPhC to the lossless MPhC is 0.868. Furthermore, since magnetic loss effects are cumulative, the EM pulse amplitude is more strongly suppressed as it penetrates more deeply into the crystal. Note, however, such ferromagnetic losses do not destroy the essential properties (wave slowdown and pulse compression) of the MPhC response.

We also evaluate the interplay of ferromagnetic losses and the total number of unit cells in the MPhC response. Fig. 2.13 plots the peak amplitude increase in lossy MPhC with different numbers of unit cells. As expected, a sufficient number of unit cells and a small ferromagnetic loss coefficient must be present to produce higher
amplitudes. It can also be seen that the relative $|E_x|$ peak amplitude ratio is nearly constant for MPhCs with more than 100 unit cells.

2.4.4 Imperfect $A$-layer Misalignment

To illustrate the effects of orientation misalignments of the $A$-layers, we incorporate random deviations in the orientation angles of $A$-layers. In this case, $\varphi_{A1}$ and $\varphi_{A2}$ are described by Gaussian random variables:

$$\varphi_{A1} = 0^\circ + N(0, \zeta_\phi^2),$$

$$\varphi_{A2} = 36.0963^\circ + N(0, \zeta_\phi^2),$$

where $N(\varpi, \zeta_\phi^2)$ indicates a Gaussian random variable with the mean $\varpi$ and variance $\zeta_\phi^2$. Four different standard deviations ($\zeta_\phi = 1.5^\circ, 3^\circ, 4.5^\circ, 6^\circ$) are considered. For each standard deviation, an ensemble with 15 realizations is used. The solid line

Figure 2.12: Snapshots of $|E_x|$ in the presence of a MPhC with lossy ($\alpha = 10^{-4}$) $F$-layers, for a narrowband incident pulse of unit amplitude.
in Fig. 2.14 interpolates the (ensemble averaged) peak value of $|E_x|$ inside lossless MPhCs for the various $\phi$. A narrowband incident pulse is used for these results. For reference, the peak $|E_x|$ for the frequency-shifted (narrowband) pulse with $\delta \omega = 0.01\%$ and $\delta \omega = 0.1\%$ and the wider band pulse with FBW = 0.1\% are also displayed at $\phi = 0^\circ$. As seen from this figure, small deviations in the misalignment angle can have a strong impact on the MPhC response.

### 2.4.5 Imperfect Layer Thickness

To elucidate the effects of variations on the layer thickness, we include (Gaussian distributed) random deviations in the thicknesses of ($A$- and $F$-) layers. Three different standard deviations ($\zeta_L = 1\%, 5\%, 10\%$) are considered. For each distribution, an ensemble with 15 realizations is used. The solid line in Fig. 2.15 interpolates the
Figure 2.14: $|E_x|_{\text{max}}$ inside lossless MPhCs with random deviations in the misalignment of $A$-layers.

(ensemble averaged) peak value of $|E_x|$ inside lossless MPhCs for various $\zeta_L$. A narrowband incident pulse is employed for these results. As seen from this figure, small deviations in the layer thickness have a strong influence on the MPhC response. For instance, in the case of a standard deviation of $\zeta_L = 5\%$, the peak amplitude is decreased to about half of that in the optimal MPhC.

2.5 Concluding Remarks

In this Chapter, the CFS-PML-FDTD method has been employed to analyze MPhCs with ferromagnetic losses. The proposed algorithm is based on the D-H and B-E formulation that decouples (anisotropic and dispersive) constitutive equations inside their MPhCs from (modified PML) Maxwell’s equations. Frequency dispersive material properties have been incorporated in the time-domain by the ADE approach,
in order to analyze frozen modes in MPhCs that require long time integrations. We note that the alternative RC approach has led to late-time instabilities. Both CFS-PML and standard PML have been implemented into the FDTD equations, leading to practically equivalent results in this case, and yielding no instabilities for simulations involving up to 160 million time steps. The proposed algorithm can be extend to 2-D parallel-plate waveguides loaded with MPhCs [32]. However, in this case, the standard PML formulation suffers from late-time instabilities and thus the CFS-PML should be employed for 2-D MPhC waveguides.

Numerical results show that the proposed algorithm can successfully analyze transient responses of MPhCs, capturing its unique characteristics such as frozen modes, pulse compression with a dramatic increase on the amplitude, and its unidirectional
properties. A sensitivity analysis was carried out to examine the effect of ferromagnetic losses, frequency mismatch, random A-layer misalignment, and random layer thickness on the electromagnetic pulse propagation inside a MPhC. As expected, the frozen mode is particularly sensitive to the center frequency of the excitation pulse, with its properties rapidly deteriorating for slight off-frequency excitations. In the examples considered, inclusion of ferromagnetic losses of $\alpha = 10^{-4}$ (typical value for the frequencies considered from off-the-shelf materials such as Calcium Vanadium Garnett (CVG), for example), has still yielded frozen modes, and an amplitude increase of about 87% compared to the optimal (lossless) case, albeit with progressive amplitude deterioration inside the MPhC. The peak amplitude also deteriorates when (Gaussian distributed) small random variations are included in the geometry of a MPhC, with a decrease of about a half on the electric field peak amplitude for a standard deviation of 1.5° in the relative misalignment of A-layers and a standard deviation of 5% in the thickness of (A- and F-) layers, respectively.
CHAPTER 3

PHOTONIC CRYSTALS WITH A DEGENERATE BAND EDGE (DBE)

3.1 Introduction

Periodic stacks composed of alternating isotropic layers with different refractive index yield a regular band edge (RBE) in the band diagram and their applications include a resonator, a Bragg reflector, and a transmission filter [33]. The dispersion relation can be further tailored by employing complicated periodic stacks. PhCs made of two misaligned anisotropic dielectric layers (A-layers) and one isotropic layer (B-layer) in each period can yield a degenerate band edge (DBE) [34]. Fig. 3.1 and Fig. 3.2 show the schematic of a DBE PhC and the $\omega$-$k$ band diagram of a DBE PhC, respectively. Near the band edge, DBE PhCs display a quartic dispersion curve and RBE PhCs show a quadratic dispersion curve:

\begin{align*}
DBE : \omega_b - \omega & \propto (k - k_b)^4, \\
RBE : \omega_b - \omega & \propto (k - k_b)^2,
\end{align*}

where $\omega_b$ and $k_b$ are the angular frequency and wavenumber, respectively, at the band edge.
Figure 3.1: Schematic of a PhC composed of two anisotropic dielectric layers (A-layers) and one isotropic dielectric layer (B-layer).

Figure 3.2: Band diagram of a PhC with a degenerate band edge (DBE).
EM waves propagate at slow group velocities below the band edge frequency. The group velocity \(v_g = \partial \omega / \partial k\) just below the band edge frequency can be approximated as

\[
DBE : v_g \propto (\omega_b - \omega)^{3/4},
\]
\[
RBE : v_g \propto (\omega_b - \omega)^{1/2}.
\]

The above indicates slow-wave propagation in DBE PhCs, compared to RBE PhCs. The wave slowdown leads the increase in the interaction of EM waves with materials and thus EM waves grow in amplitude.

Semi-infinite periodic PhCs yield poor matching properties, although they support slow-wave propagation. In the semi-infinite-media case, the transmittance decreases and gradually approaches zero as the frequency \(\omega\) approaches either the DBE or the RBE from below. In order to achieve high transmittance, Fabry-Perot resonances (associated with narrowband transmission peaks) can be exploited in finite-size periodic stacks. Fabry-Perot cavity resonances depend on the number \(N\) of unit cells. The resonances below the DBE frequency are shown for \(N = 8\) and \(N = 16\) in Fig. 3.3. As \(N\) increases, Fabry-Perot resonance frequencies move close to the DBE frequency and simultaneously the transmission bands are narrowed. As Fabry-Perot resonances move just below the band edge, a dramatic increase in field intensity is produced because of the wave slowdown, similar to what occurs in MPPhCs. Hence, larger \(N\) leads to greater growth in field intensity. Because the group velocity is smaller below the DBE frequency than the RBE frequency, a much larger increase in the field amplitude is produced at DBE-based Fabry-Perot resonances than at the RBE counterpart (for same \(N\)).
One of the main challenges in the analysis of DBE PhCs by a finite-difference technique is that the spatial discretization cell size needs to be very small in order to correctly capture the sharp field distributions inside the structure. Unfortunately, the time step size of the conventional FDTD algorithm is limited by the Courant stability criterion, which imposes an upper bound on the time step size based on the spatial cell size [12]. This leads to a prohibitive number of time steps for FDTD simulations. An alternative choice would be to employ the ADI-FDTD algorithm [35–37], which is an unconditionally stable method where the time step is not bound by the Courant criterion. However, the numerical accuracy of the ADI-FDTD algorithm deteriorates as the time step size and/or the maximum frequency increases [38, 39]. Contrary to the ADI-FDTD algorithm, the numerical accuracy of the complex-envelope (CE) ADI-FDTD [40–47] algorithm is governed by the bandwidth of the excitation, not by the maximum frequency. Therefore, the CE-ADI-FDTD algorithm is especially suited
for the analysis of DBE PhCs. Numerical aspects of the CE-ADI-FDTD algorithm can be found elsewhere in Refs. [41] and [42].

In this work, we extend the CE-ADI-FDTD algorithm to anisotropic media [48]. By employing the extended CE-ADI-FDTD algorithm, we analyze the DBE PhC response in detail, examining field enhancement effects and providing a sensitivity analysis under geometric perturbations and presence of dielectric losses. The effect of a ground plane on the DBE PhC response is also considered.

3.2 CE-ADI-FDTD Algorithm for Anisotropic Media

In this Section, we describe details on the extended CE-ADI-FDTD algorithm to anisotropic media, together with a summary of its relative computational performance for the analysis for DBE PhCs.

Consider anisotropic media with anisotropy in the $xy$ plane under a $y$-polarized plane wave propagating along $z$, as illustrated in Fig. 3.1. Both $x$ and $y$ components should be considered simultaneously due to the cross-coupling of transverse electric and magnetic components. Maxwell’s curl equations are expressed as

$$\frac{\partial}{\partial t} D_x + \frac{\sigma_z}{\epsilon_0} D_x = -\frac{\partial}{\partial z} H_y,$$

(3.5)

$$\frac{\partial}{\partial t} D_y + \frac{\sigma_z}{\epsilon_0} D_y = \frac{\partial}{\partial z} H_x,$$

(3.6)

$$\frac{\partial}{\partial t} H_x + \frac{\sigma_z}{\epsilon_0} H_x = \frac{\partial}{\mu \partial z} E_y,$$

(3.7)

$$\frac{\partial}{\partial t} H_y + \frac{\sigma_z}{\epsilon_0} H_y = -\frac{\partial}{\mu \partial z} E_x.$$

(3.8)
In the above, $\sigma_z$ is the artificial conductivity profile along the z-direction that implements a PML absorbing boundary condition [17, 19, 20]. Conventional Maxwell’s curl equations are recovered by setting $\sigma_z = 0$.

To derive the CE-ADI-FDTD formulation, we assume $\mathbf{F} = \Re e \left[ \widetilde{\mathbf{F}} \cdot e^{j\omega_c t} \right]$, where $\omega_c$ is the carrier frequency, $\mathbf{F}$ denotes the field components, and $\widetilde{\mathbf{F}}$ denotes the corresponding complex envelope. Maxwell’s curl equations in terms of the complex envelopes are expressed as

\[
\frac{\partial}{\partial t} \widetilde{D}_x + j \omega_c \widetilde{D}_x + \frac{\sigma_z}{\epsilon_0} \widetilde{D}_x = - \frac{\partial}{\partial z} \widetilde{H}_y, \tag{3.9}
\]

\[
\frac{\partial}{\partial t} \widetilde{D}_y + j \omega_c \widetilde{D}_y + \frac{\sigma_z}{\epsilon_0} \widetilde{D}_y = \frac{\partial}{\partial z} \widetilde{H}_x, \tag{3.10}
\]

\[
\frac{\partial}{\partial t} \widetilde{H}_x + j \omega_c \widetilde{H}_x + \frac{\sigma_z}{\epsilon_0} \widetilde{H}_x = \frac{\partial}{\mu \partial z} \widetilde{E}_y, \tag{3.11}
\]

\[
\frac{\partial}{\partial t} \widetilde{H}_y + j \omega_c \widetilde{H}_y + \frac{\sigma_z}{\epsilon_0} \widetilde{H}_y = - \frac{\partial}{\mu \partial z} \widetilde{E}_x. \tag{3.12}
\]

The relevant constitutive equation is written as

\[
\widetilde{D} = [\epsilon] \widetilde{E}, \tag{3.13}
\]

with permittivity tensor of the form

\[
[\epsilon] = \epsilon_0 \begin{bmatrix}
\epsilon_{xx} & \epsilon_{xy} & 0 \\
\epsilon_{xy} & \epsilon_{yy} & 0 \\
0 & 0 & \epsilon_{zz}
\end{bmatrix}
= \epsilon_0 \begin{bmatrix}
\epsilon + \delta \cos(2\varphi_A) & \delta \sin(2\varphi_A) & 0 \\
\delta \sin(2\varphi_A) & \epsilon - \delta \cos(2\varphi_A) & 0 \\
0 & 0 & \epsilon_{zz}
\end{bmatrix}, \tag{3.14}
\]

where the parameter $\delta$ is the magnitude of the in-plane anisotropy, and $\varphi_A$ is the orientation angle of the principal axis of the permittivity tensor in the $xy$ plane.
In the ADI algorithm [35, 36], the update at each time step \( n \) is divided into two sub-steps. For simplicity, we omit the tilde in update equations that follow. For the first sub-step, discretized equations from Maxwell’s curl equations (3.9)-(3.12) can be written as

\[
D_{xk}^{n+1/2} = c_{d1}D_{xk}^n - c_{d2}\left[H_{yk+1/2}^n - H_{yk-1/2}^n\right],
\]

(3.15)

\[
D_{yk}^{n+1/2} = c_{d1}D_{yk}^n + c_{d2}\left[H_{xk+1/2}^{n+1/2} - H_{xk-1/2}^{n+1/2}\right],
\]

(3.16)

\[
H_{xk+1/2}^{n+1/2} = c_{h1}H_{xk+1/2}^n + c_{h2}\left[E_{yk+1}^{n+1/2} - E_{yk}^{n+1/2}\right],
\]

(3.17)

\[
H_{yk+1/2}^{n+1/2} = c_{h1}H_{yk+1/2}^n - c_{h2}\left[E_{xk+1}^n - E_{yk}^n\right],
\]

(3.18)

where the subscript refers to spatial grid indexing along \( z \), and the superscript refers to the time step index. The coefficients above are given by \( c_{d1} = c_{h1} = \alpha_- / \alpha_+ \) and \( c_{d2} = \mu c_{h2} = \alpha_0 / \alpha_+ \), where \( \alpha_\pm = 1 \pm 0.25\Delta t \left(j\omega_c + \sigma_z / \epsilon_0\right) \) and \( \alpha_0 = 0.5\Delta t / \Delta z \). The update equation for \( \tilde{E} \) can be obtained from the constitutive equation (3.13) as

\[
E_{xk}^{n+1/2} = c_{e1x}D_{xk}^{n+1/2} + c_{e2}D_{yk}^{n+1/2},
\]

(3.19)

\[
E_{yk}^{n+1/2} = c_{e1y}D_{yk}^{n+1/2} + c_{e2}D_{xk}^{n+1/2},
\]

(3.20)

where \( c_{e1x} = \epsilon_{yy} / (\epsilon_0 \Lambda_e) \), \( c_{e1y} = \epsilon_{xx} / (\epsilon_0 \Lambda_e) \), and \( c_{e2} = -\epsilon_{xy} / (\epsilon_0 \Lambda_e) \), with \( \Lambda_e = \epsilon_{xx} \epsilon_{yy} - \epsilon_{xy}^2 \). From Eq. (3.16), we see that \( D_{y}^{n+1/2} \) cannot be updated explicitly. By substituting Eq. (3.20) into Eq. (3.17) and plugging the resulting equation into Eq. (3.16), we obtain an implicit equation for \( D_{y}^{n+1/2} \) in a form of the tridiagonal
system as follows:

\[-\gamma_{-,k} D_{y_{k-1}}^{n+1/2} + (1 + \beta_{-,k} + \beta_{+,k}) D_{y_{k}}^{n+1/2} - \gamma_{+,k} D_{y_{k+1}}^{n+1/2} =
\]

\[
c_{d1,k} D_{y_{k}}^{n} + c_{d2,k} \left[ c_{h1,k+1/2} H_{x_{k+1/2}}^{n} - c_{h1,k-1/2} H_{x_{k-1/2}}^{n} \right]
\]

\[+ \gamma_{-,k} D_{x_{k-1}}^{n+1/2} - (\beta_{-,k} + \beta_{+,k}) D_{x_{k}}^{n+1/2} + \gamma_{+,k} D_{x_{k+1}}^{n+1/2},
\] (3.21)

where

\[
\beta_{\pm,k} = c_{d2,k} c_{h2,k\pm1/2} c_{e1y_{,k}},
\]

\[
\gamma_{\pm,k} = c_{d2,k} c_{h2,k\pm1/2} c_{e1y_{,k\pm1}},
\] (3.22)

For clarity, the spatial grid indexing is presented explicitly in the coefficients. This tridiagonal system can be efficiently solved in \(O(N)\) operations using the Thomas algorithm [49]. This is detailed in Appendix A. The update procedure for the first sub-step is summarized as

Step 1. Update \(D_{x_{k}}^{n+1/2}\) explicitly from Eq. (3.15)

Step 2. Update \(D_{y_{k}}^{n+1/2}\) implicitly from Eq. (3.21)

Step 3. Update \(E_{x_{k}}^{n+1/2}\) explicitly from Eq. (3.19)

Step 4. Update \(E_{y_{k}}^{n+1/2}\) explicitly from Eq. (3.20)

Step 5. Update \(H_{x_{k}}^{n+1/2}\) explicitly from Eq. (3.17)

Step 6. Update \(H_{y_{k}}^{n+1/2}\) explicitly from Eq. (3.18).

An analogous procedure follows for the second sub-step. The update equations for Maxwell’s curl equation are

\[
D_{x_{k}}^{n+1} = c_{d1} D_{x_{k}}^{n+1/2} - c_{d2} \left[ H_{y_{k+1/2}}^{n+1} - H_{y_{k-1/2}}^{n+1} \right],
\] (3.23)
\[ D_{y_k}^{n+1} = c_{d1} D_{y_k}^{n+1/2} + c_{d2} \left[ H_{x_{k+1/2}}^{n+1/2} - H_{x_{k-1/2}}^{n+1/2} \right], \quad (3.24) \]

\[ H_{x_{k+1/2}}^{n+1} = c_{h1} H_{x_{k+1/2}}^{n+1/2} + c_{h2} \left[ E_{y_{k+1}}^{n+1/2} - E_{y_{k}}^{n+1/2} \right], \quad (3.25) \]

\[ H_{y_{k+1/2}}^{n+1} = c_{h1} H_{y_{k+1/2}}^{n+1/2} - c_{h2} \left[ E_{x_{k+1}}^{n+1} - E_{y_{k}}^{n+1} \right], \quad (3.26) \]

The update equation for the constitutive equation can be written as

\[ E_{x_{k}}^{n+1} = c_{e1x} D_{x_{k}}^{n+1} + c_{e2} D_{y_{k}}^{n+1}, \quad (3.27) \]

\[ E_{y_{k}}^{n+1} = c_{e1y} D_{y_{k}}^{n+1} + c_{e2} D_{x_{k}}^{n+1}. \quad (3.28) \]

From Eq. (3.23), we see that \( D_{x_k}^{n+1} \) cannot be updated explicitly. By substituting Eq. (3.27) into Eq. (3.26) and plugging the resulting equation into Eq. (3.23), we obtain an implicit equation for \( D_{x_k}^{n+1/2} \) in a form of the tridiagonal system as follows:

\[ -\gamma_{-k} D_{x_{k-1}}^{n+1} + (1 + \beta_{-k} + \beta_{+k}) D_{x_{k}}^{n+1} - \gamma_{+k} D_{x_{k+1}}^{n+1} = \]
\[ c_{d1, k} D_{y_{k}}^{n} + c_{d2, k} \left[ c_{h1, k+1/2} H_{y_{k+1/2}}^{n+1/2} - c_{h1, k-1/2} H_{y_{k-1/2}}^{n+1/2} \right] \]
\[ + \gamma_{-k} D_{y_{k-1}}^{n+1} - (\beta_{-k} + \beta_{+k}) D_{y_{k}}^{n+1} + \gamma_{+k} D_{y_{k+1}}^{n+1}. \quad (3.29) \]

The update procedure for the second sub-step is summarized as

Step 1. Update \( D_{y_k}^{n+1} \) explicitly from Eq. (3.24)

Step 2. Update \( D_{x_k}^{n+1} \) implicitly from Eq. (3.29)

Step 3. Update \( E_{x_k}^{n+1} \) explicitly from Eq. (3.27)

Step 4. Update \( E_{y_k}^{n+1} \) explicitly from Eq. (3.28)

Step 5. Update \( H_{x_k}^{n+1} \) explicitly from Eq. (3.25)
Step 6. Update $H_{y}^{n+1}$ explicitly from Eq. (3.26).

Note that the above algorithm recovers the conventional ADI-FDTD algorithm by setting the carrier frequency $\omega_c$ zero and by using real arithmetics.

Next, we illustrate superior computational performance of the CE-ADI-FDTD algorithm over the FDTD algorithm and the ADI-FDTD algorithm. Fig. 3.4 shows the steady-state time-averaged $|E|^2$ inside the DBE PhC with $N = 16$, calculated by the FDTD simulation and the CE-ADI-FDTD simulation with various CNs. Here, CN means the Courant number [defined in Eq. (3.30)]. Because we focus on computational performance in this section, the illustration of physical mechanism underlying the DBE PhC response will be postponed until the next section. From Fig. 3.4, very good agreement is observed between FDTD and CE-ADI-FDTD results, for all the CNs considered. On the other hand, a discrepancy is observed between ADI-FDTD and FDTD results, as shown in Fig. 3.5. The ADI-FDTD results start to be compromised for CN as low as four. The ADI-FDTD results deteriorate as the CN increases because of numerical dispersion [38].

Table 3.1 summarizes the maximum value of instantaneous field intensity ($|E|_{\text{max}}^2$) inside the DBE PhC and the normalized computation time for the three methods. We notice that the maximum value of instantaneous field intensity is twice as the maximum value of time-averaged field intensity. The difference of $|E|_{\text{max}}^2$ between the CE-ADI-FDTD simulation with CN=250 and the FDTD simulation is only about 0.03%. For same CN, the computation time of the CE-ADI-FDTD simulation is longer than the ADI-FDTD simulation because the former requires complex number arithmetic. Despite the increase of computation time for same CN, the CE-ADI-FDTD algorithm reduces computation time dramatically because it allows for much
Figure 3.4: CE-ADI-FDTD results using various CNs for the steady-state time-averaged field intensity $|E|^2$ inside the DBE PhC with $N = 16$.

Figure 3.5: ADI-FDTD results using various CNs for the steady-state time-averaged field intensity $|E|^2$ inside the DBE PhC with $N = 16$. 
| Method      | CN | $|E_{\text{max}}|^2$ | CPU time |
|-------------|----|---------------------|----------|
| FDTD        | 1  | 201.9835            | 100 %    |
| ADI-FDTD    | 4  | 158.0580            | 102.59 % |
| ADI-FDTD    | 10 | 25.6795             | 41.01 %  |
| ADI-FDTD    | 100| 0.73460             | 5.67 %   |
| CE-ADI-FDTD | 100| 201.9235            | 13.01 %  |
| CE-ADI-FDTD | 250| 201.9235            | 5.25 %   |
| CE-ADI-FDTD | 1000| 200.5322           | 1.30 %   |

Table 3.1: Comparison between FDTD, ADI-FDTD, and CE-ADI-FDTD results: DBE PhC with $N = 16$.

larger time steps. For example, the CPU time of the CE-ADI-FDTD simulation with CN=250 is reduced to circa 5.25% of the FDTD simulation within 99.97% accuracy. In terms of memory requirement, the ADI-FDTD algorithm requires 27% more memory than the FDTD algorithm and the CE-ADI-FDTD algorithm requires 72% more memory than the FDTD algorithm, due mainly to complex arithmetic requirements.

Fig. 3.6 shows the error in CE-ADI-FDTD results for various CNs in the case of the DBE PhC with $N = 8$. The difference between the CE-ADI-FDTD and the FDTD results does not increase noticeably as the time step size is increased. The accuracy of CE-ADI-FDTD results is nearly invariant unless the time-step $\Delta t$ is made close to the Nyquist limit [50]. Therefore, computational time can be greatly reduced utilizing CE-ADI-FDTD simulations, since one can choose a much larger $\Delta t$.  

40
for a given accuracy versus conventional FDTD algorithm. This makes it practical to carry out the sensitivity analysis presented in Section 3.4.

### 3.3 DBE PhC Properties

We next examine the PhC response using the proposed CE-ADI-FDTD algorithm. The schematic of PhCs is shown in Fig. 3.1, where we assume $B$-layer as air. The constitutive tensor (relative) parameters for the $A$-layers are as follows

$$
\varepsilon_{A1} = \varepsilon_{A2} = 13.61,
$$

$$
\delta_{A1} = \delta_{A2} = 12.4,
$$

$$
\varphi_{A1} = 0^\circ,
$$

$$
\varphi_{A2} = 45^\circ,
$$
\[ \epsilon_{zz, A1} = \epsilon_{zz, A2} = 1, \]

\[ \mu_{r, A1} = \mu_{r, A2} = 1. \]

The dispersion curve can be determined by a combination of geometrical and materials parameters. Either the DBE dispersion curve or the RBE dispersion curve can be achieved by changing geometrical parameters, with material properties fixed. For DBE PhCs, the layer thicknesses are as follows

\[ L_{A1} = L_{A2} = 0.270545 \text{ m}, \]
\[ L_B = 0.45891 \text{ m}. \]

For RBE PhCs, the layer thicknesses are as follows

\[ L_{A1} = L_{A2} = 0.120545 \text{ m}, \]
\[ L_B = 0.75891 \text{ m}. \]

This choice yields the angular frequency of the first resonance near \( c_0 \text{ rad/s} \) for DBE PhCs and 1.6\( c_0 \) rad/s for RBE PhCs, respectively, where \( c_0 \) is the numerical value of vacuum light speed in m/s. The excitation is a raised-cosine-ramped sine wave [51] with unit peak amplitude whose carrier angular frequency \( \omega_c \) corresponds to the first Fabry-Perot resonance. The space step is \( \Delta z = 1/400 \text{ m} \), multiplied by different \( \kappa \) factors inside each layer to match the respective thicknesses. We choose \( \kappa_{A1} = \kappa_{A2} = 0.270545/0.27 \) and \( \kappa_B = 0.45891/0.46 \) for the DBE PhC simulations here. The time step size is given by

\[ \Delta t = C N \kappa_B \Delta z / c_0, \quad (3.30) \]
Figure 3.7: Steady-state time-averaged field intensity $|E|^2$ inside a PhC with $N = 8$, under a sine-wave excitation with unit amplitude.

where CN is the Courant number. A Courant number CN=250 is used unless specified otherwise.

First, we analyze a DBE PhC with $N = 8$. Fig. 3.7 shows the steady-state time-averaged field intensity $|E|^2$ inside this finite-stack DBE PhC. The incident field has unit amplitude. The layer configuration is also displayed for DBE PhCs. Note that the field distribution has sharp variations inside the DBE PhC, which illustrates the need for a very fine mesh resolution. For comparison, we also show the results for a RBE PhC with $N = 8$. The field intensity in the DBE PhC is about twice that of the RBE PhC.

Fig. 3.8 shows the steady-state time-averaged field intensity $|E|^2$ inside the DBE PhC with $N = 16$ and that inside the RBE PhC with $N = 16$. As illustrated in Fig. 3.3, the resonance bandwidth in this case is narrower than with $N = 8$, but the
resonance closer to the band edge. The gigantic enhancement in the field intensity inside the DBE PhC is clearly visible, with the field intensity ratio of the DBE PhC to the RBE PhC being about five.

We next consider the analysis of a DBE PhC with $N = 32$. From convergence tests, it is determined that simulations with $\Delta z = 1/400$ m cannot accurately analyze a DBE PhC that long. In this case, $\Delta z = 1/1600$ m is required to capture even sharper field distributions. To make the matter worse, longer time integration times should be employed to obtain the necessary frequency resolution given the narrower Fabry-Perot resonance with $N = 32$. Those two requirements — very small $\Delta z$ and long integration times — make it very challenging to simulate DBE PhCs with $N = 32$.

We mention that it would not be practical to simulate this DBE PhC by either the FDTD method or the ADI-FDTD method under our available computing resources. For analysis of the DBE PhC with $N = 32$, the CE-ADI-FDTD simulation with
Figure 3.9: Steady-state time-averaged field intensity $|E|^2$ inside a PhC with $N = 32$, under a sine-wave excitation with unit amplitude.

CN=500 is employed. Fig. 3.9 shows the steady-state time-averaged $|E|^2$ inside the DBE PhC with $N = 32$ and that inside the RBE PhC with $N = 32$, illustrating the great difference in the intensity increase. A curve fit for these examples indicates that the peak field intensity is proportional to about $N^{3.8}$ for DBE PhCs and $N^{1.9}$ for RBE PhCs.

Next, we employ a sine-wave modulated Gaussian pulse to illustrate the impact of the FBW on field enhancement effects. In this case, CN=50 is employed. Fig. 3.10 and Fig. 3.11 show the maximum field intensity $|E|_{max}^2$ inside the DBE PhC with $N = 8$ and that inside the DBE PhC with $N = 16$, respectively. As the FBW increases, the enhancement in the field intensity decreases. Narrower transmittance bandwidth of the Fabry-Perot resonance for $N = 16$ versus $N = 8$ leads to a greater impact of the fractional bandwidth on field enhancement effects (see Fig. 3.3).
Figure 3.10: Maximum field intensity $|E|_{\text{max}}^2$ inside the DBE PhC with $N = 8$ under sine-wave modulated Gaussian pulse excitations. Here, FBW=0% means a sine-wave excitation (without Gaussian pulse modulation).

Figure 3.11: Same as Fig. 3.10 for the DBE PhC with $N = 16$. 
3.4 Sensitivity Analysis

Next, we illustrate the effects of grounding, layer thickness perturbations, and anisotropic dielectric losses on the DBE PhC response. In what follows, the time-domain excitation is again a raised-cosine-ramped sine wave.

3.4.1 Ground Plane Effects

We illustrate ground plane effects on the DBE PhC response. The ground plane is on the far end of the DBE PhC. We assume the ground plane to be a perfect electric conductor (PEC). Fig. 3.12 shows the steady-state time-averaged $|E|^2$ inside the PEC-backed DBE PhC with $N = 8$, showing an approximately five-fold increase in the field intensity compared to the case with no ground plane. We note that the spatial distributions in field intensity are not symmetric anymore. We also examine the effects of the ground plane on the DBE PhC with $N = 16$ and $N = 32$. A similar increase of the field intensity and non-symmetric field intensity distributions result from including a ground plane, as shown in Fig. 3.13 and Fig. 3.14. The peak intensity increase due to the ground plane is of 5.63, 4.03, and 4.04 for $N = 8$, $N = 16$, and $N = 32$, respectively. The increase in the field intensity can be attributed to (higher) resonance frequencies closer to the DBE frequency, thus having slower group velocity.

3.4.2 Layer Thickness Perturbations

Next, we assess the sensitivity of PhC responses to layer thickness perturbations. For this purpose, we randomly perturb the thickness of all cells, for the PhC with $N = 16$. The thickness of each cell is assumed to be a (independent) Gaussian random
Figure 3.12: Ground plane effect on the response of the DBE PhC with $N = 8$.

Figure 3.13: Ground plane effect on the response of the DBE PhC with $N = 16$. 
Figure 3.14: Ground plane effect on the response of the DBE PhC with \( N = 32 \).

Figure 3.15: Effect of layer thickness perturbations on the response of the DBE PhC with \( N = 16 \).
Figure 3.16: Effect of layer thickness perturbations on the response of the RBE PhC with $N = 16$.

variable centered on the nominal thickness. For each variance, an ensemble with 12 realizations is considered. Fig. 3.15 shows the steady-state time-averaged $|E|^2$ inside the DBE PhC with the perturbed layer thickness. As can be seen from this figure, small variations in the layer thickness can have a strong impact on the DBE PhC performance (due to the sensitivity of Fabry-Perot resonance to geometrical parameters). Fig. 3.16 shows the steady-state time-averaged $|E|^2$ inside the RBE PhC with the same thickness perturbations. It is observed that the RBE PhC is less sensitive to the layer thickness perturbations compared to the DBE PhC. Fig. 3.17 displays the peak value of $|E|^2$ inside the DBE PhC and the RBE PhC under various layer thickness perturbations and PhC sizes. The DBE PhC with $N = 16$ produces less enhancement in the field intensity than the RBE PhC with $N = 16$ when the layer thickness is perturbed by about 0.3%. We also display the peak value of $|E|^2$ inside the RBE PhC with $N=38$ (which has a similar performance in terms of intensity
0.005 0.01 0.05 0.1 0.5 1

Standard Deviation of Layer Thickness (%)

|E|^2

DBE PhC with N=16
RBE PhC with N=16
RBE PhC with N=38

Figure 3.17: Peak value of |E|^2 inside PhCs with layer thickness perturbations. The dashed lines indicate nonperturbed PhC results.

increase to the DBE PhC with N = 16). As shown in Fig. 3.17, the DBE PhC with N = 16 is similarly sensitive to the considered layer thickness perturbations as the RBE PhC with N=38, with the former yielding a little bit smaller field intensity. Table 3.4.2 summarizes the peak value of field intensity under considered layer thickness perturbations.

3.4.3 Anisotropic Dielectric Losses

For DBE PhCs with dielectric losses, we extended the CE-ADI-FDTD algorithm to general lossy anisotropic dielectrics. Details on the algorithm can be found in Ref. [52]. The sensitivity of the PhC response to dielectric losses in the A-layers is illustrated in Fig. 3.18, where a loss tangent of 10^{-4} produces a 60% decrease in the peak field intensity in the DBE PhC and a 10% decrease in the peak field intensity in the RBE PhC, for the same number of N = 16 layers. Note how the DBE PhC with
<table>
<thead>
<tr>
<th>Perturbations</th>
<th>DBE ($N = 16$)</th>
<th>RBE ($N = 16$)</th>
<th>RBE ($N = 38$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.005 %</td>
<td>98.5167</td>
<td>17.6172</td>
<td>99.7660</td>
</tr>
<tr>
<td>0.01 %</td>
<td>85.8719</td>
<td>17.5628</td>
<td>96.7120</td>
</tr>
<tr>
<td>0.05 %</td>
<td>31.4252</td>
<td>17.2379</td>
<td>37.4918</td>
</tr>
<tr>
<td>0.1 %</td>
<td>25.0403</td>
<td>16.4865</td>
<td>31.6033</td>
</tr>
<tr>
<td>0.5 %</td>
<td>1.8743</td>
<td>7.1981</td>
<td>3.1802</td>
</tr>
<tr>
<td>1 %</td>
<td>1.6433</td>
<td>3.7178</td>
<td>2.3190</td>
</tr>
</tbody>
</table>

Table 3.2: Field intensity under layer thickness perturbations.

$N = 16$ shows a very similar sensitivity curve as the RBE PhC with $N=38$. It should be further noted that dielectric losses change the resonance peak frequency somewhat, as shown in Fig. 3.19. Therefore, the results presented in Fig. 3.18 also include any detuning effect in Fabry-Perot resonances produced by the dielectric losses, since the frequency of the excitation signal is kept constant.

### 3.5 Concluding Remarks

A full-wave CE-ADI-FDTD algorithm has been developed to anisotropic media based on the D-H-E formulation to decouple the update of the constitutive equations from the update of the Maxwell’s curl equations written in terms of (complex) field envelopes. The CE-ADI-FDTD algorithm is advantageous over both conventional FDTD algorithm and ADI-FDTD algorithm for the analysis of DBE PhCs, with a dramatic reduction on the overall computation time being achieved. Contrary to the traditional ADI-FDTD method, the numerical dispersion error of the CE-ADI-FDTD
Figure 3.18: Peak value of $|E|^2$ inside PhCs with losses in $A$-layers. The dashed lines indicate lossless PhC results.

Figure 3.19: Effect of dielectric losses on the first Fabry-Perot resonance of the DBE PhC with $N = 16$. 

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method for narrowband problems remains small unless the time step size approaches the Nyquist limit.

Using the extended CE-ADI-FDTD algorithm, we examined the EM response of finite-stack DBE PhCs. The gigantic amplitude increase produced by Fabry-Perot resonances was contrasted to similar effects yielded by RBE PhCs. The numerical analysis has shown that the field intensity inside DBE PhCs increases approximately as $N^{3.8}$, where $N$ is the number of unit cells. It has been observed that a ground plane can boost the field intensity inside DBE PhCs. In particular, the peak field intensity inside DBE PhCs with $N = 8$ and $N = 16$, and backed by ground planes, is about 5.6 and 4 times larger, respectively, than the peak field intensity inside DBE PhCs with equal lengths.

We have performed a sensitivity analysis of DBE PhC responses under perturbations on geometrical and material parameters, and compared the impact of these perturbations on DBE and RBE PhC responses. As expected, the field intensity enhancement in DBE PhCs deteriorates under small perturbations of the layer thickness. On the other hand, the overall response is quite robust to the presence of dielectric losses. For the DBE PhC with $N = 16$, a loss tangent of $10^{-5}$ decrease the peak intensity by only about 10%.
CHAPTER 4

PHOTONIC CRYSTALS WITH A SPLIT BAND EDGE (SBE)

4.1 Introduction

In the previous chapter, we pointed out that PhCs made up of one isotropic layer and two misaligned anisotropic dielectric layers in each period can yield the DBE on the band diagram, with a quartic dispersion relation just below the band edge frequency $\omega_b$. Finite-size DBE PhCs yield good transmittance and a dramatic increase in the field intensity due to the interplay of vanishing group velocity near $\omega_b$ and good transmittance at the Fabry-Perot resonances close to $\omega_b$. The transmittance of DBE PhCs, however, depends on the polarization of incident waves. DBE PhCs support a reciprocal pair of propagating Bloch modes and a reciprocal pair of evanescent Bloch modes in vicinity of the band edge frequency $\omega_b$. Therefore, one (elliptical) polarization component of incident waves is matched to propagating (real wavenumber) modes and well coupled into the DBE PhCs. The other (elliptical) polarization component is only matched to evanescent (imaginary wavenumber) modes and reflected back.
To circumvent this problem while maintaining slow-wave Fabry-Perot resonances, new dispersion-engineered periodic stacks — referred to as split band edge (SBE) PhCs — have been proposed [53]. The unit cell of SBE PhCs is configured same as that of DBE PhCs, viz. one isotropic layer and two misaligned anisotropic dielectric layers. The dispersion relation $\omega(k)$ in SBE PhCs can be approximated by a sum of a quadratic term and a quartic term. In vicinity of the SBE frequency, all four (two reciprocal pairs) Bloch modes are propagating and thus good impedance matching (transmittance) is possible regardless of polarization of incident waves. In addition, for a given number of cells, it has been shown that SBE PhCs can produce stronger resonant transmissions than DBE PhCs, since transmission resonances in SBE PhCs can move closer to band edges [54].

In this chapter, we examine the behavior of the transmittance and field enhancement effects in SBE PhCs as a function of the incident wave polarization and contrast it against the DBE PhC performance. We also perform a sensitivity analysis of the SBE PhC response with respect to geometrical and material perturbations. Since the periodicity is broken in those cases, full-wave numerical techniques for solving transient Maxwell’s equations in general anisotropic media are employed. In Chapter 3, we have demonstrated the accuracy and computational suitability of the CE-ADI-FDTD algorithm for anisotropic media because of its unconditional stability (free from the Courant stability limit) and low grid-dispersion error near to the carrier frequency. Therefore, we employ the extended CE-ADI-FDTD algorithm described in Chapter 3 to analyze the SBE PhC response.
4.2 Dispersion Characteristics of SBE PhCs

Just below \( \omega_b \), the dispersion curve of the SBE is approximated as [53]

\[
\nu_{SBE}(\kappa) \approx \frac{a}{2} \kappa^2 + \frac{b}{4} \kappa^4,
\]

(4.1)

with \( \kappa = |k - k_0|L \) and \( \nu(\kappa) = [\omega(k) - \omega(k_0)]L/c_0 \), where \( k_0 \) indicates a stationary point, i.e., 0 or \( \pi/L \). Here, \( k \) and \( \omega \) are the Bloch wavenumber and the angular frequency, respectively. \( L \) is the unit cell length and \( c_0 \) is speed of light in vacuum. On the other hand, for RBE and DBE PhCs we have

\[
\nu_{RBE}(\kappa) \approx \frac{a}{2} \kappa^2,
\]

(4.2)

\[
\nu_{DBE}(\kappa) \approx \frac{b}{4} \kappa^4,
\]

(4.3)

respectively as described in Eq. (3.1) and Eq. (3.2).

A key condition for SBE behavior is

\[
a/b < 0,
\]

(4.4)

so that its dispersion curve has both concave and convex regions. In addition, the dispersion curve should satisfy the following (proximity) condition:

\[
|a/b| \ll 1.
\]

(4.5)

The above is required for gigantic field intensity enhancement as present in DBE PhCs \((a = 0)\).

For the design of a SBE PhC, we modify the DBE PhC considered in Chapter 3. As described in the previous chapter, the constitutive tensor (relative) parameters of the DBE PhC are: \( \epsilon_{A1} = \epsilon_{A2} = 13.61; \delta_{A1} = \delta_{A2} = 12.4; \phi_{A1} = 0^\circ, \phi_{A2} = 45^\circ; \mu_{r,A1} \)
Figure 4.1: Changes in the dispersion curve $\omega(k)$ by adjusting the misalignment angle $\phi_{A2}$ of $A_2$-layer.

$\mu_{r,A2} = 1$. The layer thicknesses are: $L_{A1} = L_{A2} = 0.270545$ m and $L_B = 0.45891$ m. We modify the above PhC by changing $\phi_{A2}$ while keeping the other parameters fixed. Such a change in $\phi_{A2}$ is not the sole route to achieve a dispersion curve with SBE since the latter is determined by a combination of geometrical and material parameters. As shown in Fig. 4.1, a decrease in $\phi_{A2}$ develops a SBE in the dispersion curve. On the other hand, an increase in $\phi_{A2}$ makes the dispersion relation develop a RBE. We consider two cases: $\phi_{A2} = 15^\circ$ and $\phi_{A2} = 35^\circ$. The dispersion curves of these cases can be fitted to the relation in Eq. (4.1). From Fig. 4.2 and Fig. 4.3, we have $a = 0.2486$ and $b = -0.1635$ for the former and $a = 0.0899$ and $b = -0.2163$ for the latter. Although both PhCs satisfy the condition in Eq. (4.4), only the latter satisfies the DBE proximity condition in Eq. (4.5). Hence, we consider $\phi_{A2} = 35^\circ$ in what follows. We note that there is a tradeoff between the DBE proximity condition and the SBE frequency range (i.e., the frequency range in which all four Bloch modes
propagate). As a dispersion curve deviates from the DBE (in this study: as $\phi_{A2}$ decreases), it yields a wider SBE frequency range but with more deviation from the proximity condition.

In general, the impedance mismatch gets worse as the frequency of operation approaches $\omega_b$ for a semi-infinite periodic stack. As pointed out in Chapter 3, good matching (transmittance) can be achieved by exploiting Fabry-Perot resonances associated with finite-size periodic stacks. As the number $N$ of unit cells increases, the Fabry-Perot resonance frequencies move closer to the band edge frequency and thus EM waves can propagate extremely slowly inside the crystal while maintaining good transmittance. For DBE PhCs, the choice of $N$ may be arbitrary once all other application-specific criteria (overall physical size, operating frequency, quality factor, etc.) are met. For SBE PhCs, however, $N$ should be judiciously chosen so that SBE PhCs operate at the double SBE resonance condition, viz. the condition for two

Figure 4.2: Curve fit for the PhC with $\phi_{A2} = 15^\circ$. 

\[ f(\kappa)=\frac{a}{2} \kappa^2 + \frac{b}{4} \kappa^4 \]

\[ a=0.2486 \]

\[ b=-0.1635 \]
cavity resonances (associated with two reciprocal pairs of propagating Bloch modes) occurring at the same (or nearly the same) frequency, as pointed out in Ref. [53]. Numerical examples will be provided in the next section to illustrate this point.

### 4.3 Polarization Dependence

We illustrate the transmittance of the SBE PhC versus $N$ under various incident wave polarizations in Fig. 4.4-Fig. 4.6. From these figures, it is observed that the SBE PhC with $N = 11$ leads to the polarization-independent perfect transmittance at the Fabry-Perot resonance, implying that the double SBE resonance condition is satisfied. Hence, any incident wave regardless of the polarization can be perfectly coupled into the SBE PhC with $N = 11$ at the Fabry-Perot resonance. By comparison, we illustrate the effect of polarization on transmittance in the DBE PhC with $N = 11$ in Fig. 4.7. Transmittance of the DBE PhC is highly dependent on polarization. The incident
wave with $y$ polarization is mostly coupled into the DBE PhC but the incident wave with $x$ polarization is mostly reflected back. In fact, this polarization dependence exists for DBE PhCs with any $N$.

Next, we examine the field intensity inside the SBE PhC with $N = 11$ at the Fabry-Perot resonance under the same polarization as considered previously. Fig. 4.8 shows the steady-state time-averaged field intensity $|E|^2$ inside the SBE PhC when the incident wave has unit amplitude. The SBE PhC produces gigantic field enhancement for all polarizations, although the magnitude of field intensity depends on the particular polarization. The field intensity distribution inside the SBE PhC results from the field due to two pairs of propagating Bloch modes. Each propagating pair is matched to each polarization but their group velocities (hence, the field enhancement effects) are different. The relative contribution of each Bloch mode is dictated by the incident wave polarization, which explains why the field intensity depends on
Figure 4.5: Transmittance of the SBE PhC with $N = 11$ under various polarization.

Figure 4.6: Transmittance of the SBE PhC with $N = 13$ under various polarization.
the polarization in spite of the polarization-independent perfect transmittance. By comparison, the DBE PhC with $N = 11$ is also considered in Fig. 4.9. The field intensity inside the DBE PhC under $x$ polarization is very small, since a large portion of incident wave is not coupled into the PhC but reflected back. However, a dramatic increase in field intensity is observed for $y$ polarization due to good transmittance in that case.

### 4.4 Sensitivity Analysis

Next, we illustrate the sensitivity of the SBE PhC response against geometrical and material perturbations. The field intensity enhancement effects under $y$ polarization are investigated and a contrast between SBE and DBE PhC responses is made. We consider four different perturbations: (i) anisotropic dielectric losses, (ii) layer
Figure 4.8: Steady-state time-averaged field intensity $|\mathbf{E}|^2$ inside the SBE PhC with $N = 11$, for an incident wave with unit amplitude.

Figure 4.9: Steady-state time-averaged field intensity $|\mathbf{E}|^2$ inside the DBE PhC with $N = 11$, for an incident wave with unit amplitude.
thickness perturbations, (iii) misalignment angle perturbations, and (iv) simultaneous perturbations on layer thickness and misalignment angle.

4.4.1 Anisotropic Dielectric Losses

We investigate the variation on the field intensity distribution inside the SBE PhC when dielectric losses are present in the anisotropic dielectric layers. Fig. 4.10 and Fig. 4.11 show the steady-state time-averaged $|E|^2$ inside the SBE PhC with $N = 11$ and the DBE PhC with $N = 11$, respectively. Note the order of magnitude difference in the dielectric losses considered in these two figures (cf. the indicated loss tangents). The effect of losses on the field intensity is more pronounced for the SBE PhC than the DBE PhC, while the absolute intensity enhancements in the SBE PhC are still higher than in the DBE PhC when the loss tangent is below $10^{-4}$. 
The relative field distribution in the SBE PhC changes as dielectric losses increase. On the other hand, the relative field distribution in the DBE PhC is mostly preserved, despite the decrease in magnitude. The change in the relative field distribution of the SBE PhC follows from the fact that the sensitivities of the two reciprocal Bloch mode pairs against dielectric losses are different. As alluded before, the SBE PhC response results from a superposition of (quadratic dispersion) RBE- and (quartic dispersion) DBE-related responses. As pointed out in Chapter 3, RBE responses are more robust than DBE responses against losses. Therefore, for SBE PhCs with higher losses, the RBE contribution becomes progressively more dominant, which alters the relative field distribution.

Fig. 4.12 shows the peak value of $|E|^2$ inside PhCs with losses. The DBE PhC with $N = 15$ is also included in this case, since this DBE PhC yields field enhancement effects similar to the considered SBE PhC when lossless. Comparing the SBE PhC
Figure 4.12: Peak value of $|E|^2$ inside lossy PhCs. Lossless PhC results are also displayed by dashed lines.

$N = 11$ and the DBE PhC $N = 15$ results, dielectric losses show stronger influence on SBE than DBE responses for low loss, but the reverse is true for high loss.

### 4.4.2 Layer Thickness Perturbations

Next, we examine the effect of layer thickness perturbations on the PhC response. For this purpose, we first assume the thickness of each cell to be an independent Gaussian random variable, centered on the nominal thickness. This kind of perturbation is expected from manufacturing tolerances during fabrication. The results for the peak value of $|E|^2$ inside the PhCs are shown in Fig. 4.13. For each variance, an ensemble with 12 realizations is considered and the average result is taken. As the deviation in the layer thickness increases, the field intensity in the PhCs progressively decreases, as expected.
Figure 4.13: Peak value of $|E|^2$ inside PhCs with all-layer thickness perturbations. The dashed lines indicate nonperturbed PhC results, for reference. Each cell thickness is assumed to be an independent Gaussian random variable with mean at the nominal thickness value.

Figure 4.14: Peak value of $|E|^2$ inside PhCs with all-layer thickness perturbations. In this case, the thickness of each cell is uniformly perturbed (systematic perturbation).
Next, the thickness of all cells is perturbed uniformly (systematic perturbation). This kind of perturbation is expected from calibration tolerances during fabrication. Fig. 4.14 shows the peak value of $|E|^2$ inside PhCs with perturbed layer thicknesses. It is seen that small variations in the layer thickness have a stronger impact on the SBE PhC performance than the DBE PhC performance. However, a more pronounced effect is observed on DBE than SBE for large perturbations. When the layer thickness is perturbed by 0.1%, the SBE PhC produces greater field intensity enhancement than either of the DBE PhCs considered ($N = 11, 15$). Field enhancement effects, however, are not observed for PhCs with above 1% error in the layer thickness because almost no incident power is coupled into the PhC in this case. Comparing Fig. 4.13 and Fig. 4.14, we also observe that systematic perturbations on the layer thickness have a more pronounced effect on PhC responses than random perturbations.
Figure 4.16: Effect of layer thickness perturbations on the Fabry-Perot resonance frequency for the DBE PhC with $N = 11$. The vertical dashed line indicates the original operating (resonance) frequency for the nonperturbed PhC.

Figure 4.17: Effect of layer thickness perturbations on the Fabry-Perot resonance frequency for the DBE PhC with $N = 15$. The vertical dashed line indicates the original operating (resonance) frequency for the nonperturbed PhC.
Table 4.1: Peak value of field intensity inside PhCs with misalignment angle perturbations.

<table>
<thead>
<tr>
<th>√Var(φₐ)</th>
<th>SBE, N = 11</th>
<th>DBE, N = 11</th>
<th>DBE, N = 15</th>
</tr>
</thead>
<tbody>
<tr>
<td>0°</td>
<td>78.38</td>
<td>24.74</td>
<td>79.60</td>
</tr>
<tr>
<td>0.25°</td>
<td>17.37</td>
<td>13.40</td>
<td>10.58</td>
</tr>
<tr>
<td>0.5°</td>
<td>10.36</td>
<td>8.93</td>
<td>3.26</td>
</tr>
<tr>
<td>0.75°</td>
<td>8.12</td>
<td>4.49</td>
<td>2.72</td>
</tr>
<tr>
<td>1°</td>
<td>5.39</td>
<td>4.09</td>
<td>2.03</td>
</tr>
<tr>
<td>2°</td>
<td>4.62</td>
<td>3.30</td>
<td>1.71</td>
</tr>
<tr>
<td>3°</td>
<td>2.73</td>
<td>2.25</td>
<td>1.62</td>
</tr>
</tbody>
</table>

We evaluate the transmittance τ versus layer thickness perturbations in Fig. 4.15-Fig. 4.17. As the layer thickness is perturbed, the resonance frequency is shifted to lower frequencies, leading to a poor impedance matching at the original operating frequency (resonance). It is observed that for 0.1% perturbation, τ ∼ 0.5 for the SBE PhC with N = 11, τ ∼ 0.1 for the DBE PhC with N = 11, and τ ∼ 0 the DBE PhC with N = 15. For large perturbations (above 1%), however, none of the PhCs provide good matching. Hence, the enhancement in the field intensity is not observed for the 0.5% or 1% perturbations, as illustrated in Fig. 4.14.

4.4.3 Misalignment Angle Perturbations

To illustrate the effect of orientation misalignments of the A-layers, we randomly perturb the orientation angles of A-layers. The misalignment angles are treated as independent Gaussian random variables. For each variance, an ensemble with 12
Figure 4.18: Effect of simultaneous random perturbations of layer thickness and misalignment angle on the field intensity for the SBE PhC with $N = 11$. In the legend, $\delta L$ denotes the standard deviation of the layer thickness. The curve $\delta L = 0$ indicates the result with misalignment angle perturbation only.

realizations is again used. Table 4.1 summarizes the peak value of $|E|^2$ inside PhCs under such perturbations. We note that the SBE PhC with $N = 11$ yields more field enhancement effects than DBE PhCs for the perturbations considered. For the SBE PhC with $N = 11$ and the DBE PhC with $N = 15$, the field intensity drops quickly under for $0.25^\circ$ standard deviation in the misalignment angle but decreases more gradually under higher deviations. The DBE PhC with $N = 11$ is considerably less sensitive to angle perturbations than the DBE PhC with $N = 15$.

4.4.4 Interplay of Layer Thickness and Misalignment Angle Perturbations

Finally, we assess the sensitivity of the SBE PhC response to simultaneous perturbations on the layer thickness and misalignment angle. We assume both layer
thickness and misalignment angle to be independent (each) Gaussian random variable centered on the nominal values. Fig. 4.18 shows the peak value of $|E|^2$ inside the SBE PhC with $N = 11$ under thickness and misalignment angle perturbations. For comparison, we also include SBE PhC responses for misalignment angle perturbations only. For standard deviations above $0.25^\circ$, the effect of misalignment angle errors dominates the overall degradation in response, for the layer perturbations considered.

4.5 Concluding Remarks

We have examined the transmittance behavior and field enhancement effects in finite-size periodic stacks of anisotropic layers with SBE characteristics supporting slow-wave Fabry-Perot resonances. We have contrasted the response of SBE PhCs with that of DBE PhCs. A sensitivity analysis was carried out to examine the effect of geometrical and material parameters, and the impact of these perturbations on SBE and DBE PhC responses was illustrated. In particular, we have examined the sensitivity of PhC responses to dielectric losses, layer thickness perturbations, and misalignment angle perturbations (the latter two both in isolation and combined). As expected, all above imperfections lead to a decrease in field intensity enhancement effects, for both SBE and DBE PhCs. The effect of small perturbations is in general more pronounced for SBE PhCs than for DBE PhCs, while the reverse is true for larger perturbations. For the perturbation ranges considered, it has been observed that the SBE PhC response is more sensitive to misalignment angle perturbations than layer thickness perturbations when those are considered simultaneously.
CHAPTER 5

NANORING-BASED PLASMON WAVEGUIDES

5.1 Introduction

Due to the classical diffraction limit, conventional optical devices such as dielectric waveguides have large transverse dimensions compared to the complementary metal oxide semiconductor (CMOS) scale and thus leading to an inherent dimension mismatch for optical/CMOS integration [11]. The bending loss of conventional dielectric waveguides is quite large at any sharp transitions. As a result, large curvatures are necessary, leading to a further increase in the minimum size of the optical structures. Therefore, the development of subwavelength integrated optical devices are of fundamental importance for the solution of this size incompatibility.

Surface plasmon resonances supported by plasmon structures lead to unusually localized field enhancement at the metal-dielectric interfaces. EM fields can be guided along nanoscale metallic structures with lateral confinement below the diffraction limit [55,56]. Therefore, plasmonics [11,57–59], an emerging area of researches on the interaction between light and metallic nanostructures, can open a new avenue for truly nanoscale optical devices. Apart from the optical/electronic device integration alluded
above, plasmon structures have a wide range of potential applications such as surface-enhanced Raman spectroscopy (SERS) [60, 61], near-field optical microscopy [62, 63], more recently, biosensors [64, 65]. For the latter, the ability to sense a surrounding material is based on the high dependence of surface plasmon resonance on optical properties of the dielectric background media around metallic nanoparticles.

An ordered array of metallic nanoparticles has attracted much interest for the application of subwavelength guiding structures [57, 67–78]. When EM fields penetrate metallic nanoparticles, localized surface plasmon resonances (LSPRs) are excited at the metal/dielectric interfaces, and then EM fields are guided along an ordered array of metallic nanoparticles below the diffraction limit via near-field coupling between closely spaced nanoparticles. As a result, truly nanoscale optical waveguides can be constructed by employing an array of metallic nanoparticles. Most previous works have considered nanoparticle-based plasmon waveguides operating at the UV or visible spectrum.

In this chapter, we design and investigate plasmon waveguides to operate at wavelengths $\lambda_0 \sim 1550$ nm (optical communication band), based on an array of metallic nanoparticles [79]. The LSPR must be red-shifted in order to make plasmon waveguides possible at 1550 nm. Previous works have shown that the optical response of metallic nanoparticles depends on the size and shape of particles and surrounding materials [9, 65]. Using the quasi-static approximation (Rayleigh theory) [80], it is easy to show that, in order to provide the LSPR near 1550 nm, Au (gold) nanospheres must be surrounded by a host medium with relative permittivity as high as 55, which is not practical. Therefore, better candidates should be sought among nanoparticles
with extra DoF in their geometry, such as nanodisks and nanorings. In the former case, the plasmon resonance can be further tuned by modifying the ratio of the longest axis (diameter) to the shortest axis (height) or by changing the radial thickness. Our numerical modeling has shown that the LSPR at $\lambda_0 = 1550$ nm occurs for Au nanodisks with 340 nm diameter and 35 nm height in SiO$_2$ host.

Compared to nanodisks, nanorings allow for a further size reduction and enhanced tunability. The LSPR in nanorings can be tuned by changing (i.) the radial thickness, (ii.) the outer diameter, or (iii.) the height. The EM coupling between the inner and outer ring surfaces plays an important role in optical plasmon resonance in nanorings [81–85], similarly to nanoshells [86–90].

The FDTD method is suited for modeling of plasmon resonances and energy transport in chains of nanoparticles because of its geometrical flexibility and matrix-free (explicit update) nature. The FDTD method has been successfully employed to analyze a variety of structures including nanospheres [73, 74, 91], nanoellipsoids [73], nanorods [92], nanocylinders [93], nanocubes [94], nanoholes [95], and nanoshells [86]. In particular, Maier et al [73] successfully applied the FDTD method to calculate nanosphere-based plasmon waveguide characteristics such as transmission loss and group velocity.

### 5.2 CFS-PML-FDTD Algorithm for Plasmon Nanostructures

As will be pointed out in Chapter 7, the multispecies Drude-Lorentz dispersion model (rather than monospecies Drude only) becomes necessary for Au plasmon structures when the wavelength range of interest is below 700 nm due to interband transitions. However, we use the monospecies Drude model in this study, because the
prescribed wavelength range is out of the wavelength range influenced by interband transitions. At the wavelengths of interest (\(\lambda_0 \sim 1550 \text{ nm}\)), the (complex) relative permittivity of Au is described by the monospecies Drude dispersion model given by

\[
\epsilon_r(\omega) = \epsilon_\infty + \frac{\omega_D^2}{j\omega(\Gamma_D + j\omega)},
\]

where \(\omega_D\) is the plasma frequency and \(\Gamma_D\) is the damping coefficient, with \(\epsilon_\infty = 9.5\), \(\omega_D = 13.6033 \times 10^{15} \text{ rad/s}\), and \(\Gamma_D = 10.5026 \times 10^{13} \text{ rad/s}\) [86, 96].

By introducing equivalent Drude current \(J_D\) in Maxwell’s equations, we obtain the governing equations as follows

\[
\frac{\mu_0}{\epsilon_0} \frac{\partial H}{\partial t} = -\nabla \times E,
\]

\[
\epsilon_0 \epsilon_\infty \frac{\partial E}{\partial t} + J_D = \nabla \times H,
\]

\[
\frac{\partial J_D}{\partial t} + \Gamma_D J_D = \epsilon_0 \omega_D^2 E.
\]

Using the central difference scheme in the time domain, we have the following update equations:

\[
H_n^{1/2} = H_n^{-1/2} - \frac{\Delta t}{\mu_0} \nabla \times E^n,
\]

\[
E^{n+1} = E^n + \frac{\Delta t}{\epsilon_0 \epsilon_\infty} \nabla \times H^{n+1/2} - \frac{\Delta t}{2\epsilon_0 \epsilon_\infty} (J^{n+1} + J^n),
\]

\[
J_D^{n+1} = c_D1 J_D^n + c_D2 (E^{n+1} + E^n),
\]

where

\[
c_D1 = \frac{1 - \alpha_D}{1 + \alpha_D},
\]

\[
c_D2 = \frac{0.5 \Delta t \epsilon_0 \omega_D^2}{1 + \alpha_D},
\]

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and $\alpha_D = 0.5 \Gamma_D \Delta t$.

Plugging Eq. (5.7) into Eq. (5.6), we have

$$E^{n+1} = C_a E^n + C_b \nabla \times H^{n+1/2} + C_c J^n. \quad (5.8)$$

Here, the coefficients are expressed as

$$C_a = \frac{\beta_e - c_{D2}}{\beta_e + c_{D2}},$$
$$C_b = \frac{2}{\beta_e + c_{D2}},$$
$$C_c = \frac{1 + c_{D2}}{\beta_e + c_{D2}},$$

and $\beta_e = 2\varepsilon_0 \varepsilon_\infty / \Delta t$. We note that the coefficients $(c_{D1}, c_{D2}, C_a, C_b, and C_c)$ are different from those in Chapter 7. Final update equations can be obtained by employing the central difference scheme to the nabla operator. The update procedure is summarized as

Step 1. Update $H$ from Eq. (5.5)

Step 2. Update $E$ from Eq. (5.8)

Step 3. Update $J_D$ from Eq. (5.7).

To minimize spurious reflections from the outer boundary of the computational domain, CFS-PML is utilized. For the PML implementation, we use a modified nabla operator with complex stretching variables [19, 20]:

$$\nabla \longrightarrow \tilde{\nabla} = \hat{x} \frac{1}{s_x} \frac{\partial}{\partial x} + \hat{y} \frac{1}{s_y} \frac{\partial}{\partial y} + \hat{z} \frac{1}{s_z} \frac{\partial}{\partial z}, \quad (5.9)$$

where a CFS stretching [21–23] is utilized so that

$$s_\xi = \kappa_\xi + \frac{\sigma_\xi}{\nu_\xi + j\omega \varepsilon_0}, \quad (5.10)$$
where $\xi = x, y, z$.

In all simulations, we use a mesh cell size of 2.5 nm and Courant factor of 0.95. We note that the refractive index of SiO$_2$ deviates from the nominal value within 1% in the wavelength range between 590 nm and 2500 nm [97]. Hence, we use the nominal value 1.444 in all simulations.

5.3 Plasmon Resonances of Isolated Au Nanoring in SiO$_2$ Host

We first consider the optical resonance properties of an isolated Au nanoring as depicted in Fig. 5.1. Fig. 5.1 shows the basic geometrical parameters: metallic thickness $t$, inner/core diameter $D_i$, outer diameter $D$, and height $H$. The Au nanoring is surrounded by SiO$_2$ (in the core, substrate, and host medium). The Au nanoring particle is excited by a plane-wave with modulated Gaussian pulse in time. We first investigate the LSPR behavior under variations on the inner diameter while setting $t = 30$ nm and $H = 35$ nm fixed (to compare with the nanodisk case alluded to in the Introduction). Fig. 5.2 shows that a Au nanoring with inner diameter of 175 nm leads to a plasmon resonance at 1550 nm. In this case, $D = 235$ nm, which is less than the diameter of the nanodisk (340 nm), leads to the LSPR at the same wavelength. Note that these geometrical parameters are not unique in yielding a plasmon resonance at 1550 nm, since the resonance frequency is determined by a combination of geometrical parameters and surrounding medium permittivity.

Next, we investigate the sensitivity of the plasmon resonance to variations on inner diameter, height, and thickness. For each case, one geometrical parameter is changed within $\sim 15\%$, while the others are fixed. Fig. 5.2 shows the influence of $D_i$ on the optical response. The LSPR is red-shifted by increasing $D_i$. Two distinct plasmon
Figure 5.1: Schematic illustration showing a Au nanoring surrounded by SiO$_2$ (core, substrate, and host medium). The three independent geometrical parameters $t$ (metallic thickness), $D_i$ (inner diameter), and $H$ (height) are indicated in the side view.
resonances are observed at visible ($\sim 700$ nm) and infrared ($\sim 1550$ nm) regions of optical spectrum. This plasmon hybridization [90] is caused by the interaction between the “cavity” [90] and “disk” [81] plasmons, analogous to what occurs in nanoshells. Fig. 5.3 shows the effect of $H$ on the optical response. The LSPR is red-shifted by decreasing $H$. The dependence of optical response on $D_i$ and $H$ is somewhat similar to that of a spheroidal particle. Applying a quasi-static approximation [80] to a spheroidal particle, it can be verified that the LSPR is red-shifted by increasing the eccentricity. Similarly, the LSPR is shifted to longer wavelengths by increasing the diameter-to-height ratio of the nanoring. We also evaluate the change in the plasmon resonance due to variations in $t$, as shown in Fig. 5.4. The LSPR is red-shifted by decreasing $t$, akin again to the behavior of a nanoshell. Comparing Figs. 5.2-5.4, we observe that, for similar parameter deviations of about 15% at the LSPR, the spectrum is considerably more sensitive to $D_i$ than to $H$ or $t$. This suggests the use of $D_i$ as the first parameter of choice for tunability purposes.
Figure 5.3: Effect of the height $H$ on the optical response of a Au nanoring.

Figure 5.4: Effect of the thickness $t$ on the optical response of a Au nanoring.
Figure 5.5: Effect of simultaneous variations of the inner diameter $D_i$ and thickness $t$ on Au nanoring optical response.

Figure 5.6: Effect of simultaneous variations of the inner diameter $D_i$, thickness $t$, and height $H$ on Au nanoring optical response.
We next examine the interplay among the geometrical parameters. First, we illustrate the interplay of $D_i$ and $t$ for fixed $H$ (= 35 nm). From Figs. 5.2 and 5.4, it is known that the LSPR is red-shifted or blue-shifted by increasing $D_i$ or $t$, respectively. Fig. 5.5 shows that the LSPR is red-shifted by increasing both $D_i$ and $t$ simultaneously. Compared to the case with $D_i$ increase only, red-shift on the LSPR is reduced due to the influence of $t$. Fig. 5.6 shows results when $D_i$, $t$, and $H$ are all increased simultaneously, for three value sets. The red-shift on the LSPR is smaller in this case compared with Fig. 5.5. Although an increase in only $t$ or $H$ would produce a blue-shift on the LSPR, the LSPR is still red-shifted in Fig. 5.6 because of the stronger effect from the increase in $D_i$. This again illustrates that the resonance is more sensitive to (same fractional) variations on $D_i$.

5.4 Plasmon Waveguides Based on Ordered Arrays of Au Nanoring in SiO$_2$ Host

We next analyze optical pulse propagation in plasmon waveguides based on ordered arrays of Au nanorings in SiO$_2$ host with $D_i = 175$ nm, $H = 35$ nm, and $t = 30$ nm. Seven nanoring particles with intercenter distance of 352.5 nm (= 1.5$D$) are located along the $x$ axis, forming a linear array. To study electromagnetic energy transport, non-collective modes with wavenumber $k \neq 0$ need to be excited (instead of collective modes with $k = 0$) [73]. To excite non-collective modes, a point dipole source is placed at 1.5$D$ away from the center of the first nanoring, with effective bandwidth 1530 nm - 1570 nm. We set the center of the first nanoring at reference position 0 nm.
Figure 5.7: Field intensity (circles) along a linear chain with seven nanoring particles under $T$-mode excitation. Also shown in the inset is a snapshot of the $E_y$ distribution, with polarization indicated by a gray arrow.

To examine the transmission loss, we calculate the field intensity along the linear chain when excited by a dipole pulse with transverse ($T$-mode) or longitudinal ($L$-mode) polarizations (with respect to the chain axis). Fig. 5.7 and Fig. 5.8 show the logarithm of the peak field intensity $|E|^2$ along the plasmon waveguide for $T$- and $L$-modes, respectively. Also shown in the inset are snapshots of $E_y$ for $T$-mode and $E_x$ for the $L$-mode along the nanochain. The polarization is indicated by a gray arrow. The field intensity shown is calculated by averaging the square of electric fields over the outer surface of nanoring. Due to impedance mismatch [67], reflections are observed at the first and last nanorings and hence these values are excluded when interpolating the values along the plasmon waveguide. As the pulse propagates along the waveguide, the field intensity decays in an exponential fashion $|E|^2 \propto \exp(-\gamma x)$ [67]. The transmission loss is extracted by fitting the data (indicated by circles or squares) with a linear fit in the log scale. The transmission loss factors for
Figure 5.8: Field intensity (squares) along a linear chain with seven nanoring particles under $L$-mode excitation. Also shown in the inset is a snapshot of the $E_x$ distribution, with polarization indicated by a gray arrow.

$T$-mode and $L$-mode are $\gamma_T = 3 \text{ dB/655 nm}$ and $\gamma_L = 3 \text{ dB/443 nm}$, respectively. We also display the field intensity (indicated by stars) along a shorter array missing the seventh nanoring. To illustrate the field confinement on the transverse direction, we show a 3-D sliced plot of the $E_y$ field distribution ($T$-mode) in Fig. 5.9, where it is observed that the fields are highly localized at metal/dielectric interfaces and confined transversely.

Next, we determine the group velocity by tracking the amplitude peak positions over time, as shown in Fig. 5.10. The group velocities for $T$-mode ($v_{gT}$) and $L$-mode ($v_{gL}$) are found to be about $0.177c_0$ and $0.327c_0$, respectively, where $c_0$ is the speed of light in vacuum. Note the faster group velocity of $L$-mode compared to $T$-mode, akin to the nanosphere plasmon waveguide case [73].

The influence of interelement spacing on both propagation loss and group velocity is shown in Fig. 5.11. The three interelement spacings considered (0 nm, 117.5 nm,
Figure 5.9: 3-D sliced plot of the $E_y$ field distribution under $T$-mode excitation.

Figure 5.10: Amplitude peak positions over time along a linear nanoring waveguide. Note the faster group velocity for $L$-mode compared to $T$-mode.
Figure 5.11: Influence of interelement spacing on propagation characteristics. (a) 3-dB intensity decay length. (b) Group velocity.

and 235 nm) correspond to intercenter distances $D$, $1.5D$, and $2D$, respectively. The interelement spacing of 0 nm corresponds to successive nanorings that touch each other. For the $T$-mode, the 3-dB intensity decay length decreases as the intercenter distance increases. On the other hand, for the $L$-mode, the 3-dB intensity decay length is maximum for intercenter distance of $1.5D$. Fig. 5.11 also shows that the intercenter distance of $1.5D$ supports the fastest (slowest) group velocity for the $L$-mode ($T$-mode).

The potential for subwavelength routing and switching of optical pulses is one of the major appeals of plasmon waveguides [69, 78]. L-junction (90° sharp bend) structures composed of seven nanorings (three nanorings in both horizontal and vertical arms and one nanoring at the junction position) are analyzed under $T$-mode excitation. Note that a $T$-mode excitation is converted into $L$-mode through L-junctions,
Figure 5.12: Snapshot of $E_y$ under $T$-mode excitation. Electric field is guided along the horizontal arm and coupled into the vertical arm with the bending loss of 7.3 dB.
Figure 5.13: Illustration of the constructive interference of two plasmon-polariton waves under $T$-mode excitation. Two dipole sources are employed with in-phase excitation.

Figure 5.14: Illustration of the destructive interference of two plasmon-polariton waves under $T$-mode excitation. Two dipole sources are employed with out-of-phase excitation.

and vice versa. Comparison of (time-averaged) field intensity around the last nanoparticle between this bending structure and the linear chain leads to a bending loss of 7.3 dB. The transmission performance for $90^\circ$ bends (zero radius of curvature) in nanoring plasmon waveguides is worse than in metal-dielectric-metal plasmon waveguides [98] and in photonic crystal waveguides [99], but better than in dielectric rib waveguides [100]. Fig. 5.12 shows a snapshot of the $E_y$ field along the L-junction. As can be seen, the electric field is guided along the horizontal arm and coupled into the vertical arm.

We next illustrate the coherent interference of two plasmon-polariton waves for potential switching application [78]. A linear chain composed of seven nanorings is excited at both ends with oscillating dipole sources either in-phase ("constructive"
interference) or 180° off-phase (“destructive” interference). Fig. 5.13 and Fig. 5.14 display snapshots of the $E_y$ field distribution along the linear chain, showing the interference of two plasmon-polariton waves. We note that $E_y$ field is symmetrically or anti-symmetrically distributed along the $y$-plane of the central (fourth) particle under “constructive” or “destructive” interference, respectively. Field intensity at the central particle for the “constructive” interference case is 30 dB larger than the “destructive” interference case.

5.5 Concluding Remarks

Plasmon waveguides based on ordered arrays of Au nanorings in SiO$_2$ host have been designed and investigated for use at optical communication band. The analysis was performed by the CFS-PML-FDTD algorithm that accounts for the monospecies Drude dispersion model of Au at the frequencies considered, and effectively suppresses spurious reflections from both propagating and evanescent waves on the computational grid boundaries. This leads to a decrease in the computational cost as the computational boundary can be closely placed near the nanoparticles.

Optical properties of an isolated Au nanoring were studied to determine the set of geometrical parameters producing the LSPR at 1550 nm. It has been found that a nanoring with 175 nm inner diameter, 30 nm metallic thickness, and 35 nm height in SiO$_2$ host produces the LSPR at the desired wavelength. The transmission loss and group velocity were calculated for both $T$- and $L$- polarized pulses. The $L$-mode was found to be more lossy and have a faster group velocity than the $T$-mode. The effect of the intercenter distance between nanorings on propagation characteristics was also considered. For the interelement distances considered, a spacing of about
120 nm has produced the faster group velocity and smaller loss for the $L$-mode. For the $T$ mode, the loss was found to increase with the interelement distance, being minimal for adjoining particles. Finally, more complex structures such as an $L$-junction and a linear chain with two driving dipole sources were also considered and simulated, to further illustrate the guiding properties of nanoring chains and the coherent interference of two plasmon pulses with opposite directions of propagation.
6.1 Introduction

In the previous chapter, we have illustrated that ordered arrays of Au nanorings embedded in SiO$_2$ can serve as a plasmon waveguide at optical communication band. The nanoparticle-based plasmon waveguides yield subwavelength confinement and relatively low bending losses. Recently, a 3-D surface plasmon (SP)-gap waveguide (GW) was suggested, based on a subwavelength gap in a thin metallic film [101–104]. The SP-GW yields wideband mode confinement and moderate propagation length.

Recently, Kim suggested a SP-quasi-coplanar waveguide (QCPW), in which the central metal strip is vertically misaligned to other two outer metal strips, to simplify fabrication steps and the author illustrated the effects of geometrical parameters on mode confinement [105]. In this chapter, we study a SP-coplanar waveguide (CPW) without vertical misalignment$^1$. In particular, we investigate in detail the characteristics of modes which are supported by the SP-CPW and contrast it against the SP-GW mode characteristics. It is illustrated that the SP-CPW can yield higher

$^1$The same structure was considered in Fig. 4(c) in Ref. [105] but only its mode size has been provided.
mode confinement versus the SP-GW, specially in vertical direction. In addition, we analyze 90° bending structures and investigate mode conversion loss associated with discontinuities, and we propose a modified SP-CPW to alleviate mode conversion loss.

### 6.2 SP-CPW

Fig. 6.1 shows the SP-CPW which consists of three Ag (silver) strips, where the SP-GW is also depicted. We employ the Drude model for the modeling of Ag, with $\varepsilon_\infty = 3.7$, $\omega_D = 13.8331 \times 10^{15}$ rad/s, and $\Gamma_D = 2.7362 \times 10^{13}$ rad/s [106], which is consistent with experimental data by Johnson and Christy [96]. For the refractive index of SiO$_2$, we use the nominal value of 1.444. The computational domain is terminated by the PML with large (transverse) buffer regions between plasmon structures and the PML region. As a result, the bounded SP modes are less perturbed and the leaky modes are sufficiently absorbed.
6.2.1 Mode Characteristics

To calculate the propagation constant \((\gamma = \alpha + j\beta)\) of straight plasmon structures, we employ the 3-D CFS-PML-FDTD algorithm (described in Chapter 5), with \(\Delta x = \Delta y = 2.5\) nm and \(\Delta z = 20\) nm\(^2\). After obtaining the waveforms at several positions along the \(z\)-direction (after \(z\)-directed buffer regions so that only propagating SP mode exists) and Fourier transforming the time-domain waveforms, we can obtain the propagation constant by comparing the resulting frequency domain data [107].

The fundamental SP mode of the SP-CPW is the even mode (with respect to potential). To investigate the even (odd) mode, we excite \(E_x\) inside the two gaps with opposite (same) polarizations, having a sine-modulated Gaussian pulse in the time domain. We note that an equivalent analysis can be achieved by simulating the half geometry of the SP-CPW with PMC (PEC) symmetry on the vertical plane of the central metal strip for the even (odd) mode.

Fig. 6.2 shows the effective index \((n_{\text{eff}} = \beta/\beta_0)\) of the (fundamental) even mode of the SP-CPW, where the odd mode of the SP-CPW, the SP-GW mode, and the Ag/SiO\(_2\) SP mode are also included for comparison. Here, \(\beta_0\) denotes the phase constant in vacuum. The SP-CPW even mode has higher \(n_{\text{eff}}\) than the SP-CPW odd mode and the SP-GW mode, indicating more confinement of fields and shorter propagation length \((L_p = \alpha^{-1})\). It is also observed that a decrease in the gap width leads to an increase in \(n_{\text{eff}}\) for both SP-CPW even mode and SP-GW mode, and the SP-CPW even mode has still higher \(n_{\text{eff}}\) than the SP-GW mode. At 1550 nm, we have \(n_{\text{eff}} = 2.23\) and \(L_p = 20.14\) \(\mu\)m for the SP-CPW even mode, \(n_{\text{eff}} = 1.75\) and

\(^2\)Fields change sharply near the interface of metal and dielectric on the transverse \((x-y)\) plane but smoothly in the propagation \((z-)\) direction.
Figure 6.2: Effective index $n_{\text{eff}}$ of SP modes in the SP-CPW and the SP-GW shown in Fig. 6.1. Also the SP-CPW even mode with a decreased gap width (25 nm) and the SP-GW mode with a decreased gap width (25 nm) are considered in dash lines.

$L_p = 67.5 \, \mu\text{m}$ for the SP-CPW odd mode, and $n_{\text{eff}} = 1.9$ and $L_p = 36.04 \, \mu\text{m}$ for the SP-GW mode. We note that when we employ a Drude model fitted to experimental data by Palik [97], we have almost a similar value of $n_{\text{eff}}$ but a decreased value of $L_p$.

In Fig. 6.3, we plot in dB scale the power density of the SP-CPW even mode near the central metal strip at 1550 nm, where contour plots (in gray) of -10 dB and -20 dB are also included. This fundamental SP-CPW mode is very well bounded around the central metal strip, with strong power density near the edges of the central metal strip. The mode area $A_M$ is $12.45 \times 10^3 \, \text{nm}^2$ at the -10 dB threshold and $37.8 \times 10^3 \, \text{nm}^2$ at the -20 dB threshold, excluding the physical area of the central metal strip. The vertical extent $L_v$ is 110 nm and 215 nm at the -10 dB threshold and the -20 dB
Figure 6.3: Power density of the SP-CPW even mode in dB scale at 1550 nm. Contour plots (in gray) indicating -10 dB and -20 dB are also plotted.

threshold respectively, although the horizontal extent matches to the physical size of the structure (150 nm). Fig. 6.4 shows the electric field intensity $|E|^2$ and the magnetic field intensity $|H|^2$ of the SP-CPW even mode in dB scale at 1550 nm. The electric field intensity is more confined compared to the magnetic field intensity. Electric fields are outward from the central metal strip and magnetic fields are circularly polarized. The direction of electric fields and magnetic fields indicates PMC symmetry of the SP-CPW even mode.

Next, we investigate the SP-CPW odd mode. Fig. 6.5 shows the power density of the SP-CPW odd mode near the central metal strip at 1550 nm. The SP-CPW odd mode is not well confined but it is somewhat confined inside two gaps. We observe that the power density is strong near the edges of two outer metal strips. The mode area $A_M$ is $18.23 \times 10^3$ nm$^2$ at the -10 dB threshold and $145.25 \times 10^3$ nm$^2$ at the
Figure 6.4: Field intensity of the SP-CPW even mode in dB scale at 1550 nm. The direction of fields is indicated by the arrows.
Figure 6.5: Power density of the SP-CPW odd mode in dB scale at 1550 nm. Contour plots (in gray) indicating -10 dB and -20 dB are also plotted.

-20 dB threshold, excluding the physical area of the central metal strip. The vertical extent $L_v$ is 135 nm and 400 nm at the -10 dB threshold and the -20 dB threshold, respectively. The horizontal extent matches to the physical size of the structure (150 nm), similar to the even mode case. The poor mode confinement of the SP-CPW odd mode explains why the SP-CPW odd yields the low effective index and long propagation length. Fig. 6.6 shows the electric field intensity $|E|^2$ and the magnetic field intensity $|H|^2$ of the SP-CPW odd mode in dB scale at 1550 nm. Inside two gaps, the electric field is $x$-polarized and the magnetic field is $y$-polarized, similar to the SP-GW mode [see Fig. 6.8]. This similarity indicates that the SP-CPW odd mode is equivalent to the coupled SP-GW mode [108]. We observe PEC symmetry from the direction of electric fields and magnetic fields.
Figure 6.6: Field intensity of the SP-CPW odd mode in dB scale at 1550 nm. The direction of fields is indicated by the arrows.
We also plot the power density of the \textit{SP-GW mode} near the gap at 1550 nm in Fig. 6.7. The SP-GW mode is more confined versus the SP-CPW odd mode but less confined versus the SP-CPW even mode. The mode area $A_M$ is $9 \times 10^3$ nm$^2$ at the -10 dB threshold and $61.1 \times 10^3$ nm$^2$ at the -20 dB threshold. The vertical extent $L_v$ is 125 nm and 300 nm at the -10 dB threshold and the -20 dB threshold respectively and the horizontal extent matches to the physical size of the structure (50 nm). Fig. 6.8 shows the electric field intensity $|E|^2$ and the magnetic field intensity $|H|^2$ of the SP-GW mode in dB scale at 1550 nm. Inside the gap, the electric field is $x$-polarized and the magnetic field is $y$-polarized. We also observe PEC symmetry from the direction of electric fields and magnetic fields, similar to the SP-CPW odd mode.
Figure 6.8: Field intensity of the SP-GW mode in dB scale at 1550 nm. The direction of fields is indicated by the arrows.
<table>
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<th>Mode</th>
<th>$n_{\text{eff}}$</th>
<th>$L_p$ [$\mu$m]</th>
<th>-20 dB $A_M$ [$10^3$nm$^2$]</th>
<th>-20 dB $L_v$ [nm]</th>
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<td>20.14</td>
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<td>36.04</td>
<td>61.1</td>
<td>300</td>
</tr>
</tbody>
</table>

Table 6.1: Mode characteristics at 1550 nm.

Table 6.1 summarizes mode characteristics at 1550 nm, including the effective index $n_{\text{eff}}$, the propagation length $L_p$, the mode area $A_M$ at the -20 dB threshold, and the vertical extent $L_v$ at the -20 dB threshold. For the mode area, the physical area of the central metal strip in the SP-CPW is included at this time. The SP-CPW even mode is very attractive for the application of compact (particularly low-profile) optical waveguides, since it supports better mode confinement. On the other hand, the SP-CPW odd mode is suitable for longer optical waveguides due to longer $L_p$.

### 6.2.2 Bending losses in 90° sharp bending structures

Next, we investigate 90° sharp bending structures, with FDTD meshes $\Delta x = \Delta y = \Delta z = 5$ nm in this study. We launch the SP-CPW even mode at $P_s$, with a raised-cosine-ramped sine wave in the time. Fig. 6.9 shows the snapshot of steady-state electric field intensity $|E|^2$ near a 90° bend at 1550 nm. The different path length between two gaps at the discontinuity leads to phase mismatch on the right arm. As a consequence, the SP-CPW odd mode is excited and thus (even-to-odd) mode conversion loss ensues.
Figure 6.9: Electric field intensity $|\mathbf{E}|^2$ near a $90^\circ$ bend under the SP-CPW even mode excitation at 1550 nm, on the $x$-$z$ plane at the central depth of the metal strips.

By comparing the power flow of the bending structure and that of the straight structure, we measure transmittance $T$, bending efficiency $\eta_b$, and reflectance $R$:

$$T = \frac{\text{Power, bend} @ P2}{\text{Power, straight} @ P1},$$

$$\eta_b = \frac{\text{Power, bend} @ P2}{\text{Power, straight} @ P2},$$

$$R = \frac{\text{Power, bend} @ P1 - \text{Power, straight} @ P1}{\text{Power, straight} @ P1}.$$

Here, P1 and P2 is 200 nm distant from the discontinuity. The difference between transmittance and bending efficiency indicates intrinsic ohmic loss of plasmon structures.

Fig. 6.10 shows transmittance, bending efficiency, and reflectance of a $90^\circ$ bend in the SP-CPW versus the wavelength under even mode pulse excitation. The notation
Figure 6.10: Transmittance, bending efficiency, and reflectance of a 90° bend in the SP-CPW versus the wavelength.

Figure 6.11: Transmittance, bending efficiency, and reflectance of a 90° bend in the SP-GW versus the wavelength.
“ee” indicates “even-to-even” power ratio and “oe” indicates “even-to-odd” power ratio (i.e., mode conversion). Therefore, $\eta_{bee}$ and $\eta_{boe}$ indicate bending efficiency and mode conversion loss, respectively. As the wavelength increases, bending efficiency $\eta_{bee}$ increases but mode conversion loss $\eta_{boe}$ decreases. Bending efficiency is same as mode conversion loss at 1110 nm. At 1550 nm, bending efficiency $\eta_{bee}$ is about 60% and mode conversion loss $\eta_{boe}$ is 20%. We observe very low reflectance $R$ over the wavelength band (e.g., 0.4 % at 1550 nm). For comparison, we also plot transmittance, bending efficiency, and reflectance of the 90° bending structure of the SP-GW versus the wavelength in Fig. 6.11. The SP-GW yields higher bending efficiency compared to the SP-CPW. For the SP-GW, at 1550 nm, bending efficiency and reflectance is about 80% and 1.5%, respectively.

### 6.3 SP-CPW with ground connection

We have illustrated that the SP-CPW even mode has better subwavelength confinement of fields versus the SP-GW mode, albeit with little shorter propagation length. The SP-CPW suffers from mode conversion loss at discontinuities and mode conversion loss is even larger than bending efficiency in 90° bending structures for $\lambda_0 < 1110$ nm. In this section, we modify the (original) SP-CPW to reduce mode conversion loss. We connect two ground metals so that the modified SP-CPW can not support odd modes. We consider two schemes for connecting two ground metals: one-side connection and two-side connection, as shown in Fig. 6.12. We assume Hsup equal to Hsub in two-side ground connection.
Fig. 6.13 shows the normalized $E_x$ along the modified SP-CPW under odd mode excitation. As Hsub decreases, the modified SP-CPW does not yield odd mode propagation. For one-side ground connection, odd modes are not propagating when Hsub is below 75 nm. For two-side ground connection, odd modes are strongly decaying for all considered Hsub. Therefore, we expect that the modified SP-CPW produces low mode conversion loss at discontinuities. It is interesting to investigate the effect of ground connection on mode characteristics of the SP-CPW even mode. Fig. 6.14 shows that ground connection leads to the increase in the effective index $n_{eff}$ and the decrease in the propagation length $L_p$. This effect is clearly observed for small Hsub. We note that ground connection has less effects on the SP-CPW with one-side ground connection than the SP-CPW with two-side ground connection.

Fig. 6.15 shows the power density of the even mode supported the SP-CPW with one-side ground connection (Hsub = 50 nm) at 1550 nm. The power density is little bit more dense on lower regions than upper regions, compared to the original SP-CPW.
Figure 6.13: Effects of ground connection on odd mode propagation in the modified SP-CPW.

Figure 6.14: Effects of ground connection on mode characteristics of even modes in the modified SP-CPW.
Figure 6.15: Power density of the even mode in the SP-CPW with one-side ground connection (Hsub = 50 nm) at 1550 nm.

[see Fig. 6.3]. The -20 dB vertical extent $L_v$ in this modified SP-CPW is 172.5 nm and it is smaller than $L_v$ of the original SP-CPW (215 nm). Next, we plot the power density of the even mode supported by the SP-CPW with two-side ground connection (Hsub = Hsup = 50 nm) at 1550 nm in Fig. 6.16. The power density distribution of this modified SP-CPW is quite different from that of the original SP-CPW. The vertical extent $L_v$ is 150 nm for both -10 dB and -20 dB thresholds. The -20 dB mode area $A_M$ is almost equivalent to the physical area of dielectrics surrounding the central metal strip. We note that the geometry of this modified SP-CPW resembles that of a (square) coaxial waveguide with thick metal cladding.

Next, we investigate 90° sharp bending structures in the modified SP-CPW. Fig. 6.17 shows transmittance, bending efficiency, and reflectance of a 90° bend in the SP-CPW with one-side ground connection under even mode pulse excitation. This
modified SP-CPW produces better bending efficiency $\eta_{bee}$ and less mode conversion loss $\eta_{boe}$, compared to the original SP-CPW [see Fig. 6.10]. However, ground connection somewhat increases reflectance $R$. At 1550 nm, the SP-CPW with one-side ground connection yields $\eta_{bee} = 80\%$, $\eta_{boe} = 2\%$, and $R = 5.3\%$. Bending efficiency of this modified SP-CPW is better than that of the SP-GW for $\lambda_0 > 1560$ nm. We should mention that mode conversion loss is more reduced when we measure the power flow at more far ends from discontinuities.

Fig. 6.18 shows transmittance, bending efficiency, and reflectance of a 90° bend in the SP-CPW with two-side ground connection under even mode pulse excitation. The SP-CPW with two-side ground connection yields very good bending efficiency, with almost zero loss of mode conversion. Bending efficiency of this modified SP-CPW
Figure 6.17: Transmittance, bending efficiency, and reflectance of a 90° bend in the SP-CPW with one-side ground connection.

Figure 6.18: Transmittance, bending efficiency, and reflectance of a 90° bend in the SP-CPW with two-side ground connection.
is better than that of the SP-GW. At 1550nm, the modified SP-CPW with two-side ground connection produces $\eta_{\text{bee}} = 96.6\%$ and $R = 2.5\%$.

### 6.4 Concluding Remarks

Plasmon waveguides based coplanar structures have been studied. The SP-CPW supports two SP modes, viz. even mode and odd mode, and we have investigated characteristics of these modes and compare them with those of the SP-GW mode. In the SP-CPW, the even mode yields more compact confinement of fields than the odd mode and thus the even mode is more suitable for the application of compact plasmon waveguides.

The original SP-CPW suffers from mode conversion loss at discontinuities. We modify the SP-CPW by connecting two ground metals either on one side or on two sides, so that it does not support propagating odd modes. Effects of ground connection on mode conversion loss and mode characteristics have been investigated in detail. We have demonstrated that ground connection reduces mode conversion loss at 90° bends. For example, mode conversion loss in the SP-CPW with one-side ground connection ($H_{\text{sub}} = 50 \text{ nm}$) is ten times smaller than mode conversion loss in the original SP-CPW, and the effect of ground connection on the decrease in mode conversion loss is much more pronounced for the SP-CPW with two-side ground connection. We have also observed that ground connection boosts up bending efficiency but simultaneously increases reflectance. Although we consider relatively simple schemes (with only vertical buffers, $H_{\text{sub}}$) for connecting two ground metals, more elaborate way can be employed, e.g., ground connection with both vertical and horizontal buffers.
CHAPTER 7

MULTISPECIES ADI-FDTD ALGORITHM FOR PLASMON STRUCTURES

7.1 Introduction

In this chapter, we develop an efficient time-domain algorithm to handle wideband responses of nanoscale metallic structures. The improved algorithm is based on the extension of the ADI-FDTD scheme to a complex dispersive modeling of metals, the multispecies Drude-Lorentz model, and it leads to accurate EM responses of metals in the wide bandwidth. The ADE approach is utilized to account for the time-domain modeling of metals by introducing equivalent current and polarization terms [109].

7.2 Time-Domain Modeling of Metals

Modeling of metals in the optical frequency range can be described either by the monospecies Drude model or by the multispecies Drude-Lorentz model, depending on the wavelength range of interest. For the dispersion of Au, Fig. 7.1 compares the monospecies Drude model, the multispecies Drude-Lorentz model, and experimental data by Johnson and Christy [96]. As seen from this figure, the multispecies Drude-Lorentz dispersion becomes necessary when the wavelength range of interest
Figure 7.1: Au dispersion in the visible spectrum.

has wavelengths below 700 nm due to interband transitions\(^3\) [92]. Therefore, one should choose an appropriate model according to the prescribed wavelength range.

We assume the \(e^{i\omega t}\) time convention. In the wavelength range, \(500 \text{ nm} < \lambda_0 < 1000 \text{ nm}\), the dielectric response of gold can be described by a Drude-Lorentz model as

\[
\epsilon_r(\omega) = \epsilon_\infty + \frac{\omega_D^2}{j\omega(\Gamma_D + j\omega)} + \frac{\Delta\epsilon_L\omega_L^2}{(j\omega)^2 + j\omega\Gamma_L + \omega_L^2},
\]

where \(\omega_D\) and \(\omega_L\) are pole resonances, \(\Gamma_D\) and \(\Gamma_L\) are damping coefficients, and \(\Delta\epsilon_L\) is a weighting coefficient for the Lorentz term. The following parameters [92] give a

\(^3\)For the dispersion of Ag, interband transitions become important below 350 nm.
good fit to the experimental data:

\[ \varepsilon_\infty = 5.9673, \]
\[ \omega_D = 2\pi \times 2113.6 \text{ rad/s}, \]
\[ \Gamma_D = 2\pi \times 15.92 \text{ rad/s}, \]
\[ \omega_L = 2\pi \times 650.07 \text{ rad/s}, \]
\[ \Gamma_L = 2\pi \times 104.86 \text{ rad/s}, \]
\[ \Delta\varepsilon_L = 1.09. \] (7.2)

By introducing equivalent Drude current \( J_D \) and Lorentz polarization \( Q_L \) terms in Maxwell’s equations, we obtain the governing equations as follow

\[ \mu_0 \frac{\partial \mathbf{H}}{\partial t} = -\nabla \times \mathbf{E}, \] (7.3)

\[ \epsilon_0 \varepsilon_\infty \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J}_D + \frac{\partial \mathbf{Q}_L}{\partial t} = \nabla \times \mathbf{H}, \] (7.4)

\[ \frac{\partial \mathbf{J}_D}{\partial t} + \Gamma_D \mathbf{J}_D = \epsilon_0 \omega_D^2 \mathbf{E}, \] (7.5)

\[ \frac{\partial^2 \mathbf{Q}_L}{\partial t^2} + \Gamma_D \frac{\partial \mathbf{Q}_L}{\partial t} + \omega_L^2 \mathbf{Q}_L = \epsilon_0 \Delta\varepsilon_L \omega_L^2 \mathbf{E}. \] (7.6)

Maxwell’s curl equations are described in Eq. (7.3) and Eq. (7.4) and two ADEs in Eq. (7.5) and Eq. (7.6). Alternatively, we can choose different auxiliary variable pairs, for example, \{\mathbf{J}_D and \mathbf{J}_L\}, \{\mathbf{Q}_D and \mathbf{Q}_L\}, or \{\mathbf{Q}_D and \mathbf{J}_L\}, but the above choice leads to the most memory efficient formulation.

### 7.3 ADI-FDTD Formulation

In the ADI-FDTD method, the update at each time step \( n \) is divided into two sub-steps. For the first sub-step \((n + 1/2)\), the discretized equations for the \( E_x \) and
\( H_n \) update are written as

\[
E_{n+1/2}^{x_{i+1/2,j,k}} = E_n^{x_{i+1/2,j,k}} + \frac{\Delta t}{2\varepsilon_0\varepsilon_{\infty}} \left[ \frac{H_n^{x_{i+1/2,j+1/2,k}} - H_n^{x_{i+1/2,j-1/2,k}}}{\Delta y} \right] - \frac{\Delta t}{2\varepsilon_0\varepsilon_{\infty}} \left[ \frac{H_n^{y_{i+1/2,j,k+1/2}} - H_n^{y_{i+1/2,j,k-1/2}}}{\Delta z} \right] - \frac{\Delta t}{2\varepsilon_0\varepsilon_{\infty}} \left[ \frac{Q_n^{x_{i+1/2,j,k}} - Q_n^{x_{i+1/2,j,k}}}{\Delta t/2} \right] - \frac{\Delta t}{2\varepsilon_0\varepsilon_{\infty}} \left[ \frac{J_n^{x_{i+1/2,j,k}} + J_n^{x_{i+1/2,j,k}}}{2} \right], \quad (7.7)
\]

\[
H_{n+1/2}^{z_{i+1/2,j+1/2,k}} = H_n^{z_{i+1/2,j+1/2,k}} + \frac{\Delta t}{2\mu_0} \left[ \frac{E_n^{x_{i+1/2,j+1,k}} - E_n^{x_{i+1/2,j,k}}}{\Delta y} \right] - \frac{\Delta t}{2\mu_0} \left[ \frac{E_n^{y_{i+1/2,j+1/2,k}} - E_n^{y_{i+1/2,j,k-1/2}}}{\Delta x} \right], \quad (7.8)
\]

where the subscript refers to spatial grid indexing and the superscript refers to the time step. The discretized equations for auxiliary variables can be obtained by using central differencing in time, in a standard fashion:

\[
J_D^{n+1/2} = c_{D1} J_D^n + c_{D2} (E_n^{n+1/2} + E_n^n), \quad (7.9)
\]

\[
Q_L^{n+1/2} = c_{L1} Q_L^n + c_{L2} Q_L^{n-1/2} + c_{L3} E_n^n, \quad (7.10)
\]

where

\[
c_{D1} = \frac{1 - 0.5\alpha_D}{1 + 0.5\alpha_D},
\]

\[
c_{D2} = \frac{0.25\Delta t\varepsilon_0\omega_D}{1 + 0.5\alpha_D},
\]

\[
c_{L1} = \frac{2 - 0.25(\omega_L\Delta t)^2}{1 + 0.5\alpha_L},
\]

\[
c_{L2} = \frac{0.5\alpha_L - 1}{1 + 0.5\alpha_L},
\]

\[
c_{L3} = \frac{0.25\varepsilon_0\Delta \varepsilon_L (\omega_L\Delta t)^2}{1 + 0.5\alpha_L},
\]
and $\alpha_\xi = 0.5 \Gamma_\xi \Delta t$, $\xi = D$ (Drude) or $L$ (Lorentz). From Eq. (7.7), we see that $E_{x}^{n+1/2}$ can not be updated explicitly. By substituting Eq. (7.8) and Eq. (7.9) into Eq. (7.7), we obtain an implicit equation for $E_{x}^{n+1/2}$ in a form of the tridiagonal system as follows:

$$
- \frac{C_b}{(\Delta y)^2 \beta_\mu} E_{x_i+1/2,j-1,k}^{n+1/2} + \left( 1 + 2 \frac{C_b}{(\Delta y)^2 \beta_\mu} \right) E_{x_i+1/2,j,k}^{n+1/2} - \frac{C_b}{(\Delta y)^2 \beta_\mu} E_{x_i+1/2,j+1,k}^{n+1/2} = C_a E_{x_i+1/2,j,k}^{n} + C_b \left[ \frac{H_{x_i+1/2,j+1/2,k}^n - H_{x_i+1/2,j-1/2,k}^n}{\Delta y} \right] - C_b \left[ \frac{H_{y_i+1/2,j,k+1/2}^n - H_{y_i+1/2,j,k-1/2}^n}{\Delta z} \right] - \frac{C_b}{\Delta y \Delta x \beta_\mu} [ E_{y_i+1,j+1/2,k}^n - E_{y_i,j+1/2,k}^n ] + \frac{C_b}{\Delta y \Delta x \beta_\mu} [ E_{y_i+1,j-1/2,k}^n - E_{y_i,j-1/2,k}^n ] - C_b \left[ \frac{Q_{x_i+1/2,j,k}^{n+1/2} - Q_{x_i+1/2,j,k}^n}{\Delta t/2} \right] + C_c J_{x_i+1/2,j,k}^n.
$$

(7.11)

Here, the coefficients are expressed as

$$
C_a = \frac{\beta_\epsilon - 0.5 c_{D_2}}{\beta_\epsilon + 0.5 c_{D_2}},
C_b = \frac{1}{\beta_\epsilon + 0.5 c_{D_2}},
C_c = - \frac{0.5 (1 + c_{D_2})}{\beta_\epsilon + 0.5 c_{D_2}},
$$

and $\beta_\epsilon = 2 \epsilon_0 \epsilon_\infty / \Delta t$, $\beta_\mu = 2 \mu / \Delta t$. This tridiagonal system can be easily solved with $O(N)$ complexity [49]. The other field components are obtained similarly. The update procedure for the first sub-step is summarized as

Step 1. Update $Q_L$ explicitly from Eq. (7.10)

Step 2. Update $E_x$ implicitly from Eq. (7.11), and $E_y$ and $E_z$ similarly
Step 3. Update $J_D$ explicitly from Eq. (7.9)

Step 4. Update $H_z$ explicitly from Eq. (7.8), and $H_x$ and $H_y$ similarly.

An analogous procedure is employed for the second sub-step ($n + 1$). The above recovers the standard ADI-FDTD formulation (for dielectric regions) by a proper choice of material coefficients.

### 7.4 Numerical Examples

To validate the above formulation, we analyze the localized surface plasmon resonance of an isolated Au nanosphere with radius $r = 15$ nm, in SiO$_2$ host. In the 500 – 1000 nm range, the dielectric response of gold is described in Eq. (7.1) and Eq. (7.2). The refraction index of SiO$_2$ is set to 1.444, being virtually constant in those wavelengths. The incident field is a $z$-polarized plane wave. The time-domain excitation is a Gaussian modulated sine wave having half power bandwidth (HPBW) at 500 – 1000 nm. The simulation time window is 30 fs. The CN is given by $\Delta t \sqrt{3c_0/\Delta h}$, where $c_0$ is the speed of light in vacuum.

First, we employ a grid with spatial cell size $\Delta h = 1$ nm, corresponding to 500 points per (vacuum) wavelength at the smallest wavelength. A grid with $90^3$ cells is used in this case. Fig. 7.2 shows the spectra of the Au nanosphere using both standard FDTD algorithm and proposed ADI-FDTD algorithm at a distance $4\Delta h$ away from the sphere. The spectral response is obtained by Fourier transforming the time-domain field data (with a Blackman window to remove aliasing), followed by a normalization by the excitation pulse spectrum. Very good agreement is observed between the ADI-FDTD results and the FDTD result on this mesh. Table 7.1 summarizes the normalized central processing unit (CPU) time, memory requirement, and
Figure 7.2: Spectra of a Au nanosphere ($r = 15$ nm) surrounded by SiO$_2$ with the spatial cell size $\Delta h = 1$ nm.

the surface plasmon resonance wavelengths for various CN. The ADI-FDTD method requires 7.8% more memory than the FDTD method for the same problem. For CN=6, the CPU time of the ADI-FDTD simulation is reduced to about 42% of the FDTD simulation, while the resonance wavelength (relative) error is below 0.8%. For CN=10, the relative error in the resonance wavelength is still within 1.3%. In this case, the CPU time required by the ADI-FDTD algorithm is about 32% of the FDTD algorithm.

Next, we consider a coarser grid with $\Delta h = 2$ nm and $45^3$ cells. Fig. 7.3 shows the spectra of the same structure using both FDTD method and proposed ADI-FDTD method. For large CN number, ADI-FDTD results start to deviate from the FDTD result, since the truncation error due to a larger $\Delta t$ become more pronounced. The
<table>
<thead>
<tr>
<th>Method (CN)</th>
<th>CPU Time</th>
<th>Memory Requirement</th>
<th>Res. Wavelength</th>
</tr>
</thead>
<tbody>
<tr>
<td>FDTD (CN=0.95)</td>
<td>100%</td>
<td>205 MB</td>
<td>533.62 nm</td>
</tr>
<tr>
<td>ADI-FDTD (CN=2)</td>
<td>104%</td>
<td>221 MB</td>
<td>534.76 nm</td>
</tr>
<tr>
<td>ADI-FDTD (CN=4)</td>
<td>59%</td>
<td>221 MB</td>
<td>536.48 nm</td>
</tr>
<tr>
<td>ADI-FDTD (CN=6)</td>
<td>42%</td>
<td>221 MB</td>
<td>537.63 nm</td>
</tr>
<tr>
<td>ADI-FDTD (CN=10)</td>
<td>32%</td>
<td>221 MB</td>
<td>540.54 nm</td>
</tr>
</tbody>
</table>

Table 7.1: Comparison between ADI-FDTD and FDTD results.

errors in the resonance wavelength for CN=6 and CN=10 are about 2% and 4.3%, respectively. These coarse grid results serve to illustrate that the ADI-FDTD method is more suited for very fine grids, where increase in CN produces limited truncation errors.

We also analyze the LSPR of an isolated Au nanocube with length \( l = 30 \text{ nm} \), in SiO\(_2\) host, with the cell size \( \Delta h = 1 \text{ nm} \). Fig. 7.4 shows the spectra of the Au nanocube using both FDTD method and proposed ADI-FDTD method. The resonance wavelength calculated from the ADI-FDTD algorithm deviates from the FDTD reference by 2.01% and 2.13% for CN=6 and CN=10, respectively. From Fig. 7.2 and Fig. 7.4, it is observed that the surface plasmon resonance in an isolated Au nanocube with length \( l = 30 \text{ nm} \) is located at a longer wavelength compared to an isolated Au nanosphere with diameter \( d = 30 \text{ nm} \).

We stress that, even though there is no stability limit, the CN (or, equivalently, \( \Delta t \)) in the ADI-FDTD algorithm is still limited by accuracy, for a given \( \Delta h \). In the case of dispersive media, this implies that the maximum \( \Delta t \) should be at least
Figure 7.3: Spectra of a Au nanosphere ($r = 15$ nm) surrounded by SiO$_2$ with the spatial cell size $\Delta h = 2$ nm.

Figure 7.4: Spectra of a Au nanocube ($l = 30$ nm) surrounded by SiO$_2$ with the spatial cell size $\Delta h = 1$ nm.
Figure 7.5: Snapshot of $|E_y|$ along a nanosphere-based plasmon waveguide excited by a dipole pulse with a $y$–directed polarization indicated by arrow.

about 1/10 of the smallest characteristic time constant of the media, which may include resonant frequencies and relaxation times. In the example considered, the smallest characteristic time is $t_D = 2\pi/\omega_D$. Using CN = 10 in the coarse grid, one has $t_D/\Delta t \approx 12$ and hence the accuracy starts to be compromised for CN beyond that.

Finally, we consider a plasmon waveguide based on a linear chain of Au nanospheres surrounded by SiO$_2$ host. The radius of each nanosphere is 15 nm and the intercenter distance is 45 nm. The chain is excited by a dipole with transverse polarization with respect to the chain axis. The time-domain excitation is again a Gaussian modulated sine wave with HPBW at 500 – 1000 nm. The grid has $390 \times 90 \times 90$ cells. Fig. 7.5 shows a snapshot of $E_y$ amplitude along the chain calculated by the ADI-FDTD simulation with CN=6, showing EM energy transport below the diffraction limit via near-field coupling between closely spaced nanoparticles.

7.5 Concluding Remarks

The ADI-FDTD method has been extended to multispecies dispersive media for the analysis of optical plasmon resonances in plasmon structures. Numerical results
show that the proposed ADI-FDTD algorithm is advantageous in highly refined grids and become computationally more efficient than the FDTD algorithm for moderate size CN. The present ADI-FDTD formulation has been illustrated for the two-species Drude-Lorentz dispersive media, but it can be easily applied to arbitrary multispecies dispersive media as well. By using ADEs (instead of recursive convolution), auxiliary variables associated with Lorentz dispersion terms remain real-valued and the formulation can be further extended towards nonlinear media.
CHAPTER 8

ITERATIVE LOD-FDTD ALGORITHM

8.1 Introduction

The locally-one-dimensional (LOD)-FDTD method is an attractive alternative to the ADI-FDTD method due to the reduced number of arithmetic operations with comparable accuracy [110–115]. LOD-FDTD and ADI-FDTD algorithms are unconditionally stable. However, both algorithms suffer from the splitting error, because they can be obtained from a perturbation of the Crank-Nicolson FDTD scheme. Recently, a fixed-point iterative procedure has been introduced to reduce the splitting error in two-dimensional (2-D) ADI-FDTD simulations [116–119]. This iterative procedure improves the accuracy of the ADI-FDTD method without compromising its inherent computational simplicity.

In this chapter, we introduce an iterative LOD-FDTD method with reduced splitting error based on the use of fixed-point iterations within each time step [120]. For simplicity, we consider lossless isotropic media with no dispersion, but the basic approach equally applies to complex media such as dispersive and anisotropic media.
8.2 Review of Iterative ADI-FDTD Algorithm

We consider a 2-D transverse electric (TE$_z$) problem, where Maxwell's curl equations can be written as

$$\frac{\partial \vec{u}}{\partial t} = [A] \vec{u} + [B] \vec{u}$$  \hspace{1cm} (8.1)

with $\vec{u} = [E_x, E_y, H_z]^T$ and

$$[A] = \begin{bmatrix} 0 & 0 & \frac{\partial}{\partial y} \\ 0 & 0 & 0 \\ \frac{\rho}{\mu} & 0 & 0 \end{bmatrix},$$  \hspace{1cm} (8.2)

$$[B] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\partial}{\rho} & 0 \\ 0 & -\frac{\partial}{\mu} & 0 \end{bmatrix}.$$  \hspace{1cm} (8.3)

We can write update equations for the above using the Crank-Nicolson FDTD formalism as follows

$$\left( [I] - \frac{\Delta t}{2} [A] - \frac{\Delta t}{2} [B] \right) \vec{u}^{n+1/2} = \left( [I] + \frac{\Delta t}{2} [A] + \frac{\Delta t}{2} [B] \right) \vec{u}^n,$$  \hspace{1cm} (8.4)

where the superscript denotes the time step and $[I]$ is the $3 \times 3$ identity matrix. The Crank-Nicolson FDTD algorithm is a fully-implicit method and thus its computational cost is huge.

The ADI-FDTD formulation proceeds by factoring Eq. (8.4) (in an approximate fashion) into two sub-steps

$$\left( [I] - \frac{\Delta t}{2} [A] \right) \vec{u}^{n+1/2} = \left( [I] + \frac{\Delta t}{2} [B] \right) \vec{u}^n,$$  \hspace{1cm} (8.5)

$$\left( [I] - \frac{\Delta t}{2} [B] \right) \vec{u}^{n+1} = \left( [I] + \frac{\Delta t}{2} [A] \right) \vec{u}^{n+1/2}.$$  \hspace{1cm} (8.6)
Combining Eq. (8.5) and Eq. (8.6), we can write one full time-step of the ADI-FDTD update as

\[
(I - \frac{\Delta t}{2}[A]) (I - \frac{\Delta t}{2}[B]) \vec{u}^{n+1} = (I + \frac{\Delta t}{2}[A]) (I + \frac{\Delta t}{2}[B]) \vec{u}^n.
\]  

(8.7)

Comparing (8.4) and (8.7), it is noted that the accuracy of the ADI-FDTD method can be improved using the following fixed-point iteration [116,117]:

\[
(I - \frac{\Delta t}{2}[A]) (I - \frac{\Delta t}{2}[B]) \vec{u}^{n+1}_{k} = (I + \frac{\Delta t}{2}[A]) (I + \frac{\Delta t}{2}[B]) \vec{u}^n + \left(\frac{\Delta t}{2}\right)^2 [A][B] (\vec{u}^{n+1}_k - \vec{u}^n),
\]  

(8.8)

where the subscript \(k\) denotes the \(k\)-th iteration within the time step \(n\). The two-step implementation of the iterative ADI-FDTD method can be obtained using the Peaceman-Rachford approach [116]:

\[
(I - \frac{\Delta t}{2}[A]) \vec{u}^{n+1/2} = (I + \frac{\Delta t}{2}[B]) \vec{u}^n + \frac{1}{2} \left(\frac{\Delta t}{2}\right)^2 [A][B] (\vec{u}^{n+1}_k - \vec{u}^n),
\]  

(8.9)

\[
(I - \frac{\Delta t}{2}[B]) \vec{u}^{n+1}_{k+1} = (I + \frac{\Delta t}{2}[A]) \vec{u}^{n+1/2} + \frac{1}{2} \left(\frac{\Delta t}{2}\right)^2 [A][B] (\vec{u}^{n+1}_k - \vec{u}^n).
\]  

(8.10)

### 8.3 Iterative LOD-FDTD Algorithm

Using the LOD splitting scheme [111,112], the two sub-step procedures of the LOD-FDTD algorithm are written as

\[
(I - \frac{\Delta t}{2}[A]) \vec{u}^{n+1/2} = (I + \frac{\Delta t}{2}[A]) \vec{u}^n,
\]  

(8.11)
\[
\left( [I] - \frac{\Delta t}{2} \begin{bmatrix} A \\ B \end{bmatrix} \right) \vec{u}^{n+1} = \left( [I] + \frac{\Delta t}{2} \begin{bmatrix} A \\ B \end{bmatrix} \right) \vec{u}^{n+1/2}. \quad (8.12)
\]

To illustrate the perturbation error of the LOD-FDTD algorithm, we substitute Eq. (8.12) into Eq. (8.11), and rearrange the terms to write the LOD-FDTD update as the following one-time step expression

\[
\left( [I] - \frac{\Delta t}{2} [A] \right) \left( [I] - \frac{\Delta t}{2} [B] \right) \vec{u}^{n+1} = \left( [I] + \frac{\Delta t}{2} [B] \right) \left( [I] + \frac{\Delta t}{2} [A] \right) \vec{u}^{n} \quad (8.13)
\]

\[+ \left( \frac{\Delta t}{2} \right)^2 ([B][A] - [A][B]) \vec{u}^{n+1/2}.
\]

By comparing Eq. (8.4) and Eq. (8.13), we can apply the iterative correction below to obtain a one-time step formulation of the iterative LOD-FDTD method

\[
\left( [I] - \frac{\Delta t}{2} [A] \right) \left( [I] - \frac{\Delta t}{2} [B] \right) \vec{u}^{n+1} = \left( [I] + \frac{\Delta t}{2} [B] \right) \left( [I] + \frac{\Delta t}{2} [A] \right) \vec{u}^{n} \quad (8.14)
\]

\[+ \left( \frac{\Delta t}{2} \right)^2 ([B][A] - [A][B]) \vec{u}^{n+1/2} \]

\[+ \left( \frac{\Delta t}{2} \right)^2 [A][B] (\vec{u}_{k+1}^{n+1} + \vec{u}^{n+1/2}) \]

\[\quad - \left( \frac{\Delta t}{2} \right)^2 [B][A] (\vec{u}^{n+1/2} + \vec{u}^{n}).\]

For actual implementation, a two-step implementation of the iterative LOD-FDTD algorithm is formulated as

\[
\left( [I] - \frac{\Delta t}{2} [A] \right) \vec{u}^{n+1/2} = \left( [I] + \frac{\Delta t}{2} [A] \right) \vec{u}^{n} \quad (8.15)
\]

\[+ \left( \frac{\Delta t}{2} \right)^2 [A][B] (\vec{u}_{k+1}^{n+1} + \vec{u}^{n+1/2}),
\]

\[
\left( [I] - \frac{\Delta t}{2} [B] \right) \vec{u}_{k+1}^{n+1} = \left( [I] + \frac{\Delta t}{2} [B] \right) \vec{u}^{n+1/2} \quad (8.16)
\]

\[- \left( \frac{\Delta t}{2} \right)^2 [B][A] (\vec{u}^{n+1/2} + \vec{u}^{n}).\]
To examine the consistency between the above two-step implementation Eq. (8.15), Eq. (8.16) and the (exact) one-time step formulation Eq. (8.14), we note that the two-step implementation leads to the one-time step expression Eq. (8.14) plus the following extra terms

$$+ \left( \frac{\Delta t}{2} \right)^3 [B][A][B] (\bar{u}^n_{k+1} + \bar{u}_{n+1/2}) + \left( \frac{\Delta t}{2} \right)^3 [A][B][A] (\bar{u}^{n+1/2} + \bar{u}^n). \quad (8.17)$$

In the 2-D TE\_z case, $[B][A][B] = [0]$ and $[A][B][A] = [0]$ and hence application of Eq. (8.15) and Eq. (8.16) in sequence recovers Eq. (8.14). In the 2-D TM\_z case, an analogous two-step implementation can be employed with corresponding $\bar{u}, [A],$ and $[B]$:

$$\bar{u} = [H_x, H_y, E_z]^T, \quad (8.18)$$

$$[A] = \begin{bmatrix} 0 & 0 & -\frac{\partial}{\partial y} \\ 0 & 0 & 0 \\ -\frac{\partial}{\partial y} & 0 & 0 \end{bmatrix}, \quad (8.19)$$

$$[B] = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial x} & 0 \end{bmatrix}. \quad (8.20)$$

Let us suppose that we employ the alternate choice, viz., having the $[B][A]$ term in the first sub-step and the $[A][B]$ term in the second sub-step:

$$\left([I] - \frac{\Delta t}{2} [A] \right) \bar{u}^{n+1/2} = \left([I] + \frac{\Delta t}{2} [A] \right) \bar{u}^n$$

$$- \left( \frac{\Delta t}{2} \right)^2 [B][A] (\bar{u}^{n+1/2} + \bar{u}^n), \quad (8.21)$$

$$\left([I] - \frac{\Delta t}{2} [B] \right) \bar{u}_{k+1}^{n+1} = \left([I] + \frac{\Delta t}{2} [B] \right) \bar{u}^{n+1/2}$$

$$+ \left( \frac{\Delta t}{2} \right)^2 [A][B] (\bar{u}_{k+1}^{n+1} + \bar{u}_{n+1/2}). \quad (8.22)$$
In such a case, two-step implementation leads to the one-time step expression Eq. (8.14) plus the following extra terms

\[- \left( \frac{\Delta t}{2} \right)^3 \begin{bmatrix} A \\ A \\ B \end{bmatrix} \begin{bmatrix} \vec{u}_k^{n+1} + \vec{u}^{n+1/2} \\ \vec{u}_k^{n+1} + \vec{u}^{n} \end{bmatrix} - \left( \frac{\Delta t}{2} \right)^3 \begin{bmatrix} B \\ B \\ A \end{bmatrix} \begin{bmatrix} \vec{u}_k^{n+1/2} + \vec{u}^{n} \end{bmatrix} \]. (8.23)

We note that \( [A][A][B] \neq [0] \) and \( [B][B][A] \neq [0] \) in general, and thus this alternative choice is not viable.

We next write down the field update equations for the iterative LOD-FDTD method using Eq. (8.15) and Eq. (8.16). In the first sub-step \((n + 1/2)\), we have

\[
E_x^{n+1/2} = E_x^n + \frac{\Delta t}{2\epsilon} \frac{\partial}{\partial y} \left[ H_z^{n+1/2} + H_z^n \right] - \left( \frac{\Delta t}{2} \right)^2 \frac{1}{\mu \epsilon} \frac{\partial}{\partial x} \left[ E_y^{n+1} + E_y^{n+1/2} \right]
\]

\[
E_y^{n+1/2} = E_y^n
\]

\[
H_z^{n+1/2} = H_z^n + \frac{\Delta t}{2\mu} \frac{\partial}{\partial y} \left[ E_x^{n+1/2} + E_x^n \right].
\]

In the second sub-step \((n + 1)\), we have

\[
E_{x,k+1}^{n+1} = E_x^{n+1/2}
\]

\[
E_{y,k+1}^{n+1} = E_y^{n+1/2} - \frac{\Delta t}{2\epsilon} \frac{\partial}{\partial x} \left[ H_z^{n+1} + H_z^{n+1/2} \right] + \left( \frac{\Delta t}{2} \right)^2 \frac{1}{\mu \epsilon} \frac{\partial}{\partial x} \frac{\partial}{\partial y} \left[ E_x^{n+1/2} + E_x^n \right]
\]

\[
H_{z,k+1}^{n+1} = H_z^{n+1/2} - \frac{\Delta t}{2\mu} \frac{\partial}{\partial x} \left[ E_y^{n+1} + E_y^{n+1/2} \right].
\]

In each sub-step, we solve one explicit update equation (for \(H_z\)) and one semi-implicit (tridiagonal matrix-form) update equation (for \(E_x\) in the first sub-step and \(E_y\) in the second sub-step). The same number of basic steps is involved for both iterative ADI and iterative LOD, but overall, the iterative LOD-FDTD algorithm requires a smaller number of arithmetic operations than the iterative ADI-FDTD algorithm in each full
update. Table 8.1 lists the number of arithmetic operations in the right-hand side of the update equations, illustrating the reduced operation count of the iterative LOD-FDTD algorithm versus the iterative ADI-FDTD algorithm.

### Table 8.1: Operation Count.

<table>
<thead>
<tr>
<th>Method</th>
<th>Implicit</th>
<th>Explicit</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>M,D A,S</td>
<td>M,D A,S</td>
<td>M,D A,S</td>
</tr>
<tr>
<td>ADI</td>
<td>6+i 12+8i</td>
<td>6+i 12+8i</td>
<td>12+2i 24+16i</td>
</tr>
<tr>
<td>LOD</td>
<td>4 12</td>
<td>2+2i 8+16i</td>
<td>6+2i 20+16i</td>
</tr>
</tbody>
</table>

M,D: multiplication/division, A,S: addition/subtraction, i: number of iterations.

8.4 Numerical Examples

We calculate the field distribution in the vicinity of two (2 m-long) parallel PECs with separation of 0.2 m, and surrounded by perfect magnetic conductor walls, as shown in Fig. 8.1. The EM field in this example exhibits a sharp spatial distribution leading to large spatial derivatives near the PEC edges. This serves to illustrate the effect of the iterative procedure in reducing the splitting error. The excitation is a hard source with unit voltage amplitude between the two conductors. The time-domain excitation is given by \( v(t) = 0.5[1 - \cos(2\pi f_0 t)] \) for \( 0 \leq t \leq 0.66 \mu s \) and \( v(t) = 1 \) for \( t \geq 0.66 \mu s \), with \( f_0=750 \) KHz. The cell size is \( \Delta h = \Delta x = \Delta y = 0.2 \) m, corresponding to 2,000 points-per-wavelength at \( f_0 \). The Courant factor \( s \) is given as \( s = c_0 \Delta t/\Delta h \), where \( c_0 \) is the speed of light in vacuum. Fig. 8.2 displays \( E_y \) along the observation plane at \( t = 10 \mu s \), calculated using the FDTD method,
the iterative LOD-FDTD method, and the iterative ADI-FDTD method. We observe very good agreement between LOD-FDTD and ADI-FDTD results for the various iteration numbers and convergence towards FDTD results. This also shows that the extra noncommutativity error specific to the LOD-FDTD algorithm is negligible in this example, in concordance with the findings in [111]. Fig. 8.3 shows the $L_2$ norm $\| \delta \|_2$ of the relative error for $E_y$ (along the observation plane) using FDTD simulations as reference:

$$\| \delta \|_2 = \sqrt{\frac{\sum_{x=0m}^{10m} (E_{y,iter} - E_{y,FDTD})^2}{\sum_{x=0m}^{10m} (E_{y,FDTD})^2}}.$$ 

Similarly to the iterative ADI-FDTD case, the error of the iterative LOD-FDTD simulation decreases with the number of iterations. Note that the decrease in error is slightly smaller than that obtained by otherwise decreasing the time step size, while implying similar computational overhead. The main advantage of a fixed-point iterative approach as proposed here is that it allows for adaptivity (both in space
Figure 8.2: Electric field $E_y$ along the $x$-axis calculated by the FDTD method, the iterative LOD-FDTD method, and the iterative ADI-FDTD method.

Figure 8.3: The $L_2$ norm of the error of the iterative LOD-FDTD method and the iterative ADI-FDTD method for various Courant factor $s$ and iteration numbers.
and time) at less cost. In other words, the number of iterations can be varied locally in space and/or time, i.e., in regions with large spatial derivatives [117] and/or at particular time steps. The accuracy of the iterative LOD-FDTD method can also be further improved by choosing appropriate initial guesses at each iteration [116].

In its present form, the iterative LOD-FDTD method cannot be readily extended to 3-D problems, since the extra terms concomitant to the two-step implementation are not equal to zero in 3-D. Note that a direct extension of the iterative ADI-FDTD method for 3-D problems with TE/TM coupling is also problematic [119]. The generalization of the iterative LOD-FDTD algorithm to 3-D is under investigation.

8.5 Concluding Remarks

We have introduced the iterative LOD-FDTD method to reduce the splitting error based on a fixed-point iteration at each time step. Numerical examples have demonstrated the efficacy of the iterative LOD-FDTD algorithm for spatially oversampled 2-D problems. Due to the reduced number of arithmetic operations, the iterative LOD-FDTD method is in general less costly than the iterative ADI-FDTD method. We believe that the proposed algorithm can be extended to dispersion-engineered and plasmon structures, although we consider simple examples to show the computational efficiency.
CHAPTER 9

NUMERICAL ARTIFACTS OF CE-ADI-FDTD ALGORITHM

9.1 Introduction

The ADI-FDTD method can be obtained from a perturbation of the Crank-Nicolson FDTD scheme. This perturbation produces a splitting error that is proportional to the time step size and to the magnitude of spatial derivatives [38]. Another numerical error inherent to the ADI-FDTD method is numerical dispersion. Since the numerical dispersion error increases with the time step size and/or the peak excitation frequency, the time step size is limited for a given (desired) accuracy and excitation spectrum [39, 121, 122]. Differently from the Crank-Nicolson FDTD method, the ADI-FDTD method produces two unwelcome numerical artifacts, viz. spurious charges and anomalous-mode propagation (i.e., negative group-velocity modes with positive phase velocities) [123].

The CE-ADI-FDTD method is an unconditionally stable method with better numerical dispersion properties than conventional ADI-FDTD method [40–45, 47]. In the CE-ADI-FDTD method, the maximum numerical dispersion error is determined by the fractional bandwidth rather than by the highest frequency of excitation. Hence,
the CE-ADI-FDTD method is ideally suited for narrowband problems. The carrier frequency information is incorporated analytically by means of modified field update equations in terms of the slowly-varying complex field envelopes.

In this chapter, we examine in detail spurious numerical artifacts present in the CE-ADI-FDTD algorithm, viz. spurious charges and anomalous-wave propagation. We contrast the ensuing properties of the numerical solutions versus those of the FDTD method and the conventional ADI-FDTD method. In particular, we address the fact that spurious charges in the CE-ADI-FDTD method have a fundamental difference from those of the ADI-FDTD method: they are static in the latter but implicitly time-harmonic in the former. These spurious charges are particularly detrimental to CE-ADI-FDTD simulations because they produce secondary radiation. We also show how the spurious charges in the CE-ADI-FDTD algorithm can be mitigated by a fixed-point iterative correction.

9.2 Numerical Dispersion Relation

The investigation of numerical artifacts in the CE-ADI-FDTD method is based on the dispersion relation. This follows the general approach employed in [123] for the conventional ADI-FDTD method. We briefly review that approach to fix the notation and contrast it with the CE case considered in sequence.

9.2.1 ADI-FDTD Algorithm

Three-dimensional (3-D) Maxwell’s curl equations for source-free, linear isotropic homogeneous media with no losses can be written as

\[ \partial_t \vec{U} + [\mathcal{R}] \vec{U} = [0], \quad (9.1) \]
where \( \vec{U} = (E_x, E_y, E_z, H_x, H_y, H_z)^T \) and

\[
[R] = \begin{pmatrix}
\frac{1}{\mu}[C] & -\frac{1}{\epsilon}[C] \\
\frac{1}{\mu}[C] & \frac{1}{\epsilon}[C] \\
0 & 0 \\
0 & 0
\end{pmatrix}.
\]

Here, \([0]_a\) is the \(a \times a\) zero matrix and \([C]\) is the curl matrix

\[
[C] = \begin{bmatrix}
0 & -\partial_z & \partial_y \\
\partial_z & 0 & -\partial_x \\
-\partial_y & \partial_x & 0
\end{bmatrix}.
\]  

Using the Crank-Nicolson FDTD formalism, update equations for the above can be written as

\[
\frac{\vec{u}^{n+1/2}_{i,j,k} - \vec{u}^n_{i,j,k}}{\Delta t} + [R] \frac{\vec{u}^{n+1}_{i,j,k} + \vec{u}^n_{i,j,k}}{2} = [0]_6,
\]  

where \(\vec{u}^n_{i,j,k}\) is the discrete field on the grid point \((i\Delta x, j\Delta y, k\Delta z)\) at time step \(n\), and \([R]\) is the discrete operator corresponding to \([R]\). We use calligraphic characters for fields and operators in the continuum and non-calligraphic characters for their discrete counterparts.

As described in Chapter 8, the ADI-FDTD formulation proceeds by factoring Eq. (9.3) (in an approximate fashion) into two sub-steps

\[
\left( [I]_6 + \frac{\Delta t}{2} [A] \right) \vec{u}^{n+1/2}_{i,j,k} = \left( [I]_6 - \frac{\Delta t}{2} [B] \right) \vec{u}^n_{i,j,k},
\]

\[
\left( [I]_6 + \frac{\Delta t}{2} [B] \right) \vec{u}^{n+1}_{i,j,k} = \left( [I]_6 - \frac{\Delta t}{2} [A] \right) \vec{u}^{n+1/2}_{i,j,k},
\]
where $[I]_a$ is the $a \times a$ identity matrix and $[R] = [A] + [B]$ with

$$[A] = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & \delta_y/\epsilon \\
0 & 0 & 0 & \delta_z/\epsilon & 0 & 0 \\
0 & 0 & 0 & 0 & \delta_x/\epsilon & 0 \\
0 & \delta_z/\mu & 0 & 0 & 0 & 0 \\
0 & 0 & \delta_x/\mu & 0 & 0 & 0 \\
\delta_y/\mu & 0 & 0 & 0 & 0 & 0
\end{bmatrix}, \quad (9.6)$$

$$[B] = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & \delta_z/\epsilon \\
0 & 0 & 0 & 0 & 0 & \delta_x/\epsilon \\
0 & 0 & \delta_y/\epsilon & 0 & 0 & 0 \\
0 & 0 & \delta_y/\mu & 0 & 0 & 0 \\
0 & \delta_x/\mu & 0 & 0 & 0 & 0 \\
\delta_z/\mu & 0 & 0 & 0 & 0 & 0
\end{bmatrix}, \quad (9.7)$$

where $\delta_\varsigma$ is the central difference operator corresponding to $\partial_\varsigma$, $\varsigma \in \{x, y, z\}$. Combining Eq. (9.4) and Eq. (9.5), we can write one full time-step of the ADI-FDTD update as

$$\left( [I]_6 + \frac{\Delta t^2}{4} [A][B] \right) \frac{\vec{u}^{n+1}_{i,j,k} - \vec{u}^n_{i,j,k}}{\Delta t} + \frac{[R]}{2} \frac{\vec{u}^{n+1}_{i,j,k} + \vec{u}^n_{i,j,k}}{2} = [0]_6. \quad (9.8)$$

In order to derive the dispersion relation, let us express the numerical field vector in terms of plane waves:

$$\vec{u}^n_{i,j,k} = \vec{u}_0 e^{j \omega n \Delta t} e^{-j (i \Delta x \beta_x + j \Delta y \beta_y + k \Delta z \beta_z)}, \quad (9.9)$$

where $(\beta_x, \beta_y, \beta_z)$ are real wavenumber components, $\omega$ is the complex frequency, and $j = \sqrt{-1}$. The above is a discrete analogue of $\vec{U} = \vec{U}_0 e^{j \omega t} e^{-j (\beta_x x + \beta_y y + \beta_z z)}$. Plugging Eq. (9.9) into Eq. (9.8), we have

$$\left\{ \left( [I]_6 + \frac{\Delta t^2}{4} [K_A][K_B] \right) \frac{2j \sin(\omega \Delta t/2)}{\Delta t} + \frac{[K]}{2} \frac{2 \cos(\omega \Delta t/2)}{2} \right\} \vec{u}_0 = [0]_6. \quad (9.10)$$

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with

\[
[K_A] = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & j\beta_{ny}/\epsilon \\
0 & 0 & 0 & j\beta_{nz}/\epsilon & 0 & 0 \\
0 & j\beta_{nz}/\mu & 0 & 0 & 0 & 0 \\
0 & 0 & j\beta_{nx}/\mu & 0 & 0 & 0 \\
j\beta_{ny}/\mu & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\] (9.11)

\[
[K_B] = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & -j\beta_{nz}/\epsilon \\
0 & 0 & 0 & 0 & 0 & -j\beta_{nx}/\epsilon \\
0 & 0 & -j\beta_{ny}/\mu & 0 & 0 & 0 \\
0 & -j\beta_{nz}/\mu & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\] (9.12)

\[
[K] = [K_A] + [K_B] = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{1}{\mu}[KC] & 0 & 0 & 0 & 0 \\
0 & [KC] & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\] (9.13)

Here, \(\beta_{nc}\) is the numerical wavenumber related to the real wavenumber as follows

\[
\beta_{nc} = \frac{2}{\Delta\varsigma} \sin \left(\frac{\beta \Delta\varsigma}{2}\right).
\] (9.14)

We note that \([KC]\) is equivalent to the cross product of the numerical wavenumber vector \(\vec{\beta}_n\) multiplied by \(-j\), i.e.,

\[
[K_C] = \begin{bmatrix}
0 & -(-j\beta_{nz}) & (-j\beta_{ny}) \\
(-j\beta_{nz}) & 0 & -(-j\beta_{nx}) \\
(-j\beta_{ny}) & (-j\beta_{nx}) & 0
\end{bmatrix} \mapsto -j\vec{\beta}_n \times
\] (9.15)

with \(\vec{\beta}_n = (\beta_{nx}, \beta_{ny}, \beta_{nz})\).

After some manipulations, we can simplify Eq. (9.10) to

\[
\left\{ \frac{2j}{\Delta t} \tan \left(\frac{\omega \Delta t}{2}\right) [I]_6 + [K]_{ADI} \right\} \vec{u}_0 = [0]_6,
\] (9.16)

with

\[
[K]_{ADI} = \left([I]_6 + \frac{\Delta t^2}{4}[K_A][K_B]\right)^{-1} [K].
\]

It is obvious that a non-trivial solution of Eq. (9.16) exists if

\[
\frac{2}{\Delta t} \tan \left(\frac{\omega \Delta t}{2}\right) = j\kappa
\] (9.17)
where $\kappa$ is an eigenvalue of $[K]_{ADI}$. It turns out that

$$\kappa = \pm j \sqrt{\frac{\beta^2_n + \zeta^2}{\mu \epsilon + \xi^2}},$$

(9.18)

with

$$\beta^2_n = \beta^2_{nx} + \beta^2_{ny} + \beta^2_{nz},$$

$$\zeta^2 = \frac{t^2}{4\mu \epsilon} (\beta^2_{nx} \beta^2_{ny} + \beta^2_{ny} \beta^2_{nz} + \beta^2_{nz} \beta^2_{nx}),$$

$$\xi^2 = \frac{t^6}{64 \mu^2 \epsilon^2} \beta^2_{nx} \beta^2_{ny} \beta^2_{nz}.$$  

Combining Eq. (9.17) and Eq. (9.18), we have the dispersion relation of the ADI-FDTD method [123]:

$$\frac{2}{\Delta t} \tan \left( \frac{\omega \Delta t}{2} \right) = \pm \sqrt{\frac{\beta^2_n + \zeta^2}{\mu \epsilon + \xi^2}}.$$  

(9.19)

### 9.2.2 CE-ADI-FDTD Algorithm

To construct the CE version of Maxwell’s curl equations, we write $\vec{U} = \Re \{ \tilde{\vec{U}} e^{j \omega_c t} \}$, where $\omega_c$ represents a carrier frequency. Note that $\vec{U}$ indicates actual components and $\tilde{\vec{U}}$ indicates the CE components. Hereafter, tilde characters indicate the CE fields.

We write modified Maxwell’s curl equations in terms of the CE components as

$$\partial_t \tilde{\vec{U}} + [\tilde{\mathcal{R}}] \tilde{\vec{U}} = [0]_6,$$

(9.20)

with $\tilde{\vec{U}} = \left( \tilde{\vec{E}}_x, \tilde{\vec{E}}_y, \tilde{\vec{E}}_z, \tilde{\vec{H}}_x, \tilde{\vec{H}}_y, \tilde{\vec{H}}_z \right)^T$ and $[\tilde{\mathcal{R}}] = j \omega_c [I]_6 + [\mathcal{R}]$. Using the Crank-Nicolson scheme, we can write the CE version of Crank-Nicolson FDTD update equations as follows

$$\frac{\tilde{u}_{i,j,k}^{n+1} - \tilde{u}_{i,j,k}^n}{\Delta t} + \frac{[\tilde{\mathcal{R}}] \tilde{u}_{i,j,k}^n + \tilde{u}_{i,j,k}^n}{2} = [0]_6.$$  

(9.21)
Following the ADI approach [49], we obtain one full time-step of the CE-ADI-FDTD update as

\[
\left( I_6 + \frac{\Delta t^2}{4}[\tilde{A}][\tilde{B}] \right) \frac{z^n_{i,j,k} - z^n_{i,j,k}}{\Delta t} + [\tilde{R}] \frac{z^n_{i,j,k} + z^n_{i,j,k}}{2} = [0]_6, \tag{9.22}
\]

where \([\tilde{R}] = [\tilde{A}] + [\tilde{B}], [\tilde{A}] = \frac{3\omega_c}{2}[I]_6 + [A], \) and \([\tilde{B}] = \frac{3\omega_c}{2}[I]_6 + [B] \). For actual implementations, the two-step of the CE-ADI-FDTD update is obtained by employing the Peaceman-Rachford approach [49]:

\[
\begin{align*}
&\left( I_6 + \frac{\Delta t}{2}[\tilde{A}] \right) \frac{z^{n+1/2}_{i,j,k}}{\Delta t} = \left( [I]_6 - \frac{\Delta t}{2}[\tilde{B}] \right) \frac{z^n_{i,j,k}}{\Delta t}, \tag{9.23} \\
&\left( I_6 + \frac{\Delta t}{2}[\tilde{B}] \right) \frac{z^{n+1}_{i,j,k}}{\Delta t} = \left( [I]_6 - \frac{\Delta t}{2}[\tilde{A}] \right) \frac{z^{n+1/2}_{i,j,k}}{\Delta t}. \tag{9.24}
\end{align*}
\]

Comparing Eq. (9.8) and Eq. (9.22), we notice that the CE-ADI-FDTD formulation can be constructed similarly from the ADI-FDTD formulation by employing the modified complex matrices ([\tilde{A}] and [\tilde{B}]).

In order to obtain the dispersion relation of the CE-ADI-FDTD method, we express the numerical CE field vector in terms of plane waves:

\[
\tilde{u}^n_{i,j,k} = \tilde{u}_0 e^{j\omega n \Delta t} e^{-j(i\Delta x\beta_x + j\Delta y\beta_y + k\Delta z\beta_z)}, \tag{9.25}
\]

where \((\beta_x, \beta_y, \beta_z)\) are real wavenumber components for the actual time-domain field and \(\omega\) is the complex envelope frequency. Substituting Eq. (9.25) into Eq. (9.22), we obtain

\[
\left\{ \frac{2j}{\Delta t} \tan \left( \frac{\omega \Delta t}{2} \right) [I]_6 + [\tilde{K}]_{ADI} \right\} \tilde{u}_0 = [0]_6, \tag{9.26}
\]

with

\[
[\tilde{K}]_{ADI} = \left( [I]_6 + \frac{\Delta t^2}{4}[\tilde{K}_A][\tilde{K}_B] \right)^{-1} [\tilde{K}].
\]
We note that $[\tilde{K}_A] = \frac{j\omega}{2}[I]_6 + [K_A]$, $[\tilde{K}_B] = \frac{j\omega}{2}[I]_6 + [K_B]$, and $[\tilde{K}] = [\tilde{K}_A] + [\tilde{K}_B] = j\omega_e[I]_6 + [K]$.

We can find out the dispersion relation of the CE-ADI-FDTD method by determining an eigenvalue $\tilde{\kappa}$ of $[\tilde{K}]_{ADI}$:

$$\frac{2}{\Delta t} \tan \left( \frac{\omega}{2} \right) = j\tilde{\kappa}. \quad (9.27)$$

The above dispersion relation can be solved numerically and recovers to the dispersion relation of the ADI-FDTD method Eq. (9.19) by setting $\omega_c = 0$.

### 9.3 Spurious Charges

We next consider the homogeneous system Eq. (9.26) by taking into account Eq. (9.27):

$$\left( -\tilde{\kappa}[I]_6 + [\tilde{K}]_{ADI} \right) \vec{u}_0 = [0]_6. \quad (9.28)$$

We can rewrite the above as

$$\left\{ -\tilde{\kappa} \left( [I]_6 + \frac{\Delta t^2}{4} [\tilde{K}_A][\tilde{K}_B] \right) + [\tilde{K}] \right\} \vec{u}_0 = [0]_6. \quad (9.29)$$

Let us denote $j\tilde{\kappa}$ as $\tilde{\kappa}_r$. After some manipulations, we express Eq. (9.29) in terms of the CE electric field and the CE magnetic field as

$$j \left( \omega_c + \tilde{\kappa}_r (1 - \alpha^2) \right) \begin{bmatrix} [I]_3 & [0]_3 \end{bmatrix} \begin{bmatrix} \vec{E}_0 \\ \vec{H}_0 \end{bmatrix} + \left( 1 - \tilde{\kappa}_r \frac{\Delta t}{2} \frac{1}{\mu} \right) \begin{bmatrix} [0]_3 \\ \frac{1}{\epsilon} [K_C] \end{bmatrix} \begin{bmatrix} \vec{E}_0 \\ \vec{H}_0 \end{bmatrix} + j\tilde{\kappa}_r \frac{\Delta t^2}{4 \mu \epsilon} \begin{bmatrix} [Q] \\ [0]_3 \end{bmatrix} \begin{bmatrix} \vec{E}_0 \\ \vec{H}_0 \end{bmatrix} = [0]_6,$$ \quad (9.30)
with
\[
\alpha = \frac{\omega_c \Delta t}{4},
\]
\[
[Q] = \begin{bmatrix}
0 & \beta_{nx} \beta_{ny} & 0 \\
0 & 0 & \beta_{ny} \beta_{nz} \\
\beta_{nz} \beta_{nx} & 0 & 0
\end{bmatrix}.
\]

Using Eq. (9.15), we finally obtain the plane-wave relation of the CE-ADI-FDTD method as
\[
\vec{E}_0 + \frac{\Delta t^2}{4 \mu \varepsilon} \left( \frac{1}{\omega_c + \tilde{\kappa}_r (1 - \alpha^2)} \right) [Q] \vec{E}_0 = -\frac{\beta_n}{\varepsilon} \left( \frac{1 - \tilde{\kappa}_r \Delta t \alpha}{\omega_c + \tilde{\kappa}_r (1 - \alpha^2)} \right) \beta_n \times \vec{H}_0, \quad (9.31)
\]
\[
\vec{H}_0 + \frac{\Delta t^2}{4 \mu \varepsilon} \left( \frac{1}{\omega_c + \tilde{\kappa}_r (1 - \alpha^2)} \right) [Q]^T \vec{H}_0 = \frac{\beta_n}{\mu} \left( \frac{1 - \tilde{\kappa}_r \Delta t \alpha}{\omega_c + \tilde{\kappa}_r (1 - \alpha^2)} \right) \beta_n \times \vec{E}_0, \quad (9.32)
\]

Similar to the ADI-FDTD method, the orthogonality between the electric and magnetic field vectors does not hold in the CE-ADI-FDTD method. Applying \( \hat{\beta}_n \cdot \) to Eq. (9.31), we can reveal the non-divergence free nature (spurious charges) in the CE-ADI-FDTD method:
\[
\hat{\beta}_n \cdot \vec{E}_0 = -\frac{\Delta t^2}{4 \mu \varepsilon \beta_n} \left( \frac{1}{1 + \omega_c / \tilde{\kappa}_r - \alpha^2} \right) \cdot \left( \beta_{nx}^2, \beta_{ny}^2, \beta_{nz}^2 \right) \cdot \vec{E}_0. \quad (9.33)
\]

It is clear that both non-orthogonality (between the CE electric field and the CE magnetic field) and non-divergence free behavior of the CE field are consequence of the splitting error. This will be illustrated in the numerical examples in Section 9.5.

We stress that \( \left[ \frac{1}{1 + \omega_c / \tilde{\kappa}_r - \alpha^2} \right] \) is a distinct factor in the field divergence of the CE-ADI-FDTD method, compared to the conventional ADI-FDTD method. As mentioned, setting \( \omega_c = 0 \) in Eq. (9.33) leads to the field divergence in the conventional ADI-FDTD method [123]. In Fig. 9.1, we plot in dB scale the dependency of the spurious field divergence on the CN and the FBW by calculating \( \frac{\Delta t^2}{1 + \omega_c / \tilde{\kappa}_r - \alpha^2} \) in free space (\( \mu = \varepsilon = 1 \)). Here CN= \( \sqrt{3} c_0 \Delta t / \Delta h \), where \( c_0 \) is speed of light in free space and
Figure 9.1: Effects of the CN and the FBW on the field divergence of the CE-ADI-FDTD method with PPW (points per wavelength) = 1000 at a carrier frequency.

$\Delta h (= \Delta x = \Delta y = \Delta z)$ is the spatial grid size. The field divergence is proportional to the bandwidth and also to the time step size.

According to Eq. (9.33), the spurious charges are larger at regions with sharp field distributions (i.e., large $\beta_n$). Although both ADI-FDTD and CE-ADI-FDTD simulations produce spurious charges, their nature is fundamentally different. Spurious charges in ADI-FDTD are truly static. On the other hand, spurious charges in CE-ADI-FDTD simulations are inherently time-harmonic and hence produce secondary radiation. This difference will be illustrated in Section 9.5.

### 9.4 Anomalous-Wave Propagation

To investigate anomalous-wave propagation in CE-ADI-FDTD simulations, we consider a plane wave along a 3-D diagonal grid direction ($\theta = \phi = 45^\circ$) on a grid with
\( \Delta h = 1 \text{ m} \) in free space. We define the normalized wavenumber and the normalized frequency as \( R_s = \beta \Delta h / 2 \) and \( R_t = (\omega + \omega_c)\Delta t / 2 \), respectively. Note that \( \beta \) is the wavenumber for the actual frequency \( (\omega + \omega_c) \) \([42, 45]\).

We consider two different mesh resolutions (points per wavelength, PPW) at a fixed carrier frequency. Fig. 9.2 shows the dispersion relation of the CE-ADI-FDTD simulation with PPW=1000 at a carrier frequency. We also plot the dispersion relation of the ADI-FDTD simulation, where \( R_t = \omega \Delta t / 2 \) with \( \omega \) being the actual frequency. Negative group-velocity modes with positive phase velocities may exist for large CNs. The dispersion relation of the CE-ADI-FDTD method is similar to that of the ADI-FDTD method at low wavenumbers, but starts to deviate for large CNs. Fig. 9.3 shows the dispersion relation of the CE-ADI-FDTD simulation with PPW=300 at the carrier frequency, where it is observed that the dispersion of the CE-ADI-FDTD method deviates from that of the ADI-FDTD method at high wavenumbers. We observe that anomalous-wave propagation modes are supported for \( \beta_{nx}\beta_{ny}\beta_{nz} \neq 0 \). Hence, anomalous-wave propagation modes are not supported in 1-D or 2-D. In addition, for 3-D problems, anomalous-wave propagation modes are supported only when the numerical wavenumber vector \( \vec{\beta}_n = (\beta_{nx}, \beta_{ny}, \beta_{nz}) \) has non-zero components in all three directions. To illustrate this point, we plot the dispersion relation for a 3-D problem with propagation direction \( \theta = 45^\circ, \phi = 0^\circ \) in Fig. 9.4. As can be seen from this figure, anomalous-wave propagation modes do not exist in this case.
Figure 9.2: Dispersion relation of the 3-D CE-ADI-FDTD simulation with PPW=1000 at a carrier frequency for a diagonal grid propagation ($\theta = 45^\circ, \phi = 45^\circ$), indicated in solid lines. Also the dispersion relation of the 3-D ADI-FDTD simulation is plotted in dash lines.

Figure 9.3: Same as Fig. 9.2 with PPW=300.
9.5 Numerical Examples

In this section, we illustrate the effect of spurious charges in CE-ADI-FDTD and ADI-FDTD simulations, stressing their differences. We simulate the radiation of \( z \)-directed magnetic current source \( M_z \) in a 2-D \( TE_z \) free-space problem. A Gaussian pulse modulated by a sine-wave located at the center of the computational domain is used as time-domain excitation. The computational domain has 1000 \( \times \) 1000 cells and is terminated by perfect magnetic conductor walls. The carrier frequency is \( f_c = 300 \) KHz and the space step size is \( \Delta h = 1 \) m (corresponding to PPW=1000 at \( f_c \)). The HPBW of 0.1\( f_c \) is used unless specified otherwise. In this 2-D problem, \( CN = \sqrt{2c_0\Delta t/\Delta h} \). Since the fields change sharply near the source, large spurious charges are expected to be produced in the near-field.
Figure 9.5: $\nabla \cdot \vec{E}$ in the ADI-FDTD simulation with CN=50 at $t = 37.7\mu s$. The spatial coordinates ($x$ and $y$) are in meters.

Figure 9.6: Same as Fig. 9.5 with CN=10.
Figs. 9.5 and 9.6 show snapshots of $\nabla \cdot \vec{E}$ in ADI-FDTD simulations with CN=50 and CN=10 respectively. The non-divergence free behavior of the field is clearly observed near the excitation. As the CN increases, the spurious charges also increase. Fig. 9.7 shows $|\nabla \cdot \vec{E}|$ and $|\vec{E}|^2$ in the ADI-FDTD simulation with CN=50 at the same time step in dB scale. The top snapshots [(a) and (b)] are taken when the excitation pulse is around its peak value while the bottom snapshots [(c) and (d)] are taken when the excitation pulse has already died off. The field distributions [(b) and (d)] result from the superposition of the field due to the magnetic current source $M_z$ and from the distributed spurious (static) charges. Note that the amplitude scales in Fig. 9.7 (c) and Fig. 9.7 (d) are not the same as in Fig. 9.7 (a) and Fig. 9.7 (b), for visibility purposes. Fig. 9.8 shows another ADI-FDTD simulation with CN=50, where $[A]$ and $[B]$ are interchanged. In this case, the spurious charges are distributed along the $x$ axis. For 2-D $TE_z$ problems, $E_x$ field is directly related to the splitting error $[A][B]$ in Fig. 9.7 while $E_y$ field is directly related to the splitting error $[B][A]$ in Fig. 9.8, which explains the difference in the distribution of spurious charges. The CN=10 case is shown in Fig. 9.9, where less spurious charges are produced compared to the CN=50 case.

Next, we illustrate the non-divergence free nature of the CE-ADI-FDTD method. Figs. 9.10 and 9.11 show snapshots of $\nabla \cdot \vec{E}$ in the CE-ADI-FDTD simulations with CN=50 and CN=10 respectively. Similar to ADI-FDTD simulations, spurious charges are produced by sharp field variations near the excitation (near-field) and also increase as the CN increases. For same CN, the CE-ADI-FDTD simulation produces, at early times, less spurious charges near the excitation than the ADI-FDTD simulation. This
Figure 9.7: $|\nabla \cdot \vec{E}|$ and $|\vec{E}|^2$ in the ADI-FDTD simulation with CN=50 (dB scale). The spatial coordinates $(x$ and $y)$ are in meters. The upper snapshots [(a) and (b)] are taken at $t = 37.7\mu s$ (excitation pulse still on). The lower snapshots [(c) and (d)] are taken at $t = 66\mu s$ (excitation pulse has died off). Note the different amplitude scales.
Figure 9.8: Same as Fig. 9.7 with [A] and [B] interchanged.

Figure 9.9: Same as Fig. 9.7 with CN=10. Note that the amplitude scales for showing the late-time responses [(c) and (d)] are decreased compared to the CN=50 case.
Figure 9.10: $\nabla \cdot \vec{E}$ in the CE-ADI-FDTD simulation with CN=50 at $t = 37.7\mu s$. The spatial coordinates ($x$ and $y$) are in meters.

is because the additional factor $\left[ \frac{1}{1+\omega \kappa_\gamma - \alpha^2} \right]$ in the CE-ADI-FDTD algorithm is less than one in this case.

Figs. 9.12 and 9.13 show snapshots of $|\nabla \cdot \vec{E}|$ and $|\vec{E}|^2$ in the CE-ADI-FDTD simulation with CN=50 for $[A][B]$-associated splitting error and $[B][A]$-associated splitting error, respectively. The CE-ADI-FDTD simulation with CN=10 is also shown in Fig. 9.14. Similar to ADI-FDTD simulations, the field distributions result from the superposition of the physical source $M_z$ and spurious charge effects. At early times [(a) and (b)], spurious charges are smaller in the CE-ADI-FDTD simulation, compared to the ADI-FDTD simulation. However, at later times [(c) and (d)], spurious charges in the CE-ADI-FDTD simulation have a stronger effect than those in the ADI-FDTD simulation due to their radiating nature of the former.
Figure 9.11: Same as Fig. 9.10 with CN=10.

Figure 9.12: $|\nabla \cdot \vec{E}|$ and $|\vec{E}|^2$ in the CE-ADI-FDTD simulation with CN=50 in dB scale. The spatial coordinates ($x$ and $y$) are in meters. The upper snapshots [(a) and (b)] are taken at $t = 37.7\mu s$. The lower snapshots [(c) and (d)] are taken at $t = 66\mu s$. The same amplitude scales are used as the ADI-FDTD case of Fig. 9.7. In (d), $|\vec{E}|^2$ near the center is too large in this amplitude scale and thus its distribution is not distinct. Compare these results with Fig. 9.7 results.
9.6 Fixed-Point Iterative Correction

The splitting error in (CE) ADI-FDTD simulations that contributes to the numerical artifacts discussed above can be mitigated by employing an iterative fixed-point correction. As a result, the incorporation of such iterative correction into the (CE) ADI-FDTD method leads to a reduction in the spurious charges. To demonstrate that, we introduce a figure of merit to measure the global amount of field divergence in the computational domain. Since $|\nabla \cdot \vec{E}|$ varies in both space and time, we consider the (time and space) average $|\nabla \cdot \vec{E}|$ in a square domain of size $(0.25\lambda_0)^2$ centered around the source position (where $|\nabla \cdot \vec{E}|$ is larger) and for the entire simulation time.
Figure 9.14: Same as Fig. 9.12 with CN=10. Note that the amplitude scales for showing the late-time responses [(c) and (d)] are decreased compared to the CN=50 case. In the lower snapshots, both $|\nabla \cdot \vec{E}|$ and $|\vec{E}|^2$ near the center are too large for the scale considered and thus their distributions are not distinct. Compare these results with Fig. 9.9 results.
Figure 9.15: Time- and space-averaged $|\nabla \cdot \vec{E}|$ versus the number of fixed-point iterations in ADI-FDTD and CE-ADI-FDTD simulations, for various CNs.

window, as follows

$$|\nabla \cdot \vec{E}|_{avg} = \frac{1}{250^2 N_{max}} \sum_{n=1}^{N_{max}} \sum_{i=375}^{625} \sum_{j=375}^{625} |\nabla \cdot \vec{E}_{n,i,j}|.$$  \hspace{1cm} (9.34)

Fig. 9.15 shows the effect of the iterative correction on $|\nabla \cdot \vec{E}|_{avg}$. As the number of iterations increases, $|\nabla \cdot \vec{E}|_{avg}$ decreases. The iterative correction is particularly effective for the CE-ADI-FDTD case with CN=10.

Finally, we illustrate the dependency of $|\nabla \cdot \vec{E}|_{avg}$ on the FBW of the excitation pulse in Fig. 9.16. In the conventional ADI-FDTD algorithm, spurious charge production does not depend on the FBW. However, for the CE-ADI-FDTD algorithm, spurious charges decrease as the bandwidth decreases. Furthermore, the effect of the FBW on $|\nabla \cdot \vec{E}|_{avg}$ becomes more pronounced as the CN decreases.
Figure 9.16: Time- and space-averaged $|\nabla \cdot \vec{E}|$ versus the FBW in ADI-FDTD and CE-ADI-FDTD simulations.

9.7 Concluding Remarks

In this work, we have illustrated that the CE-ADI-FDTD method supports spurious charges and anomalous-wave propagation modes, similar to the conventional ADI-FDTD method. These characteristics are ascribed to the splitting error. We note that spurious charges affect only 2-D and 3-D simulations. They do not affect 1-D (CE) ADI-FDTD simulations because there is no splitting error in that case. Therefore, DBE PhCs and SBE PhCs can be accurately analyzed by employing the CE-ADI-FDTD method in Chapter 3 and Chapter 4. Anomalous-wave propagation modes are not supported in 1-D or 2-D. For 3-D problems, anomalous-wave propagation modes are supported only when the numerical wavenumber vector $\vec{\beta}_n = (\beta_{nx}, \beta_{ny}, \beta_{nz})$ has non-zero components in all three directions.
We have stressed that the non-divergence free nature of the CE-ADI-FDTD method is fundamentally different from that of the ADI-FDTD method because spurious charges are implicitly dynamic in the CE-ADI-FDTD algorithm but static in the ADI-FDTD algorithm. As a consequence, the spurious charges in the CE-ADI-FDTD algorithm behave as secondary radiating sources. We have shown that a fixed-point iterative correction procedure can be used to reduce the spurious charges in the computational domain in both CE-ADI-FDTD and conventional ADI-FDTD simulations.
Both dispersion-engineered materials and plasmon waveguides are of great interest due to their extraordinary EM properties such as wave slowdown, EM unidirectionality, field enhancement, subwavelength confinement, etc. In this dissertation, we have developed time-domain algorithms intended for the study of dispersion-engineered materials and plasmon waveguides.

In Chapter 2, we have developed late-time stable FDTD algorithms for the analysis of MPhCs with ferromagnetic losses. This has been achieved by means of the combination of (1) the material-independent CFS-PML formulation and (2) the ADE scheme for modeling of fully dispersive (lossy) ferromagnetic materials. Employing the proposed method, we have illustrated unusual properties of MPhCs, viz. wave slowdown, field enhancement, and EM unidirectionality.

The study on slow-wave Fabry-Perot resonances in DBE PhCs and SBE PhCs has been performed in Chapter 3 and Chapter 4 respectively. Toward this purpose, we have extended the CE-ADI-FDTD method to anisotropic media. The total simulation time of the developed algorithm is reduced approximately two digit over the conventional FDTD algorithm with no loss of accuracy. We have found that the DBE
PhC response is more sensitive to the RBE PhC response under perturbations on geometrical and material parameters in Chapter 3. In Chapter 4, we have pointed out that the SBE dispersion curve can be obtained from the DBE dispersion curve by modifying geometrical parameters, e.g., the misalignment angle in anisotropic dielectrics in our study. We have figured out that the SBE PhC response is in general more sensitive to small (material and geometrical) perturbations versus the DBE PhC response, while the SBE PhC response is more sensitive to larger perturbations versus the DBE PhC response.

In Chapter 5, we have proposed a novel compact plasmon waveguide operating at optical communication band, based on an ordered array of Au nanorings. The CFS-PML-FDTD algorithm has been employed to determine proper geometrical parameters of nanorings yielding the plasmon resonance at $\lambda_0 \sim 1550$ nm. We have validated the subwavelength guiding, routing, and switching function of the proposed plasmon waveguide. Apart from the waveguiding application, ring-shaped nanostructures are also attractive for chemical and biological sensing applications, due to their high tunability and ability to contain high volumes of molecules [85].

In Chapter 6, we have studied a compact optical waveguide based on a coplanar structure. We have illustrated subwavelength confinement and moderate propagation loss of the SP-CPW. We have found out that ground connection leads to a reduction in mode conversion loss at discontinuities. We note that the SP-CPW has longer propagation length versus the nanoring-based plasmon waveguide, since the former does not rely on (lossy) near-field coupling mechanism.

In Chapter 7, we have introduced an efficient time-domain algorithm for wideband responses of plasmon structures. The multispecies Drude-Lorentz dispersion model
should be employed for plasmon structures in the visible spectrum due to interband transitions. The ADI scheme is incorporated into the FDTD modeling of the multispecies model, based on equivalent Drude current and Lorentz polarization terms. Numerical examples show its improved computational performance.

The splitting error is inherent to either the ADI-FDTD method or the LOD-FDTD method and it is proportional to the time step size and the magnitude of spatial derivatives. Therefore, the time step size in unconditionally stable FDTD algorithms above should be limited by a given accuracy, not by stability issues. In Chapter 8, we have introduced a novel LOD-FDTD method with reduced splitting error. Our techniques are based on the use of fixed-point iterations within each time step. This approach allows for spatial and/or temporal adaptivity and thus it can reduce overall computational overheads. Unfortunately, the direct incorporation of the iterative correction technique into either ADI- or LOD-FDTD algorithms in 3-D problems (with TE/TM coupling) suffers from stability issues. To extend the usefulness of iterative unconditionally stable algorithms, these problems must be solved.

In Chapter 9, we have contrasted the effect of the splitting error on CE-ADI-FDTD simulations versus those of ADI-FDTD simulations. We have in particular emphasized that spurious charges inherent to the splitting error have a deleterious effect on CE-ADI-FDTD simulations due to their time-harmonic nature. We have also shown that spurious charges can be reduced by a fixed-point iterative correction in the CE-ADI-FDTD algorithm, similar to the conventional ADI-FDTD algorithm.
APPENDIX A

THOMAS ALGORITHM: TRIDIAGONAL MATRIX SYSTEM SOLVER

The ADI-FDTD method needs to solve the tridiagonal matrix system. The implicit update equations in the ADI-FDTD algorithm can be formed as

\[
\begin{bmatrix}
  b_1 & c_1 & 0 & \cdots & 0 & 0 & 0 \\
  a_2 & b_2 & c_2 & \cdots & 0 & 0 & 0 \\
  0 & a_3 & b_3 & \cdots & 0 & 0 & 0 \\
  0 & 0 & a_4 & \cdots & c_{N-3} & 0 & 0 \\
  0 & 0 & 0 & \cdots & b_{N-2} & c_{N-2} & 0 \\
  0 & 0 & 0 & \cdots & a_{N-1} & b_{N-1} & c_{N-1} \\
  0 & 0 & 0 & \cdots & 0 & a_N & b_N
\end{bmatrix}
\begin{bmatrix}
  u_1 \\
  u_2 \\
  u_3 \\
  \vdots \\
  u_{N-2} \\
  u_{N-1} \\
  u_N
\end{bmatrix}
= \begin{bmatrix}
  r_1 \\
  r_2 \\
  r_3 \\
  \vdots \\
  r_{N-2} \\
  r_{N-1} \\
  r_N
\end{bmatrix}, \quad (A.1)
\]

where \( u_i \) represents an unknown field component and \( r_i \) is a known value. The above can be efficiently solved using the Thomas algorithm [49] as follows:

\( i = 1 \) :

\[
\begin{align*}
  u_i &= c_i / b_i \\
  g_i &= r_i / b_i
\end{align*}
\]

Loop on \( i \) from 2 to \( N - 1 \)

\[
\begin{align*}
  u_i &= c_i / (b_i - a_i u_{i-1}) \\
  g_i &= (r_i - a_i g_{i-1}) / (b_i - a_i u_{i-1})
\end{align*}
\]

End of loop on \( i \)
\[i = N:\]
\[u_i = (r_i - a_i g_{i-1}) / (b_i - a_i u_{i-1})\]

Loop on \(i\) from \(N - 1\) to 1

\[u_i = g_i - u_i u_{i+1}\]

End of loop on \(i\),

where \(g_i\) is the auxiliary term in the implementation of the Thomas algorithm. The above algorithm first eliminates the subdiagonal terms \((a_i)\) and then employ an backward substitution to obtain the solution. In fact, the Thomas algorithm is a simplified form of Gaussian elimination and its complexity is \(O(N)\).


