FDTD Analysis of a Metal Grating Structure at Oblique Incidence

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Abstract
To analyze a periodic structure consisting of a dispersive medium at oblique incidence, we apply the piecewise linear recursive convolution technique to the FDTD method with the split-field procedure. The validation of the present algorithm is confirmed through the analysis of a metal grating structure.

Keywords: Finite-difference time-domain method Oblique incidence Split-field procedure Dispersive medium Piecewise linear recursive convolution

1. Introduction
The finite-difference time-domain (FDTD) method with the periodic boundary condition (PBC) [1] has frequently been used to analyze a periodic structure. To treat a dispersive medium, the frequency-dependent (FD) FDTD methods have also been proposed. Recently, we have analyzed a polarizer based on a surface plasmon (SP) resonance [2] using the FD-FDTD method with the PBC. However, our previous work was limited to the analysis at normal incidence. This fact motivates us to extend the previous algorithm to the oblique incidence case [3].

The purpose of this paper is to formulate the FD-FDTD method with the PBC at oblique incidence in more detail [4]. Although Baida and Belkhir [5] also independently developed the algorithm at oblique incidence, they used the auxiliary differential equation (ADE) and the recursive convolution (RC) technique to treat a dispersive medium. In this paper, we use the piecewise linear (PL) RC technique [6], which requires less memory than that for the ADE technique and provides higher accuracy than that for the RC technique. We employ the Drude model to express a metal dispersion. For simplicity, the two-dimensional transverse-magnetic (TM) case is treated.

2. Numerical Method
At oblique incidence, the relationships between fields at the periodic boundary include a phase shift: 

\[ E_z(x = x_p, z) = E_z(x = 0, z) \exp(-jk_0 \Delta x \sin \theta), \]

\[ H_y(x = -\Delta x/2, z) = H_y(x = x_p - \Delta x/2, z) \exp(jk_0 \Delta x \sin \theta), \]

where \( x_p \) is the periodicity, \( k_0 \) is the free-space wavenumber, and \( \Delta x \) is the sampling width. To remove this phase shift, we introduce the field-transformation (FT) technique [1]:

\[ P = E \exp(jk_0 x), \quad Q = \eta_0 H \exp(jk_0 x), \]

where \( \eta_0 \) is the intrinsic impedance of free space. In addition, to treat the extra terms resulting from the FT technique, we apply the split-field procedure [7] to Maxwell’s equations. As a result, for the TM case we obtain the following equations:

\[ \frac{\partial P_x}{\partial t} = -c \frac{\partial Q_z}{\partial z} \] (1), \quad \[ \frac{\partial P_{za}}{\partial t} = c \frac{\partial Q_y}{\partial x} \] (2), \quad \[ \frac{\partial Q_y}{\partial t} = -c \frac{\partial Q_z}{\partial z} + c \frac{\partial Q_y}{\partial x} \] (3), \quad \[ (\varepsilon_r - \sin^2 \theta)P_z = \varepsilon_r P_{za} - Q_{ya} \sin \theta \] (4), \quad \[ Q_y = Q_{ya} - P_z \sin \theta \] (5),

where \( \varepsilon_r \) is the relative permittivity.
In a dispersive medium, \( \varepsilon_r \) is expressed as a function of frequency. We define the electric flux density with the FT technique as

\[
R = \varepsilon_0 \varepsilon_r P
\]

where \( \varepsilon_0 \) is the permittivity of free space. The relation between \( R \) and \( P \) in the time domain is approximately written as

\[
\Phi^{n-1} = \sum_{m=0}^{n-2} \left\{ P^{n-1-m} e^{- \gamma_m t} + P^{n-2-m} - P^{n-1-m} \varepsilon_m \right\}
\]

where \( \Phi \) is

\[
\Phi^{n-1} = \sum_{m=0}^{n-2} \left\{ P^{n-1-m} e^{- \gamma_m t} + P^{n-2-m} - P^{n-1-m} \varepsilon_m \right\}
\]

We express the dispersion of a metal as the Drude model. Therefore, \( \chi \) and \( \xi \) are, respectively, defined as

\[
\chi = \frac{\omega_p^2}{v_e} \left[ \Delta t \left( 1 - e^{-v_e \Delta t} \right) e^{-v_e \Delta t} \right],
\]

\[
\xi = \frac{\omega_p^2}{v_e} \left[ \frac{\Delta t}{2} \left( 1 - e^{-v_e \Delta t} \right) e^{-v_e \Delta t} + \frac{1}{v_e} e^{-v_e (m+1) \Delta t} \right],
\]

where \( \omega_p \) is the electron plasma frequency and \( v_e \) is the effective electron collision frequency.

Usually, Eq. (6) is transformed into a discrete-time form. This transformation is suitable for the treatment of Eqs. (1) and (2) because of the existence of the time derivative. Note that there is no time derivative in Eq. (4), so that the discrete-time form of Eq. (6) cannot be directly applied to Eq. (4). To tackle this problem, Baida and Belkhir [5] differentiated Eq. (4) with respect to time. This differential, however, leads to additional data storage. In this paper, we present another way to apply the PLRC technique to Eq. (4). More specifically, we express Eq. (6) as a recursive equation in the following way.

From Eq. (8), \( \chi_{m+1} \) is rewritten as

\[
\chi_{m+1} = \frac{\omega_p^2}{v_e} \left[ \Delta t \left( 1 - e^{-v_e \Delta t} \right) e^{-v_e \Delta t} \right] + \frac{\omega_p^2}{v_e} \Delta t e^{-v_e \Delta t} - \frac{\omega_p^2}{v_e} \Delta t e^{-v_e \Delta t}.
\]

Note that we have added extra terms, which cancel out each other. With the help of these terms, Eq. (10) can be transformed into

\[
\chi_{m+1} = \frac{\omega_p^2}{v_e} \Delta t \left( 1 - e^{-v_e \Delta t} \right) e^{-v_e \Delta t} + e^{-v_e \Delta t} \chi_m.
\]

It is found that Eq. (11) satisfies the recursive relation because \( \chi \) is obtained with the previous time step. In the same way as that for the \( \chi_{m+1} \), we represent \( \xi_{m+1} \) as a recursive equation:

\[
\xi_{m+1} = \frac{\omega_p^2}{2v_e} \Delta t \left( 1 - e^{-v_e \Delta t} \right) e^{-v_e \Delta t} + e^{-v_e \Delta t} \xi_m.
\]

We next substitute Eqs. (11) and (12) into Eq. (7), and eventually obtain

\[
\Phi^{n-1} = e^{-v_e \Delta t} \left[ \left( \chi^0 - \xi^0 \right) P^{n-1} + \xi^0 P^{n-2} \right] + \frac{\omega_p^2}{v_e} \Delta t \left( 1 - e^{-v_e \Delta t} \right) \left( \Psi^{n-1} - \frac{1}{2} P^{n-1} \right) e^{-v_e \Delta t} \Phi^{n-2},
\]

where \( \Psi \) is defined as \( \Psi^{n-1} = P^{n-1} + \Psi^{n-2} \). The use of Eq. (13) enables us to express Eq. (6) as a recursive equation.

Finally, we combine Eq. (6) with Eq. (4), and then obtain the following equation:

\[
\left( 1 + \chi^0 - \xi^0 - \sin^2 \theta \right) P^n = \varepsilon_p P^n - Q_{ya} \sin \theta - \xi^0 P^{n-1} - \Phi^{n-1}.
\]

Note that \( \varepsilon_p \) remains in the first term on the right-hand side of Eq. (14). This term can be calculated with \( \partial(c \varepsilon_p P_{za}) / \partial t = c \partial Q_y / \partial x \), which corresponds to Eq. (2). Thus, there is no need to apply the PLRC technique to Eq. (2).
3. Metal Grating Structure

To confirm the validity of the present algorithm, we analyze the metal gratings on a substrate shown in Fig. 1. The configuration is the same as that treated in Ref. [8]. The refractive indices of the metal (Ag) grating and the substrate are, respectively, set to be \( n_m = 0.144 - j11.214 \) at \( \lambda = 1.55 \) \( \mu \)m [9] and \( n_s = 1.51 \). The numerical parameters are chosen to be \( \Delta x = \Delta z = 0.005 \) \( \mu \)m. The TM wave is incident towards the direction defined by \( \theta \).

The incident wave is diffracted by the metal gratings. Then the propagation constant of the diffracted wave parallel to the grating surface is defined by

\[
k_d = k_0 \sin \theta + m \frac{2\pi}{\Lambda},
\]

where \( m \) is the diffraction order (\( m = \pm 1, \pm 2, \ldots \)). When \( k_d \) agrees with the propagation constant of the SP modes \( k_{sp} \), the SP is excited either at the Ag-air or at the Ag-substrate interface.

Fig. 2 shows the transmissivity as a function of wavelength. It is found for \( \theta = 0^\circ \) that the transmissivity approaches zero at \( \lambda = 1.25 \) and 1.63 \( \mu \)m. A similar tendency is also observed for \( \theta = 5^\circ \), although the minima are obtained at \( \lambda = 1.17, 1.31, 1.48, \) and 1.76 \( \mu \)m. It is worth mentioning that good agreement is found between our numerical results and the experimental results shown in Ref. [8].

We now investigate the propagation constants against wavelength. It should be noted that \( k_{sp} \) is obtained by the eigenmode analysis, in which the grating part is approximately modelled as a homogeneous layer. Figs. 3 and 4 show the results with \( k_d \) for \( \theta = 0^\circ \) and 5\(^\circ\), respectively, where all the data are normalized to \( 2\pi/\Lambda \). For \( \theta = 0^\circ \), \( k_d \) is determined by the second term on the right-hand side of Eq. (15). That is, \( k_d \) is equal to the integral multiple of \( 2\pi/\Lambda \). On the other hand, for \( \theta = 5^\circ \), we need to consider the effect of the first term of the right-hand side of Eq. (15). Therefore, \( k_d \) for each diffraction order is separated into two values.

It is seen for \( \theta = 0^\circ \) that \( k_d \) crosses \( k_{sp} \) at \( \lambda = 1.25 \) and 1.63 \( \mu \)m. These wavelengths correspond to those at which the minimal transmissivities are obtained. This correspondence is also found in the results for \( \theta = 5^\circ \).

4. Conclusions

We have extended the FDTD method with the periodic boundary condition to the analysis of a dispersive medium at oblique incidence. To treat the dispersive medium, we have applied the PLRC technique without using the discrete-time form. Through the analysis of the silver grating structure, we confirm the validity of the present algorithm. It is revealed that the transmissivity approaches zero, when the propagation constant of the diffracted wave agrees with that of the surface plasmon mode.

![Figure 1: Configuration.](image1)

![Figure 2: Transmissivity as a function of wavelength.](image2)
Figure 3: Normalized propagation constants for $\theta = 0^\circ$.

Figure 4: Normalized propagation constants for $\theta = 5^\circ$.

References


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