A General ADE-FDTD Algorithm for the Simulation of Dispersive Structures

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***Abstract*—A finite-difference time-domain general algorithm, based on the auxiliary differential equation (ADE) technique, for the analysis of dispersive structures is presented. The algorithm is suited for cases where materials having different types of dispersion are modeled together. While having the same level of accuracy, the proposed algorithm finds its strength in unifying the formulation of different dispersion models into one form. Consequently, savings in both memory and computational requirements, compared to other ADE-based methods that model each dispersion type separately, are possible. The algorithm is applied in the simulation of surface plasmon polaritons using the multipole Lorentz–Drude dispersion model of silver.**

***Index Terms*—Auxiliary differential equation (ADE), finite-difference time-domain (FDTD) method, material dispersion, surface plasmon polariton (SPP), Lorentz–Drude model.**

I. Introduction

A NUMBER of finite-difference time-domain (FDTD)-based algorithms for the analysis of dispersive materials have already been proposed in literature. These frequency-dependent algorithms can be categorized into three types: 1) the auxiliary differential equation (ADE) method [1]–[4]; 2) the Z-transform methods [5]; and 3) methods based on the discrete convolution of the dispersion relation [6]. The ADE method offers a more general representation for the dispersion relation with high flexibility in fitting arbitrary permittivity functions. Because no assumption of the linearity of the medium is made, the ADE method is particularly attractive for modeling nonlinear effects [2]. However, when the problem space involves materials having different types of dispersion with or without multipoles, the solution algorithms become complicated. The existing algorithms require a separate formulation for each dispersion type. To remove this complication, a recent ADE approach based on the formulation of the permittivity function as the sum of multiple complex-conjugate pole-residue pairs (CC-PR) has been reported [7]. The CC-PR approach offers two main advantages. First, it provides an additional degree of freedom in the parameter fitting process. Second, it unifies the treatment of different dispersion models within the general formulation. These advantages, however, come with a heavy computational cost as several complex-domain operations have to be performed in the FDTD algorithm every time step. Furthermore, this computational cost is justified only for the very limited number of cases and/or frequency ranges for which fitting using the classical dispersion models is not satisfactory. A computationally more efficient approach that serves the majority of dispersive materials is clearly needed. The ADE-FDTD algorithm proposed in this letter finds its strength in unifying the formulation of different dispersion models into one form. Consequently, savings in both memory and computational requirements are possible. The proposed algorithm is not only a significant improvement to the existing ADE methods for dispersive materials but is also very competitive to the CC-PR approach.

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II. Formulations and FDTD Algorithm

Starting with the most general form of dispersion, the Lorentzian form, the polarization field in the frequency domain can be written as

$$P(\omega) = \frac{a}{b + jc\omega - d\omega^2} E(\omega). \tag{1}$$

Shifting to the time domain through inverse Fourier transform gives

$$bP(t) + cP'(t) + dP''(t) = aE(t). \tag{2}$$

The key step towards the formulation of a consistent and general FDTD algorithm is approximating the time derivatives in (2) at time instant $n - 1$. Thus, one obtains the following update equation:

$$bP^{n-1} + c\frac{P^n - P^{n-2}}{2\Delta t} + d\frac{P^n - 2P^{n-1} + P^{n-2}}{\Delta t^2} = aE^{n-1} \tag{3}$$

or

$$P^n = \frac{4d - 2b\Delta t^2}{2d + c\Delta t} P^{n-1} + \frac{-2d + c\Delta t}{2d + c\Delta t} P^{n-2} + \frac{2a\Delta t^2}{2d + c\Delta t} E^{n-1} \tag{4}$$

which can be written in the form

$$P^n = C_1 P^{n-1} + C_2 P^{n-2} + C_3 E^{n-1}. \tag{5}$$

The constants C_1, C_2, and C_3 can be found for any form of dispersion relation (see Table I). In the case of multipole dispersion, the same relation is written for each pole with appropriate

TABLE I
SEVERAL DISPERSION TYPES AND THE CORRESPONDING COEFFICIENTS

Dispersion term in frequency domain	C_1	C_2	C_3
Lorentz Pole $P=\frac{a}{b+jc\omega-d\omega^2}E$	$\frac{4d-2b\Delta t^2}{2d+c\Delta t}$	$\frac{-2d+c\Delta t}{2d+c\Delta t}$	$\frac{2a\Delta t^2}{2d+c\Delta t}$
Drude Pole $P=\frac{a}{jc\omega-d\omega^2}E$	$\frac{4d}{2d+c\Delta t}$	$\frac{-2d+c\Delta t}{2d+c\Delta t}$	$\frac{2a\Delta t^2}{2d+c\Delta t}$
Plasma Frequency $P=\frac{a}{\omega^2}E$	2	-1	$2a\Delta t^2$
Debye term $P=\frac{a}{b+jc\omega}E$	$\frac{-2b\Delta t}{c}$	1	$\frac{2a\Delta t}{c}$
Conductivity term $P=\frac{a}{jc\omega}E$	0	1	$\frac{2a\Delta t}{c}$

values of the three constants. The update equation for the electric field intensity is given by

$$E^n=\frac{D^n-\sum_i^N P_i^n}{\varepsilon_0\varepsilon_\infty} \tag{6}$$

where N is the number of poles and the updated value of the electric flux density D^n is obtained using the standard Yee's algorithm.

III. SIMULATION RESULTS

First, the validity of the proposed algorithm is tested. A wideband pulse of the form $E_s(t)=e^{-(t-t_0)^2/T^2}$ with $t_o=0.1$ ns and $T=6$ ps, is normally incident from air onto a dispersive heterogeneous structure. The structure is composed of a 12-mm-thick Debye material sandwiched between air and a multipole Lorentzian material. The dispersion relation of the Debye medium is given by

$$\varepsilon_r(\omega)=\varepsilon_\infty+\frac{(\varepsilon_s-\varepsilon_\infty)}{1+j\omega\tau} \tag{7}$$

where $\varepsilon_s=81, \varepsilon_\infty=1.8$, and $\tau=5$ ns. The dispersion relation of the two-pole Lorentzian medium is given by

$$\varepsilon_r(\omega)=\varepsilon_\infty+(\varepsilon_s-\varepsilon_\infty)\sum_{p=1}^{2}\frac{G_p\omega_p^2}{\omega_p^2+j2\delta_p\omega-\omega^2} \tag{8}$$

where $\varepsilon_s=3, \varepsilon_\infty=1.5, \omega_1=40\pi\times10^9$ rad/s, $G_1=0.4, \delta_1=0.1\omega_1, \omega_2=100\pi\times10^9$ rad/s, $G_2=0.6$ and $\delta_2=0.1\omega_2$. The reflection coefficient at the air interface is theoretically given by

$$\Gamma=\frac{\Gamma_{AD}+\Gamma_{DL}e^{j2\beta_D d}}{1+\Gamma_{AD}+\Gamma_{DL}e^{j2\beta_D d}} \tag{9}$$

where d is the thickness of the Debye layer and β is the phase constant. The subscripts A, D and L designate, respectively, the air, Debye and Lorentz layers. Fig. 1 shows the simulated and exact reflection coefficient at the air interface. The agreement between the two curves is excellent. It should be noted here that, for this example, the FDTD solution algorithms proposed in [1] and [3] would require eight constants instead of just three. Next, the general algorithm is applied to simulate the propagation of a surface plasmon polariton (SPP) along a nanofilm. The simulated structure has been experimentally studied by Onuki *et al.* [8]. The guiding structure consists of a 30-nm thick Ti oxide layer deposited on a 30-nm thick Ag film. The SPP is excited using an input light of different wavelengths at the interface between the two layers. The dispersion relation of the Ag film is modeled into the FDTD algorithm using the six-pole Lorentz–Drude model with parameters as in [9]. In this case, the electric flux density is given by

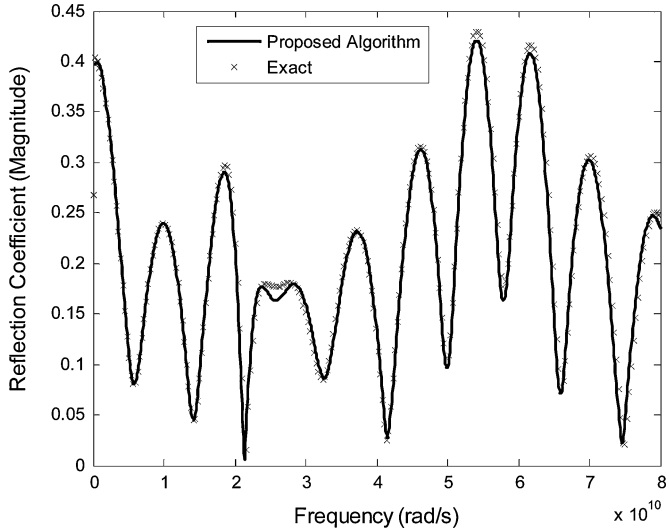

Fig. 1. Reflection coefficient as calculated by the proposed general algorithm and compared to exact solution.

$$D(\omega)=\varepsilon_0\left(1+\sum_i^N\frac{f_i\omega_i^2}{j\omega\tau_i+\omega^2}+\sum_p^M\frac{f_p\omega_p^2}{\omega_p^2+j\omega\Gamma_p-\omega^2}\right)E(\omega) \tag{10}$$

where f_i represents the weight of the ith Drude pole and f_p represents the weight of the pth Lorentz pole. Using the general algorithm, one immediately obtains

$$P^n=\frac{4}{2+\tau_i\Delta t}P^{n-1}-\frac{2-\tau_i\Delta t}{2+\tau_i\Delta t}P^{n-2}+\frac{2\varepsilon_0 f_i\omega_i^2\Delta t^2}{2+\tau_i\Delta t}E^{n-1} \tag{11}$$

for each Drude pole, and

$$P^n=\frac{4-2\omega_p^2\Delta t^2}{2+\Gamma_p\Delta t}P^{n-1}-\frac{2-\Gamma_p\Delta t}{2+\Gamma_p\Delta t}P^{n-2}+\frac{2\varepsilon_0 f_p\omega_p^2\Delta t^2}{2+\Gamma_p\Delta t}E^{n-1} \tag{12}$$

for each Lorentz pole. The computational domain is surrounded by a material-independent perfectly matched layer [10] to reduce the overall artificial reflections. A spherical point source pulse with carrier wavelengths of 532 and 830 nm is used for excitation. The point source is located close to the tip of the nanofilm at one of the ends. The SPP is excited and propagated

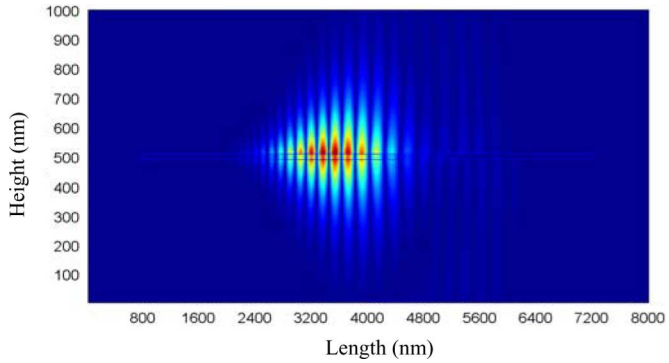

Fig. 2. SPP propagation in an Ag film modeled by Lorentz–Drude model (six poles); a snapshot of E_x.

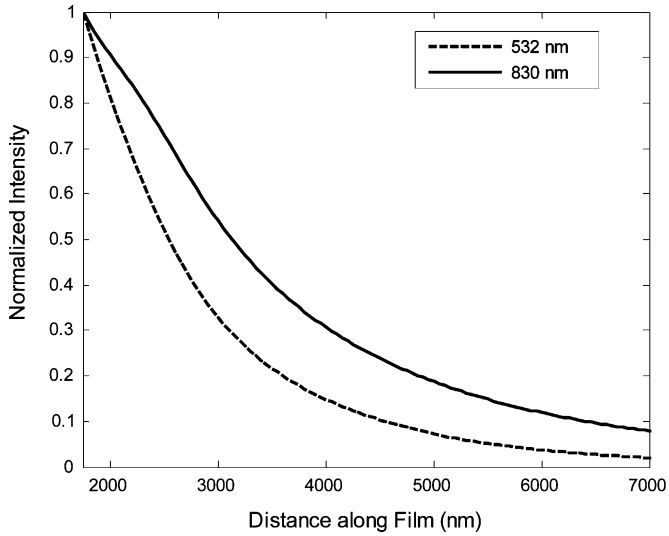

Fig. 3. Simulated propagation length of the SPP for carrier wavelengths of 532 and 830 nm.

along the nanofilm. Fig. 2 shows a snapshot of the E_x field component of the SPP corresponding to the 830-nm carrier wavelength, 23 fs into the simulation. The SPP is well-shaped with dispersion effects clearly demonstrated. In their experimental work, Onuki *et al.* studied the propagation length of the excited SPP for two different excitation wavelengths; namely, 532 and 830 nm. The propagation length was determined from intensity curves along the device. It is defined as the length where the intensity is reduced to $1/e$ of its value at the input side. The simulated results of the propagation length (Fig. 3) qualitatively agree with the experimental ones. The slight differences in the values of the propagation lengths for the two wavelengths are attributed to the difficulty in determining the exact location along the nanofilm where the SPP becomes mature and the normalization of the intensity becomes reliable. Also, in the FDTD algorithm, a constant permittivity has been assumed for the oxide layer. It should be noted here that the CC-PR approach would involve the storage of several complex-valued constants and the solution of six complex-domain equations [7, eq. (7)] in addition to several complex-domain multiplications and summations [7, eq. (6)]. It is also important to note that, within this energy range, the fitting of Lorentz–Drude pole pairs to experimental data is excellent [7], [9].

IV. Conclusion

An ADE-FDTD general algorithm for the analysis of dispersive structures is presented. The algorithm is suited for cases where materials having different types of dispersion are modeled together. In these situations, the same algorithm is used to fit all dispersion types. The accuracy of the algorithm was tested against analytical solutions. Furthermore, the algorithm was successfully applied in the simulation of SPP propagation along an Ag-based nanofilm having a multipole Lorentz–Drude dispersion relation.

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