Efficient Treatment of Dispersive Electric Permittivity in Finite-Difference Time-Domain Simulations of Advanced Photonic Devices

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***Abstract*—In this talk we demonstrate that when using the finite-difference time-domain simulations to study an interested photonic device, the dispersive electric permittivity of an involved medium can be modeled with the complex-conjugate pole-residue pairs very effectively. The theoretical foundation of the method is presented first, followed by a recent application example of simulating the single-molecule fluorescence enhancement by a gold bowtie nanoantenna.**

The finite-difference time-domain (FDTD) method is arguably the most popular numerical method for studying electromagnetic field distribution and wave propagation in a photonic device with complex geometry. Yet as a time-domain method, one challenge it often faces is the incorporation of the experimentally determined electric permittivity of a certain dispersive medium, which is normally available as a discrete dataset with varying values over a range of frequencies. In conventional FDTD practice, the typical approach is to fit such a dataset as the sum of multiple Debye poles and Lorentz pole pairs [1]. The computational cost incurred, however, can be significant for many realistic optical media, when a large number of poles are required in order to obtain a satisfactory fit.

To address this problem, we propose in [2] an alternative method that instead uses the complex-conjugate pole-residue (CCPR) pairs as the standard fitting basis for any given electric permittivity

$$\varepsilon(\omega) = \varepsilon_0\varepsilon_\infty + \varepsilon_0 \sum_{p=1}^{P} \left[\frac{c_p}{j\omega - a_p} + \frac{c_p^*}{j\omega - a_p^*} \right], \qquad (1)$$

where $(c_p,\ c_p^*)$ and $(a_p,\ a_p^*)$ are complex conjugate pairs. In fact, when $c_p = \Delta\varepsilon_p/(2\tau_p)$ and $a_p = -1/\tau_p$, (1) would represent a medium entirely modeled by Debye poles; on the other hand, when $c_p = j\Delta\varepsilon_p\omega_p^2/\left(2\sqrt{\omega_p^2 - \delta_p^2}\right)$ and $a_p = -\delta_p - j\sqrt{\omega_p^2 - \delta_p^2}$, (1) would represent a medium entirely modeled by Lorentz pole pairs. Here we adopt the same notation convention as in [1]. Nevertheless, despite that Debye poles and Lorentz pole pairs are special cases of CCPR pairs, there is some important distinction between them and general CCPR pairs. For a Debye pole, both c_p and a_p must be real. For a Lorentz pole pair, c_p must be imaginary. In contrast, for a general CCPR pair, both c_p and a_p can have a nonzero real part as well as a nonzero imaginary part, which adds additional degree of freedom in finding appropriate fitting parameters. Hence to achieve a particular modeling accuracy, one can usually expect to introduce fewer poles by using general CCPR pairs as the fitting basis than Debye poles and Lorentz pole pairs, which directly translates to lower computational cost.

The implementation of the method of CCPR pairs in a FDTD simulation can be done through either the piecewise-linear recursive convolution (PLRC) method or the auxiliary differential equation (ADE) method. For example, if the ADE method is used, which has the advantages when nonlinear effects need to be considered and when other differential equations such as the rate equation in laser simulations need to be included, with respect to each term in the summation in (1) two current items $\overrightarrow{J_p}(\omega)$ and $\overrightarrow{J_p'}(\omega)$ are introduced, where $\overrightarrow{J_p}(\omega) = \varepsilon_0\, c_p/\left(j\omega - a_p\right) j\omega\vec{E}(\omega)$ and $\overrightarrow{J_p'}(\omega) = \varepsilon_0\, c_p^*/\left(j\omega - a_p^*\right) j\omega\vec{E}(\omega)$. That leads to a set of time-domain differential equations, as in

$$\begin{aligned} \frac{d}{dt}\overrightarrow{J_p}(t) - a_p\overrightarrow{J_p}(t) &= \varepsilon_0 c_p \frac{d}{dt}\vec{E}(t) \\ \frac{d}{dt}\overrightarrow{J_p'}(t) - a_p^*\overrightarrow{J_p'}(t) &= \varepsilon_0 c_p^* \frac{d}{dt}\vec{E}(t). \end{aligned} \qquad (2)$$

Since according to (2), $\overrightarrow{J_p}(t)$ and $\overrightarrow{J_p'}(t)$ are always complex conjugate to each other in standard FDTD implementations, one only needs to store and update either one of them rather than both. For example, if $\overrightarrow{J_p}(t)$ is selected, the corresponding time-marching formulation can be derived by combining the auxiliary differential equation in (2) and Maxwell's curl equations, which is

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$$\vec{E}^{(n+1)\Delta t} = \left[\frac{2\varepsilon_0\varepsilon_\infty + \sum_{p=1}^{P} 2R_e(\beta_p) - \sigma\Delta t}{2\varepsilon_0\varepsilon_\infty + \sum_{p=1}^{P} 2R_e(\beta_p) + \sigma\Delta t}\right]\vec{E}^{n\Delta t} + \frac{2\Delta t \cdot \left[\nabla \times \vec{H}^{(n+1/2)\Delta t} - R_e \sum_{p=1}^{P}(1+k_p)\vec{J}_p^{\,n\Delta t}\right]}{2\varepsilon_0\varepsilon_\infty + \sum_{p=1}^{P} 2R_e(\beta_p) + \sigma\Delta t}$$

$$\vec{J}_p^{\,(n+1)\Delta t} = k_p \vec{J}_p^{\,n\Delta t} + \beta_p\left(\frac{\vec{E}^{(n+1)\Delta t} - \vec{E}^{n\Delta t}}{\Delta t}\right). \quad (3)$$

The notation definitions are omitted here due to space limitation. Please refer to [2] for details. As can be seen, in a given FDTD simulation, each new time step starts with computing $\vec{E}$, and then updating every $\vec{J_p}(1 \le p \le P)$, and finally obtaining $\vec{H}$ in the same way as in the case of a simple nondispersive medium.

The effectiveness of the method of CCPR pairs is demonstrated convincingly in the design of a gold bowtie nanoantenna structure that achieves an enhancement factor of single-molecule fluorescence ten times higher than what reported previously [4]. As shown in Fig. 1(a), the structure consists of a SiO_2 substrate, an indium tin oxide (ITO) layer, and a Poly(methyl methacrylate) (PMMA) layer. Inside the PMMA layer is a 20nm thick gold (Au) layer deposited on a titanium (Ti) layer of 4nm thick. The bowtie shape of the Au layer is clearly indicated in the simulated local electric field intensity profile in Fig. 1(b). To ensure an accurate FDTD simulation result over the entire interested wavelength range, general CCPR pairs are used to model Au's dispersive electrical permittivity. As shown in Fig. 2, with six CCPR pairs, one can find a permittivity function that is in excellent

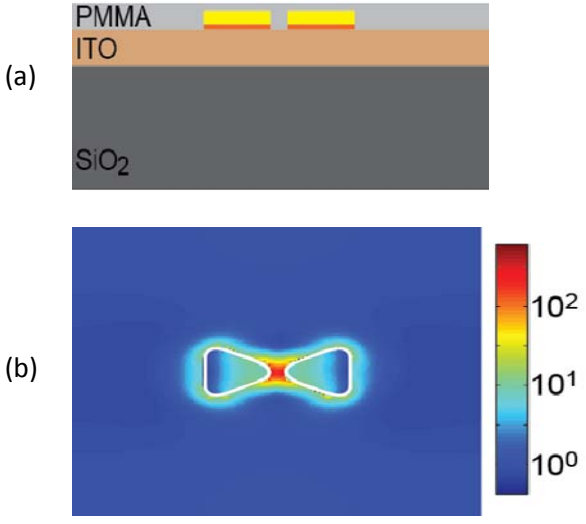

Fig. 1 (a) Side view of the bowtie antenna described in [4] that consists of a SiO_2 substrate (n=1.47), a 50nm ITO (n=2) layer, and a 30nm PMMA (n=1.49) layer, inside which is a gold bowtie structure of 20nm thick sitting on top of a Ti layer of 4nm. (b) Top view of the local electric field enhancement from the FDTD simulation.

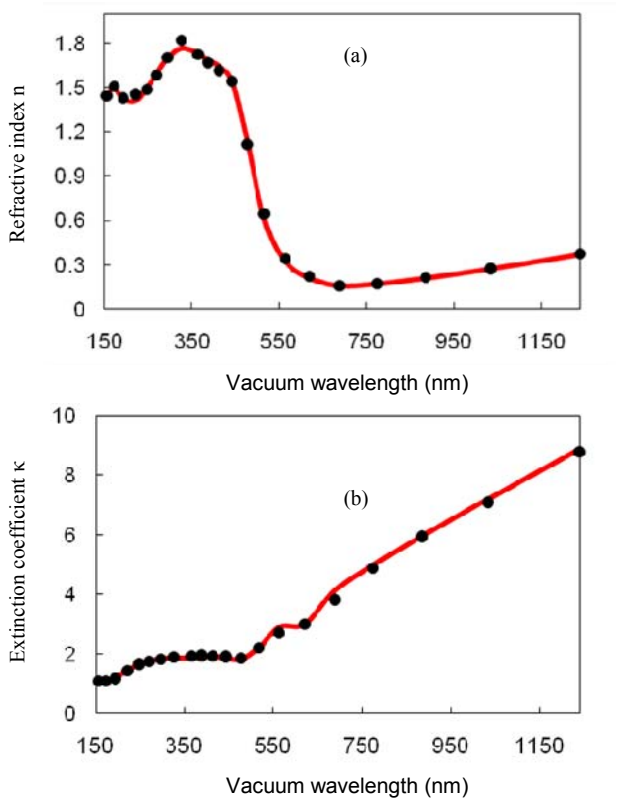

Fig. 2 (a) Real (b) Imaginary part of Au's complex refractive index *n-ik*. The black circles represent the experimental data taken from [3], and the red line represents the fitting result with 6 CCPR pairs.

agreement with the tabulated experimental data in [3]. In consequence, the fluorescence enhancement factor estimated from the FDTD simulation matches the values measured from the fabricated devices quite well.

Besides Au, other dispersive media such as metal silver (Ag), semiconductor quantum well $GaAs/Al_{0.4}Ga_{0.6}As$, and metal Tungsten (W) have also been proven [2][5] that their electric permittivity can be modeled with general CCPR pairs much more efficiently than the conventional approach.

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