General Dispersive Hybrid Implicit-Explicit Finite Difference Time Domain Formulations for Nanomaterial and Graphene Simulations

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Abstract

This paper presents general dispersive hybrid implicit-explicit finite difference time domain (HIE-FDTD) formulations for the simulation of nanomaterials, like Graphene. In the presented formulations, the material dispersion is modeled by a generalized dispersive model (GDM) that allows the description of wide range of dispersive media. The validity of the formulations is demonstrated by studying the surface plasmon polaritons (SPPs) waves in graphene nanomaterial.

Keywords: Nanomaterial, Graphene, Hybrid implicit-explicit finite difference time domain (HIE-FDTD), generalized dispersive model (GDM), surface plasmon polaritons (SPPs).

1. Introduction

In recent years, Graphene [?], which is considered to be one-atom two-dimensional (2-D) material, has recently attracted tremendous interest due to its unique electrical and mechanical properties [?]. This increases the interest in developing accurate and efficient numerical models to simulate graphene. In the last decade, considerable attention has been devoted for incorporating the hybrid implicit-explicit finite difference time domain (HIE-FDTD) technique [?] into the simulation of electromagnetic wave propagation in nanomaterials, such as graphene [?]-[?]. The advantage of this technique is that the temporal discretization is not confined by the structure smallest

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space cell size and, therefore, it increases the time step size considerable as compared with the classical explicit FDTD approach.

This paper presents general dispersive HIE-FDTD formulations for the simulation of nanomaterial. In the presented formulations, the material dispersion is described by a generalized dispersive model (GDM) [?], which allows the description of wide range of dispersive models, like Debye, for biological tissu in the MHz regime, Drude and Drude-Lorentz, for transition metals in the THz regime, and Sellmeier's law, for glass in the THz regime. The validity of the formulations is demonstrated by studying the surface plasmon polaritons (SPPs) waves in graphene nanomaterial.

2. Formulations

Considering a linear, isotropic and electrically dispersive medium, the frequency-domain Maxwell's curl equations can be written as

$$\nabla \times \widetilde{\mathbf{E}} = -\mathbf{j}\omega\mu_0\widetilde{\mathbf{H}} \tag{1}$$

$$\nabla \times \widetilde{\mathbf{H}} = \mathbf{j}\omega\varepsilon_0\varepsilon_\infty\widetilde{\mathbf{E}} + \mathbf{j}\omega\varepsilon_0\chi(\omega)\,\widetilde{\mathbf{E}} \tag{2}$$

where ε_∞ is the permitivity at infinite frequency and $\chi(\omega)$ is the electric susceptibility, which can be expressed in a generalized [1/2] Pade approximant as [?]

$$\chi(\omega) = \frac{\mathbf{j}\omega e_1 + e_0}{(\mathbf{j}\omega)^2 + \mathbf{j}\omega f_1 + f_0} \tag{3}$$

where e_1, e_0, f_1, and f_0 are constants. This generalized model unifies the common dispersive models in a single formulation. Substituting (3) into (2), and re-arranging the term $\mathbf{j}\omega(\omega)$ as

$$\mathbf{j}\omega\chi(\omega) = e_1 + \frac{(e_0 - e_1 f_1) - \frac{e_1 f_0}{\mathbf{j}\omega}}{\mathbf{j}\omega + f_1 + \frac{f_0}{\mathbf{j}\omega}} \tag{4}$$

the following time-domain equations describing the propagation of electromagnetic waves in a generalized dispersive medium can be obtained

$$
\begin{aligned}
-\mu_0 \frac{\partial \mathbf{H}}{\partial t} &= \nabla \times \mathbf{E} && (5)\\
\varepsilon_0 \varepsilon_\infty \frac{\partial \mathbf{E}}{\partial t} &= \nabla \times \mathbf{H} - \varepsilon_0 e_1 \mathbf{E} - \varepsilon_0 \mathbf{J} && (6)\\
\frac{\partial \mathbf{J}}{\partial t} &= \left(e_0 - e_1 f_1\right) \mathbf{E} - f_1 \mathbf{J} - f_0 \mathbf{P} && (7)\\
\frac{\partial \mathbf{P}}{\partial t} &= e_1 \mathbf{E} + \mathbf{J} && (8)
\end{aligned}
$$

Assuming that the nanomaterial sheet is located in the $x - z$ plane, and applying the standard HIE-FDTD implementation [**?**], the curl equations of (5) and (6) can be written in the discrete time domain as

$$
\begin{aligned}
\frac{\delta_t}{\Delta_t} H_x^{n+\frac{1}{2}} &= -\frac{1}{\mu_0}\left[\mu_t \delta_y E_z^{n+\frac{1}{2}} - \delta_z E_y^{n+1}\right] && (9)\\
\frac{\delta_t}{\Delta_t} H_y^{n+\frac{1}{2}} &= -\frac{1}{\mu_0}\left[\delta_z E_x^{n} - \delta_x E_z^{n}\right] && (10)\\
\frac{\delta_t}{\Delta_t} H_z^{n+\frac{1}{2}} &= -\frac{1}{\mu_0}\left[\delta_x E_y^{n+1} - \mu_t \delta_y E_x^{n+\frac{1}{2}}\right] && (11)\\
\frac{\delta_t}{\Delta_t} E_x^{n+\frac{1}{2}} &= \frac{1}{\varepsilon_0 \varepsilon_\infty}\left[\mu_t \delta_y H_z^{n+\frac{1}{2}} - \delta_z H_y^{n+1}\right] - \frac{e_1}{\varepsilon_\infty} \mu_t E_x^{n+\frac{1}{2}} - \frac{1}{\varepsilon_\infty} \mu_t J_x^{n+\frac{1}{2}} && (12)\\
\frac{\delta_t}{\Delta_t} E_y^{n+\frac{1}{2}} &= \frac{1}{\varepsilon_0 \varepsilon_\infty}\left[\delta_z H_x^{n} - \delta_x H_z^{n}\right] - \frac{e_1}{\varepsilon_\infty} \mu_t E_y^{n+\frac{1}{2}} - \frac{1}{\varepsilon_\infty} \mu_t J_y^{n+\frac{1}{2}} && (13)\\
\frac{\delta_t}{\Delta_t} E_z^{n+\frac{1}{2}} &= \frac{1}{\varepsilon_0 \varepsilon_\infty}\left[\delta_x H_y^{n+1} - \mu_t \delta_y H_x^{n+\frac{1}{2}}\right] - \frac{e_1}{\varepsilon_\infty} \mu_t E_z^{n+\frac{1}{2}} - \frac{1}{\varepsilon_\infty} \mu_t J_z^{n+\frac{1}{2}} && (14)
\end{aligned}
$$

where the field's spatial indices are not shown for the sake of brevity, $\mathbf{G}^n = \mathbf{G}\left(n\Delta_t\right)$, $(\mathbf{G} = \mathbf{E},\, \mathbf{H},\, \mathbf{J})$, δ_η, $(\eta = x,\, y,\, z)$, is the central difference operator with respect the coordinate η defined as

$$
\delta_\eta u^n = \frac{u^n(\eta + \frac{\Delta_\eta}{2}, \cdots) - u^n(\eta - \frac{\Delta_\eta}{2}, \cdots)}{\Delta_\eta} \qquad (15)
$$

where Δ_η is the space cell size in the η-direction, and δ_t, and μ_t are, respectively, the center difference and the central average operators with respect to time defined as

$$\delta_t u^n = u^{n+\frac{1}{2}} - u^{n-\frac{1}{2}} \tag{16}$$

$$\mu_t u^n = \frac{u^{n+\frac{1}{2}} + u^{n-\frac{1}{2}}}{2} \tag{17}$$

and finally, the **J** and **P** auxiliary variables are incorporated into the HIE-FDTD algorithm by discretizing (7) and (8) using a central difference and average operators approximated over one time step as

$$\frac{\delta_t}{\Delta_t}\mathbf{J}^{n+\frac{1}{2}} = (e_0 - e_1 f_1)\,\mu_t \mathbf{E}^{n+\frac{1}{2}} - f_1 \mu_t \mathbf{J}^{n+\frac{1}{2}} - f_0 \mu_t \mathbf{P}^{n+\frac{1}{2}} \tag{18}$$

$$\frac{\delta_t}{\Delta_t}\mathbf{P}^{n+\frac{1}{2}} = e_1 \mu_t \mathbf{E}^{n+\frac{1}{2}} + \mu_t \mathbf{J}^{n+\frac{1}{2}} \tag{19}$$

The advantage of the above formulations is that (18) and (19) can be used for implementing different models by setting the e and f coefficients accordingly. Consider, for example, the one-atom graphene material with thickness d and with an electric susceptibility expressed in the 1-10 THz frequency range as [?]

$$\chi(\omega) = \frac{\sigma_0/d\varepsilon_0}{j\omega(1 + j\omega\tau)} \tag{20}$$

where $\sigma_0 = e^2\tau k_B T\left(\frac{\mu_c}{k_B T} + 2\ln\left(e^{-\mu_c/k_B T} + 1\right)\right)/\pi\hbar^2$, τ is the scattering time, μ_c is the chemical potential, T is the temperature, $-e$ is the electron charge, $\hbar$ is the reduced Planck's constant, and k_B is the Boltzmann's constant. For this Drude dispersive material, e and f coefficients of the GDM model of (3) are found as $e_1 = 0$, $e_0 = \sigma_0/d\varepsilon_0\tau$, $f_1 = 1/\tau$, $f_0 = 0$, and $\varepsilon_\infty = 1$. Finally, it must be noted that the fields are updated from (9)-(14), (18) and (19), by following the same steps of the classical dispersive HIE-FDTD formulations [?]-[?].

3. Simulation study

In this section, numerical verification of the obtained formulations is discussed by studying the existence of the surface plasmon polaritons (SPPs) wave created at the interface between the graphene sheet and dielectric material. For this purpose, the graphene sheet with the parameters of: $T = 300$ Kelvin, $\mu_c = 0.5$ eV, $\tau = 0.5$ ps is positioned in the middle

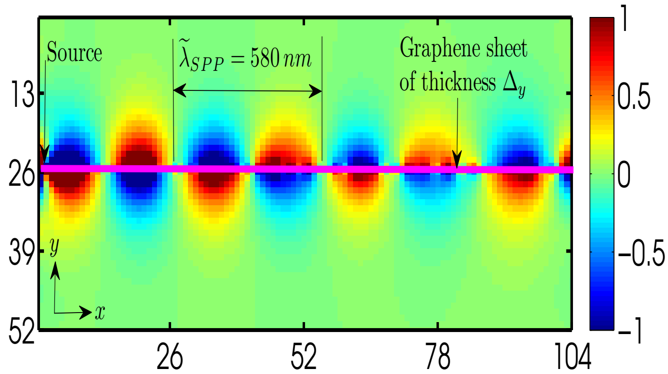

Figure 1: Spatial distribution of E_y electric field component at time step 20000 showing the SPP surface wave on the Graphene layer.

of a two-dimensional (2D) vacuum domain with a size of $104\Delta_x \times 52\Delta_y$, where $\Delta_x = 20$ nm, and $\Delta_y = 1$ nm. The graphene thickness is $d = 1$ nm, which is equivalent to one cell in the y-direction, i.e., Δ_y. The time step is selected to satisfy the classical HIE-FDTD limit for the 2D case, i.e., $\Delta_{t_{\max}}^{\mathcal{HIE}} = \Delta_x/c_0 = 6.6713 \times 10^{-18}$s [?]. The computational domain is terminated by 10 additional convolutional perfectly matched layer (CPML) cells [?]. The graphene sheet is excited by a sinusoidal dipole electric source with a frequency of 30 THZ. Fig. 1 shows the spatial distribution of E_y field component on the graphene sheet after 20,000 time steps, when the fields reach the steady state. The SPP surface wave on the graphene layer can be seen clearly from Fig. 1. The SPP guided wavelength $\left(\widetilde{\lambda}_{SPP}\right)$ can be extracted from Fig. 1 as $\widetilde{\lambda}_{SPP} = 29\Delta_x = 580$ nm, which is very close to the analytical guided wavelength computed from [?]

$$\lambda_{SPP} = \frac{\lambda_0}{\sqrt{1 - (2/\eta_0\sigma_{gr})^2}} = 584.79nm \tag{21}$$

where λ_0 and η_0 are the wavelength and intrinsic impedance in vacuum, respectively.

4. Conclusion

General HIE-FDTD formualtions of nanomaterial structures, like Graphene, is presented in this paper. The formulations allow the description of wide range of dispersive models. The conducted numerical example that investigates the existence of the SPP surface wave created at the interface between the graphene sheet and dielectric material validates the accuracy of the presented formulations.

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