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Wideband Finite-Difference Time-Domain Modeling of Graphene via Recursive Fast Fourier Transform

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Abstract—An efficient method based on the recursive fast Fourier transform (FFT) to incorporate both the intra-band and inter-band conductivity terms of graphene into the finite-difference time-domain (FDTD) method is proposed. As it only requires numerical values of the conductivity, it not only does not enforce any restrictions on the conductivity models, but also can directly take into account material properties obtained from measurement. It reduces the total computational cost from $O(N^2)$ to $O(N \log^2 N)$ where N is the length of the unknown. The FDTD method is also modified and proven to retain the stability condition of the standard FDTD method.

1. INTRODUCTION

Graphene is a 2-D sheet of bonded carbon atoms that form a honeycomb network, which has outstanding electrical, mechanical, thermal and magnetic properties [1]. Due to these unique properties, it has attracted much attention in the electromagnetic community, resulting in strong interest for studying it's electromagnetic behavior. Since in most cases obtaining the analytic solution of Maxwell's equations is impossible, the use of numerical simulation methods comes in helpful. Among various numerical methods, the finite-difference time-domain method has been shown to model graphene in a simpler and more efficient manner [2–7] in which graphene is modeled as a thin resistive sheet with a frequency-dependent conductivity (σ) consisting of two terms, namely the inter-band and the intra-band [8] terms. Modeling a frequency-dependent material, e.g., graphene, in finite-difference time-domain (FDTD) involves evaluation of a convolution: $\sigma(t) * E(t)$. The intra-band conductivity is defined by a Drude-like expression, which can be simply implemented in the FDTD using the standard approaches [2, 3]. However, the convolution involving the logarithmic approximation of the inter-band term can't be evaluated efficiently in a recursive manner and the computation cost increases as the time-stepping proceeds [5]. Several authors have alleviated this problem by approximating the inter-band term using high-order rational functions [4–6]. The order of the approximating function can be very high, which consequently increases the complexity and cost of the implementation. Furthermore, these methods require an accurate conductivity model of graphene, which may not be available in some applications such as graphene nanocomposites [9]. In these scenarios, measurement might be the primary approach to obtain electromagnetic properties in an accurate manner, which cannot be directly implemented into the FDTD code.

In this paper, we employ the recursive fast Fourier transform (FFT) to evaluate the time convolution in order to incorporate both inter-band and intra-band conductivity in the FDTD. This implementation needs only the values of the conductivity functions instead of the closed-form models as required by previous approaches. It reduces the complexity of brute-force evaluation of the convolution from $O(N^2)$ to $O(N \log^2 N)$. In addition, the FDTD algorithm is modified, and we prove that it preserves the stability condition of the standard FDTD algorithm compared to our previous paper [2] where the stability condition is a little limiting. Various numerical examples are presented to validate the method.

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2. FORMULATION

2.1. Graphene Conductivity Model

The graphene surface conductivity ($\sigma(\omega) = \sigma_{intra}(\omega) + \sigma_{inter}(\omega)$) is given by the Kubo formula in an integral form. The simplified Kubo formula for the intra-band conductivity term is [8]

$$\sigma_{intra}\left(\omega, \mu_c, \gamma, T\right) = \frac{je^2 k_B T}{(\omega - j2\gamma)\pi\hbar^2}\left(\frac{\mu_c}{k_B T} + 2ln\left(exp^{(-\mu_c/k_B T)} + 1\right)\right) \tag{1}$$

and the inter-band conductivity can be approximated by

$$\sigma_{inter}\left(\omega, \mu_c, \gamma\right) = -j\frac{\sigma_0}{\pi}\ln\left(\frac{2\left|\mu_c\right| - (\omega - j2\gamma)\hbar}{2\left|\mu_c\right| + (\omega - j2\gamma)\hbar}\right) \tag{2}$$

in which, ω is the angular frequency in radians per second, and γ is the scattering rate in s^{-1}. Also, μ_c is the chemical potential in eV, which can be controlled by chemical doping or by applying a bias voltage, T the temperature in Kelvin, e the electron charge, $\hbar$ the reduced Planck's constant, and k_B the Boltzmann constant.

The intra-band conductivity in Eq. (1), as expressed by a Drude-like expression [10], can be directly implemented in the FDTD formulation [2]; however, due to the complexity of the inter-band term in Eq. (2), it cannot be directly converted into a discrete-time relation.

2.2. Modeling Graphene in the FDTD Method

The FDTD method described here is motivated by the easy-to-implement formulation presented in our previous work [2]; however, the previous formulation imposes an extra constraint on the stability condition. Here, a modified formulation is presented to retain the stability condition of the standard FDTD. Maxwell's time-dependent curl equations used for FDTD method are

$$\frac{1}{\mu}\nabla \times E = -\frac{\partial H}{\partial t} \tag{3}$$

$$\frac{1}{\varepsilon}\nabla \times H = \frac{\partial E}{\partial t} + \frac{J}{\varepsilon} \tag{4}$$

where $J(t) = \sigma(t) * E(t)$ represents the integral convolution pertaining to the graphene conductivity. By discretizing Eqs. (3) and (4) in space and considering $\delta\{\cdot\}$ as the discrete curl operator, we will have the discrete form of the fields as

$$\frac{\delta\left\{E\right\}}{\mu} = -\frac{\partial H}{\partial t} \tag{5}$$

$$\frac{\delta\left\{H\right\}}{\varepsilon} = \frac{\partial E}{\partial t} + \frac{J}{\varepsilon}. \tag{6}$$

Using the leap-frog method to obtain the discrete form of Eqs. (5) and (6) in time and taking the average value of J results in the following equations

$$\frac{\delta\left\{E\right\}^{n+1}}{\mu} = -\frac{H^{n+\frac{3}{2}} - H^{n+\frac{1}{2}}}{\Delta t} \tag{7}$$

$$\frac{\delta\left\{H\right\}^{n+\frac{3}{2}}}{\varepsilon} = \frac{E^{n+1} - E^{n}}{\Delta t} + \frac{J^{n+1} + J^{n}}{2\varepsilon}. \tag{8}$$

Applying the trapezoidal integration rule to evaluate $J^n = \sigma * E^n$ over each interval yields

$$J^n = \frac{\Delta t}{2}\left(\sigma^1 E^n + \sigma^n E^1\right) + \Delta t\sum_{m=2}^{n-1}\sigma^{n-m+1}E^m. \tag{9}$$

Since calculating J^n requires having the value of E^n, we take the term containing E^n out of Eq. (9) and consider the rest as

$$G^n = \frac{\Delta t}{2}\left(\sigma^n E^1\right) + \Delta t \sum_{m=2}^{n-1} \sigma^{n-m+1} E^m \tag{10}$$

which clearly results in

$$J^n = \frac{\Delta t}{2}\left(\sigma^1 E^n\right) + G^n. \tag{11}$$

Subsequently, substituting Eq. (11) into Eq. (8) and taking the E^{n+1} to the left-hand side yields

$$E^{n+1} = \frac{1}{X}\left(\frac{\delta\left\{H\right\}^{n+\frac{3}{2}}}{\varepsilon} + \frac{E^n}{\Delta t}\right) - \frac{Y}{X} \tag{12}$$

in which $X{=}(1{+}\frac{\Delta t^2\sigma^1}{4\varepsilon})$ and $Y{=}\frac{\Delta t}{2\varepsilon}(G^{n+1}{+}J^n)$.

As can be seen in Eq. (12), the electric field update equation for the unknowns residing on the graphene sheet will have a correction term. After the standard update process is performed, Y can be updated separately and added to the electric field update followed by a division by the constant value of X. This approach greatly simplifies implementation without changing the standard FDTD update process. Needless to mention that the update equation for the magnetic field is not changed in this approach.

2.3. Recursive fast Fourier transform

Applying the trapezoidal integration rule to $J^n = \sigma(t) * E^n$ transforms the evaluation of the convolution integral into calculation of a summation with the basic form of

$$J^n = \sum_{m=1}^{n} \sigma^{n-m} E^m. \tag{13}$$

In order to evaluate Eq. (13) with the recursive FFT algorithm, we need to divide Eq. (13) into summations of lengths of 2^p (except the last one) starting with N the biggest possible 2^p, and in an descending order [11]

$$J^n = \sum_{m=1}^{N} \cdot + \sum_{m=N+1}^{N+2^{p_1}} \cdot + \sum_{m=N+2^{p_1}+1}^{N+2^{p_1}+2^{p_2}} \cdot + \ldots + \sum_{m=\ldots}^{n} \cdot \qquad p > p_1 > p_2 > \ldots \tag{14}$$

It is optimal to keep the length of 2^p-long summations equal to or greater than 64 [12]. Therefore, the length of the last summation will be less than 64, which should be evaluated directly.

In order to explain it clearly, we consider evaluation of Eq. (13) at the 890th time-step ($n = 890$). We first break Eq. (13) into several summations each of the length $2^p; p > 5$:

$$J^{(890)} = \sum_{m=1}^{\mathbf{512}} \cdot + \sum_{m=513}^{512+\mathbf{256}} \cdot + \sum_{m=769}^{768+\mathbf{64}} \cdot + \sum_{m=833}^{832+\mathbf{58}} \cdot \tag{15}$$

By breaking this summation to the lengths of 2^p, we can efficiently evaluate the first three summations using FFT. However, we need to calculate last remaining summation directly, as it is not efficient to further break a summation shorter than 64 to apply FFT which has been explained in [12].

It should be noted that only one summation has to be calculated (either directly or using FFT) at each time-step, because the length of a discrete convolution containing two vectors each with m entries is $2m - 1$. For example, once we evaluate the first summation at 512th time-step, we do not need to re-evaluate it until $n = 1024$. Similarly, we do not reevaluate the first three summations in Eq. (15) for any values of n between 833 and 895. The last two summations will be replaced by one summation from 769 to $768 + 128$ once we reach 896, which should be evaluated by FFT. When this process is applied recursively, more convolutions can be evaluated by FFT, and the total cost of evaluating the entire summation containing N steps is eventually reduced to $O(N\log^2 N)$ [12].

$$O\left(N\log N + 2\left(\frac{N}{2}\log\frac{N}{2}\right) + 4(\frac{N}{4}\log\frac{N}{4})\right) = O(N\log^2 N) \tag{16}$$

3. STABILITY ANALYSIS

Our stability analysis is based on the well-known von Neumann method, which involves substituting a traveling plane-wave trial function $E_\alpha = E_{\alpha 0} e^{-j(ik_x\Delta x + jk_y\Delta y)}$; $j=\sqrt{-1}$ into the FDTD equations and rewrite them in the form $X^{n+1} = \Lambda X^n$. In order to have a non-growing solution during time stepping, the eigenvalue of Λ with the largest magnitude should not lie outside of the unit circle in the complex plane [13]. For the sake of brevity, we only study the 2-D TM_z case here for which the governing equations are

$$\frac{\partial H_x}{\partial t} = -\frac{1}{\mu}\frac{\partial E_z}{\partial y} \tag{17}$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu}\frac{\partial E_z}{\partial x} \tag{18}$$

$$\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon}\left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}\right) - J_z/\varepsilon. \tag{19}$$

By discretizing (16)–(18) in space and time and substituting the trial functions, we reach

$$H_{x0}^{n+\frac{1}{2}} = H_{x0}^{n-\frac{1}{2}} - \frac{A\Delta t}{\mu} E_{z0}^n \tag{20}$$

$$H_{y0}^{n+\frac{1}{2}} = H_{y0}^{n-\frac{1}{2}} + \frac{B\Delta t}{\mu} E_{z0}^n \tag{21}$$

$$E_{z0}^{n+1} = E_{z0}^n + \left(\frac{B\Delta t}{\varepsilon} H_{y0}^{n+\frac{1}{2}} - \frac{A\Delta t}{\varepsilon} H_{x0}^{n+\frac{1}{2}}\right) - \frac{\Delta t}{2\varepsilon}\left(J_z^{n+1} + J_z^n\right) \tag{22}$$

where $A = \frac{j2}{\Delta y}\sin(k_y\frac{\Delta y}{2})$ and $B = \frac{j2}{\Delta x}\sin(k_x\frac{\Delta x}{2})$.

In the evaluation of J_z^n, we only take into account the intra-band conductivity term $\sigma(t) = \sigma_{intra}(t) = Ke^{-\alpha t}u(t)$, as the exponential form allows us to write the time-discrete convolution in a recursive fashion. However, the non-linear inter-band term does not possess such a property and makes the stability analysis complicated. Substituting the conductivity term into Eq. (9) and making some simplifications yields the following recursive relation

$$J^{n+1} = e^{-\alpha\Delta t}J^n + \frac{K\Delta t}{2}e^{-\alpha\Delta t}\left(E^n + e^{\alpha\Delta t}E^{n+1}\right). \tag{23}$$

Now, we write (19)–(22) in the matrix form shown below

$$\mathbf{M}\left[H_x^{n+\frac{1}{2}}; H_y^{n+\frac{1}{2}}; E_z^{n+1}; J_z^{n+1}\right] = \mathbf{N}\left[H_x^{n-\frac{1}{2}}; H_y^{n-\frac{1}{2}}; E_z^n; J_z^n\right] \tag{24}$$

in which

$$\mathbf{M} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ A\Delta t/\varepsilon & -B\Delta t/\varepsilon & 1 & \Delta t/2 \\ 0 & 0 & -Ke^{\alpha\Delta t}\Delta t/\varepsilon & e^{\alpha\Delta t} \end{bmatrix} \tag{25}$$

and

$$\mathbf{N} = \begin{bmatrix} 1 & 0 & -A\Delta t/\mu & 0 \\ 0 & 1 & B\Delta t/\mu & 0 \\ 0 & 0 & 1 & -\Delta t/2 \\ 0 & 0 & K\Delta t/2 & 1 \end{bmatrix}. \tag{26}$$

Studying the eigenvalue of $\mathbf{\Lambda}=\mathbf{M^{-1}N}$ shows that to meet $\max(|\mathrm{eig}(\mathbf{\Lambda})|) \le 1$ requirement, the time step should satisfy the following condition

$$\Delta t \le \frac{\sqrt{\mu\varepsilon}}{\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}}} \tag{27}$$

which is identical to the conventional stability condition, hence the new method does not limit the stability of the underlying FDTD method. Our stability analysis for the 3-D case yields the same result.

4. NUMERICAL RESULTS

To demonstrate the validity of the proposed formulation, we simulate the problem of plane-wave reflection by transmission through an infinite graphene sheet with $T = 300\,\mathrm{K}$, $\mu_c = 0.6\,\mathrm{eV}$ and $\Gamma = 11\,\mathrm{meV}/\hbar$ [4] using the 2-D FDTD method. The graphene sheet was located inside a parallel-plate waveguide with PEC walls and was truncated by a 10-layer thick perfectly matched layer (PML). As shown in Fig. 1, the computational domain contains 200×200 cells with $\Delta x = \Delta y = 2\,\mu\mathrm{m}$.

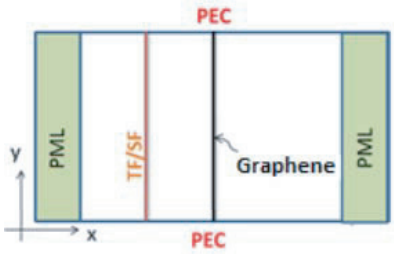

Figure 1. Graphene sheet in 2-D FDTD computational domain truncated by PML and PEC boundaries.

The transmission and reflection coefficients are obtained using discrete Fourier transform and are compared with the analytical solutions calculated by $Tr = 2/(2+\eta_0\sigma_{gr})$ and $\Gamma = Tr - 1$, in which η_0 is free space impedance, and σ_{gr} is the graphene conductivity including both inter-band and intra-band terms.

Figure 2 shows a comparison of the numerical and analytical results, for both the transmission and reflection coefficients; it demonstrates excellent agreement with the proposed method. The relative error between the analytical results and the proposed method is less than 0.05% in the considered frequency range.

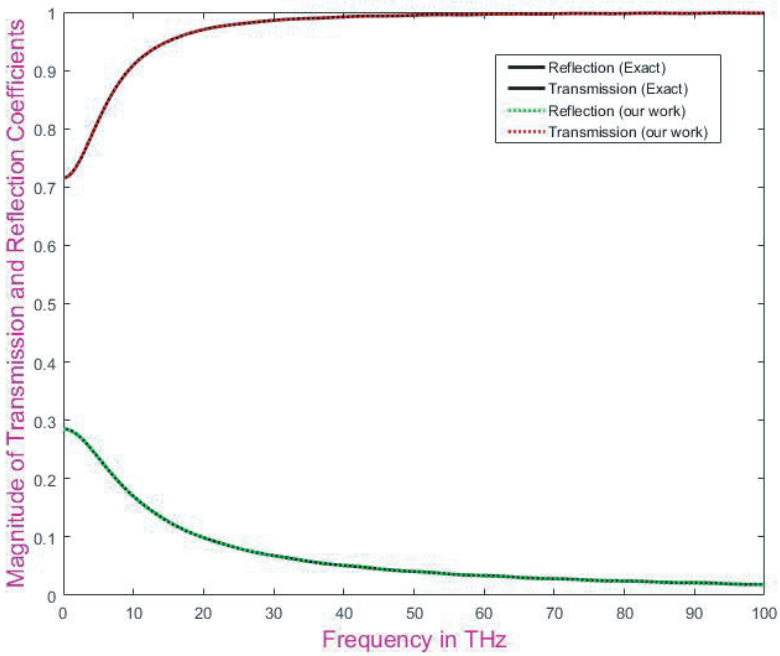

Figure 2. Comparison between transmission and reflection coefficients for a normally incident plane-wave.

Since graphene supports TM surface plasmon polariton (SPP) waves [14], it gives rise to micrometer size antennas resonating in the terahertz frequency range, yielding an advantage over their metallic counterparts. For this reason, as a second example, we simulate a SPP surface wave on two graphene layers excited by a sinusoidal dipole electric source at 30 THz frequency, as the SPP surface source in between the layers.

Figure 3 shows the spatial distribution of E_z at time step 40,000 when the field reaches steady-state. Our domain has 120×200 cells and $\Delta x = \Delta y = 20\,\text{nm}$. The time step is calculated as $\Delta t = \Delta x/(2c_0) = 3.3 \times 10^{-17}\,\text{s}$. In order to avoid spurious reflections from the boundary, the graphene layer is extended to PML regions of 10 cells. From the field distribution, we can easily extract the guided wavelength $\lambda_{SPP} = 29 \times 20 = 580\,\text{nm}$ while the results of the analytically calculated guided wavelength is $\lambda_{SPP} = \dfrac{\lambda_0}{re\sqrt{1-(\frac{2}{\eta_0\sigma_{gr}})^2}} = 577\,\text{nm}$.

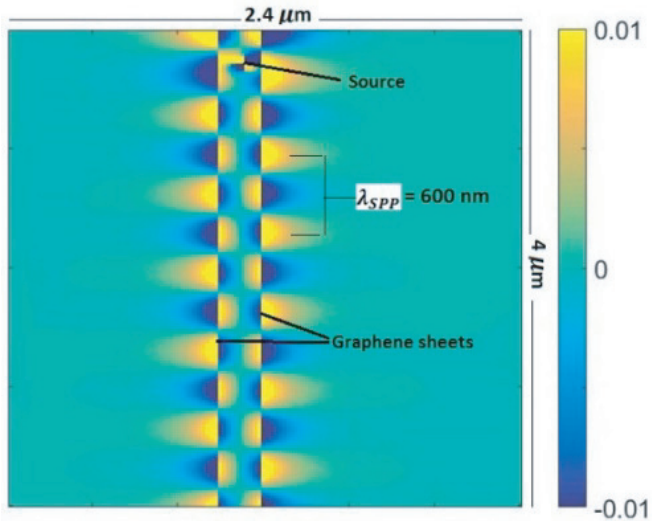

Figure 3. Shows the calculated field of the SPP-mode propagating along two graphene sheets with the dipole source located in between.

5. CONCLUSION

This work presents an efficient method to model graphene layers based on the recursive fast Fourier transform (FFT), in which both the intra-band and inter-band terms of its surface conductivity are modeled. This new approach only requires numerical values of the conductivity directly obtained from measurement, as opposed to the exact conductivity model required by previous methods. It is also shown to be fast and very cost effective.

Moreover, the new FDTD method can be implemented with minimal modifications using an existing code and leaves the stability condition of the underlying FDTD method intact.

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