Precise Modeling of Magnetically-Biased Graphene through a Recursive Convolution FDTD Method

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The consistent analysis and accurate implementation of magnetically-biased graphene layers is presented in this paper by means of a novel technique. After applying a magnetic bias perpendicular to graphene, its surface conductivity exhibits an anisotropic behavior and this significant effect is systematically modeled through a recursive convolution formulation combined with the 3-D finite-difference time-domain algorithm. The featured technique is applied to diverse graphene configurations and the extracted results are compared with those obtained from analytical expressions, thus revealing its efficiency over a wide frequency range.

***Index Terms*—Anisotropic conductivity, FDTD methods, magnetic bias, recursive convolution, surface boundary conditions.**

I. Introduction

FEW years ago, graphene, the one-atom thick carbon allotrope, was isolated to stable state [1], triggering an escalating research, due to its outstanding properties in a broad frequency range. Particularly, in the microwave spectrum, some noticeable attributes can be detected, if a magnetic bias, perpendicular to graphene, is applied, thus revealing its anisotropic nature [2], [3]. Although, this effect has been studied analytically for simple geometries, modern devices opt for more complex designs and specifications. As a consequence, for the numerical investigation of graphene, several modifications in the conventional algorithms, such as the finite-difference time-domain (FDTD) one, should be conducted. To this aim, in this paper, a new scheme, which employs the recursive convolution method (RCM), is introduced in order to effectively and rigorously model magnetically-biased graphene sheets by means of the FDTD technique. The proposed formulation is applied to an assortment of graphene arrangements, whereas all outcomes are compared to analytically-derived ones to verify its promising advantages as a potential simulation tool for such problems.

II. Theoretical Aspects

Throughout our analysis, graphene is deemed as an infinitesimally thin layer, defined by its anisotropic surface conductivity, which may be expressed as the two-dimensional dyad [4]

$$\overline{\overline{\sigma}}(\omega) = \begin{bmatrix} \sigma_{xx}(\omega) & \sigma_{xy}(\omega) \\ \sigma_{yx}(\omega) & \sigma_{yy}(\omega) \end{bmatrix}, \tag{1}$$

whose individual elements are calculated through

$$\sigma_{xx}(\omega) = \sigma_{yy}(\omega) = \sigma_o \frac{1 + j\omega\tau}{(\omega_c\tau)^2 + (1 + j\omega\tau)^2}, \tag{2a}$$

$$\sigma_{yx}(\omega) = -\sigma_{xy}(\omega) = \sigma_o \frac{\omega_c\tau}{(\omega_c\tau)^2 + (1 + j\omega\tau)^2}. \tag{2b}$$

Here, τ is the electron relaxation time that is independent of energy, ω_c the cyclotron frequency determined via the magnetic bias B, and σ_o a constant depending on temperature and the chemical potential μ_c of graphene. The latter is incorporated in the FDTD grid as the surface current $\vec{\mathbf{J}}_{gr}$ at the $z = k_0 + \frac{1}{2}$ plane (Fig. 1) and calculated via the surface conductivity and the corresponding electric field, $\vec{\mathbf{E}}$, as

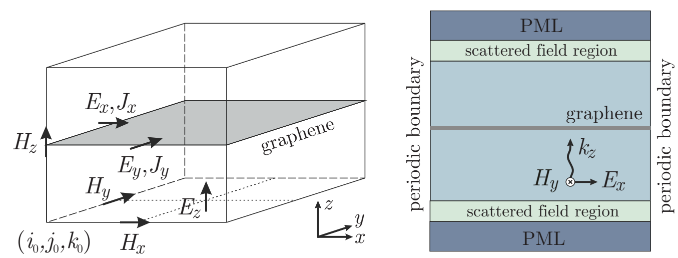

Fig. 1. The modified Yee cell including the contribution of graphene and the computational setup with the PML absorber and the periodic boundaries.

$$\vec{\mathbf{J}}_{gr} = \begin{bmatrix} J_x \\ J_y \end{bmatrix} = \overline{\overline{\sigma}}(\omega) \begin{bmatrix} E_x \\ E_y \end{bmatrix}. \tag{3}$$

Then, the contribution of graphene is imported in the FDTD method in the form of a surface current source [5], although other efficient techniques [6] can be used, owing to the generalized character of our concept. Essentially, the primary issue is to define the connection between the surface current and the electric field in the time domain. Thus, starting from (3), the surface current component is evaluated in terms of

$$\vec{\mathbf{J}}_{gr}(t) = \overline{\overline{\sigma}}(t) * \vec{\mathbf{E}}(t), \tag{4}$$

where $*$ denotes the convolution between the time-dependent surface conductivity and the electric field data. The preceding equation can be numerically implemented as a discrete convolution for the two components of the surface current, namely

$$\begin{bmatrix} J_x[(n+\frac{1}{2})\Delta t] \\ J_y[(n+\frac{1}{2})\Delta t] \end{bmatrix} = \sum_{m=0}^{n-1} \overline{\overline{\sigma}}[(n-m)\Delta t] \begin{bmatrix} E_x[(m+1)\Delta t] \\ E_y[(m+1)\Delta t] \end{bmatrix} \Delta t, \tag{5}$$

at the nth time-step of the simulation. Moreover, the surface conductivity in the time domain can be derived by applying the inverse Fourier transformation in (2). Hence, one acquires

$$\sigma_{xx}(t) = \frac{\sigma_o}{\tau} \cos(\omega_c t) \mathrm{e}^{-t/\tau} u(t) = \mathrm{Re}\{\sigma_c(t)\}, \tag{6a}$$

$$\sigma_{yx}(t) = \frac{\sigma_o}{\tau}\sin(\omega_c t)\mathrm{e}^{-t/\tau}u(t) = \mathrm{Im}\{\sigma_c(t)\}. \quad (6b)$$

In fact, (6) are the real and imaginary part of the complex time-dependent conductivity $\sigma_c(t)$, given by

$$\sigma_c(t) = \frac{\sigma_o}{\tau}\mathrm{e}^{-\gamma t}u(t), \quad (7)$$

where $\gamma = {}^1/_\tau - j\omega_c$. Correspondingly with $\sigma_c(t)$, we define the complex time-dependent surface currents J_{cx} and J_{cy} that determine the numerical discrete convolution of the complex-valued $\sigma_c(t)$ with the real-valued E_x and E_y, respectively

$$J_{cx}\left[(n+\tfrac{1}{2})\Delta t\right] = \sum_{m=0}^{n-1}\sigma_c[(n-m)\Delta t]E_x[(m+1)\Delta t]\Delta t, \quad (8a)$$

$$J_{cy}\left[(n+\tfrac{1}{2})\Delta t\right] = \sum_{m=0}^{n-1}\sigma_c[(n-m)\Delta t]E_y[(m+1)\Delta t]\Delta t. \quad (8b)$$

These complex-valued currents include the necessary terms of (5), which are extracted through the appropriate selection of the complex part (real or imaginary)

$$J_x = \mathrm{Re}\{J_{cx}\} - \mathrm{Im}\{J_{cy}\}, \quad J_y = \mathrm{Im}\{J_{cx}\} + \mathrm{Re}\{J_{cy}\}. \quad (9)$$

Note that the computation of J_{cx} and J_{cy} requires the solution of the discrete convolution that would, theoretically, need all the previous electric field values. However, based on the RCM notion [7], that all convolution terms, except the last one, can be recursively derived through the previous time-step, we get

$$J_{cx}\big|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k_0+\frac{1}{2}} = \mathrm{e}^{-\gamma\Delta t}\ J_{cx}\big|^{n-\frac{1}{2}}_{i,j+\frac{1}{2},k_0+\frac{1}{2}} + \frac{\sigma_o}{\tau}\mathrm{e}^{-\gamma\Delta t}\Delta t\ E_x\big|^{n}_{i,j+\frac{1}{2},k_0+\frac{1}{2}}, \quad (10a)$$

$$J_{cy}\big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j,k_0+\frac{1}{2}} = \mathrm{e}^{-\gamma\Delta t}\ J_{cy}\big|^{n-\frac{1}{2}}_{i+\frac{1}{2},j,k_0+\frac{1}{2}} + \frac{\sigma_o}{\tau}\mathrm{e}^{-\gamma\Delta t}\Delta t\ E_y\big|^{n}_{i+\frac{1}{2},j,k_0+\frac{1}{2}}. \quad (10b)$$

Now, (9) are easily derived and the real-valued J_x and J_y can be, finally, substituted in the FDTD update equations.

III. Numerical Validation and Conclusions

The effect of a normal incident plane wave on an infinite graphene sheet, inside vacuum, is examined for the verification of the proposed scheme. The setup of Fig. 1 consists of graphene's surface boundary perpendicular to z axis at the center of the domain, with periodic boundary conditions applied to attain the infinite graphene surface. Also, the total-field/scattered-field formulation is utilized to excite the normal incident wave, while an 8-cell thick perfectly matched layer (PML) terminates open boundaries along z axis. The computational space is divided into $20 \times 20 \times 120$ cells of $\Delta x = \Delta y = \Delta z = 1\,\mu$m, with a time-step of $\Delta t \simeq 1.9\,$fs, and a total simulation time set to $T_{\mathrm{total}} = 0.8\,$ns for the desired frequency response. Graphene parameters are selected as $\mu_c = 0.116\,$eV and $\tau = 0.129\,$ps, (extracted from typical graphene values of mobility $\mu = 10000\,\mathrm{cm}^2/(\mathrm{Vs})$ and carrier density $n_s = 10^{12}\,\mathrm{cm}^{-2}$) at room's temperature $T = 300\,$K, whereas magnetic field bias B can vary from 0.5 to 2 T with an increment of 0.5 T.

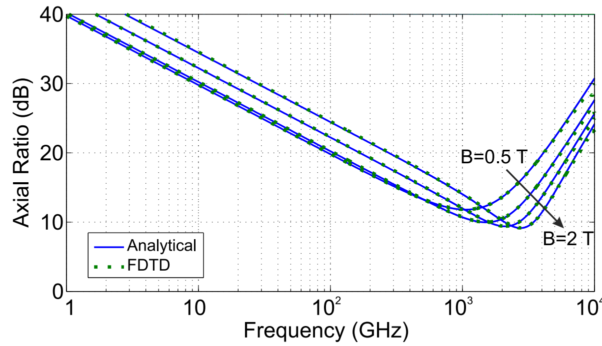

Fig. 2. Axial ratio of the transmitted wave versus frequency for different magnetic field bias values, increasing with an increment of 0.5 T.

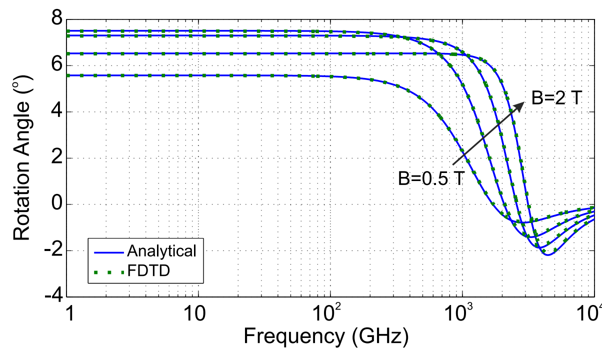

Fig. 3. Rotation of the transmitted wave versus frequency for different magnetic field bias values, increasing with an increment of 0.5 T.

The results, so extracted, are in excellent agreement with the theoretical estimations [8], with regard to the axial ratio of the transmitted wave and its rotation angle relative to the incident one, as, respectively, illustrated in Figs 2 and 3. Furthermore, the algorithm remains stable for over 10^6 time-steps and total computational resources are approximately limited to 5 MB. This performance leads to the conclusion that the developed method is highly accurate and stable over a wide frequency spectrum mandated by the presence of graphene sheets.

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