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Modified Perfectly Matched Layers in Finite-Difference Time-Domain Schemes for the Efficient Truncation of Propagating Graphene Surface Waves

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***Abstract* – The extension of the perfectly matched layer (PML) for the effective absorption of propagating graphene surface waves in finite-difference time-domain (FDTD) schemes is developed in this paper. Graphene is accurately modelled through its surface conductivity and is imported in the FDTD algorithm as a surface boundary condition. Also, the conventional PML equations are properly modified to include graphene's contribution. The validity of the proposed technique is numerically investigated in order to prove its noteworthy performance.**

I. Introduction

Recently, conspicuous advances have been conducted on the evolution of graphene, the truly two-dimensional carbon allotrope, that triggered the interest of the research community because of its extraordinary features at a broad frequency spectrum. Specifically, at the far-infrared region, graphene can support highly limited transverse magnetic surface plasmon polariton (SPP) waves that facilitate the design of two-dimensional devices for advanced configurations [1]. The performance of such structures is usually examined through numerical algorithms, including the finite-difference time-domain (FDTD) method, whose robustness and flexibility in the truncation of infinite computational domains renders it ideal for waveguiding systems. However, the popular perfectly matched layer (PML) absobing boundary condition fails to drastically attenuate graphene surface waves and thus appropriate modifications are required. Although, a modified PML scheme has been lately proposed [2], it treats graphene as a subcell of the entire Yee cell, while methods that model the material as a surface boundary condition are also very efficient owing to their accuracy [3]. Hence, it is the purpose of this paper to present a modified PML which can consistently consider the contribution of graphene in 2D and 3D computational domains. Finally, the merits of the proposed method are thoroughly validated by measuring the relative error generated by the featured PML region.

II. Theoretical Analysis

In our formulation, graphene is deemed as an infinitesimally thin, local two-sided layer, featured by a surface conductivity $\sigma(\omega, \mu_c, \Gamma, T)$, with ω the radian frequency, μ_c the chemical potential regulated by a gate voltage, Γ a phenomenological scattering rate assumed to be energy independent, and T the temperature. As in the frequency range under study, interband contributions are trivial, only the intraband term of the above conductivity is computed via the general Kubo formula as

$$\sigma_{\text{intra}}(\omega, \mu_c, \Gamma, T) = \frac{e^2 k_B T}{\pi \hbar^2 (j\omega + 2\Gamma)} \left[\frac{\mu_c}{k_B T} + 2 \ln \left(e^{-\mu_c / k_B T} + 1 \right) \right] = \frac{A}{j\omega + 2\Gamma}, \tag{1}$$

with $-e$ the electron's charge, $\hbar$ the reduced Planck's constant, and k_B the Boltzmann's constant. In this context, graphene is imported in the modified FDTD algorithm as a surface boundary condition placed, at the typical Yee cell, on the same location as the corresponding electric field component, namely E_x for the 2D case and E_x, E_z for the 3D case, as depicted in Fig. 1. Consequently, surface current $\vec{J}_{gr} = \sigma_{\text{intra}} \vec{E}$, due to graphene's surface conductivity, can be precisely incorporated in Ampere's law

$$\nabla \times \vec{H} = \varepsilon \frac{\partial \vec{E}}{\partial t} + \vec{J}_{gr}. \tag{2}$$

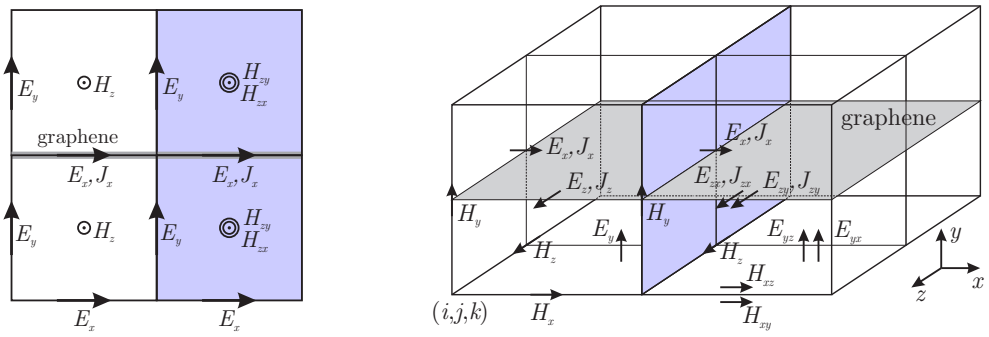


Fig. 1: The modified Yee cell including graphene's contribution for (a) a 2D and (b) a 3D computational domain.

The update equations to be altered are those that include graphene's surface conductivity, while the remaining components are extracted by means of the conventional FDTD algorithm [3, 4].

Firstly, the 2D TE mode grid is investigated. The particular scenario is quite simple as the electric field component in the PML region, is not split in two different components and graphene is straightforwardly included (Fig. 1a). Note that magnetic component H_z is updated through the original PML scheme [5]. Thus, one obtains

$$\varepsilon_0 \frac{\partial E_x}{\partial t} + \sigma_y E_x + J_x = \frac{\partial (H_{zx} + H_{zy})}{\partial y}. \tag{3}$$

Conversely, the 3D case is far more involved owing to the mandatory inevitable of electric field components, that contain graphene's contribution, in the PML region [6]. This difficulty is overcome by splitting graphene surface current into two different components, in accordance to the electric field (Fig. 1b), and separately solving the resulting equations, while all other components are time-advanced on terms the regular PML concept. The aforementioned analysis leads to

$$\varepsilon_0 \frac{\partial E_{zx}}{\partial t} + \sigma_x E_{zx} + J_{zx} = \frac{\partial (H_{yx} + H_{yz})}{\partial x}, \tag{4a}$$

$$\varepsilon_0 \frac{\partial E_{zy}}{\partial t} + \sigma_y E_{zy} + J_{zy} = -\frac{\partial (H_{xy} + H_{xz})}{\partial y}. \tag{4b}$$

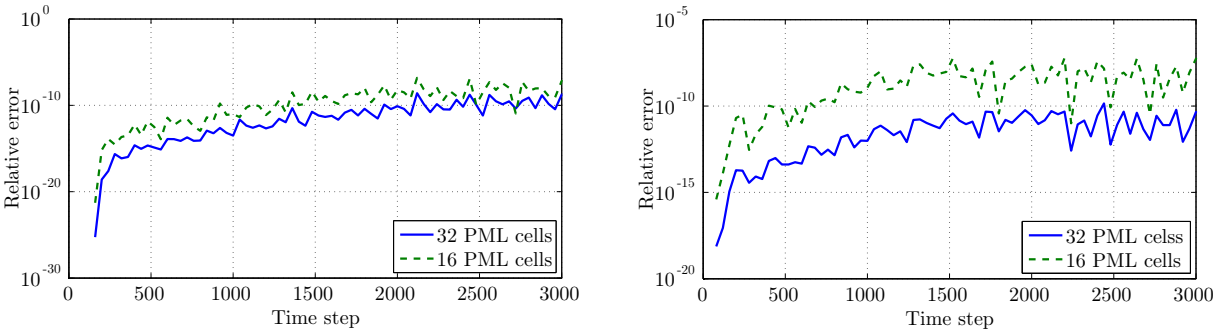
Having determined the pertinent formulas, central differences are, next, applied in order to extract the desired components. Notice that since (3) and (4) are similar, we focus, for brevity, only on the temporal integration of (3), which becomes

$$\begin{aligned} E_x\Big|_{i+1/2,j}^{n+1} &= E_x\Big|_{i+1/2,j}^{n} \frac{2\varepsilon_0 - \sigma_y \Delta t}{2\varepsilon_0 + \sigma_y \Delta t} + \\ &+ \frac{2\Delta t}{2\varepsilon_0 + \sigma_y \Delta t} \left[\frac{1}{\Delta y} \left(H_z\Big|_{i+1/2,j+1/2}^{n+1/2} - H_z\Big|_{i+1/2,j-1/2}^{n+1/2} \right) - \frac{1}{\Delta z} J_x\Big|_{i+1/2,j}^{n+1/2} \right]. \end{aligned} \tag{5}$$

It is stessed that surface current J_x, in the time domain, is normally calculated through an auxiliary differential equation (ADE) scheme, because of its frequency dependent nature [4].

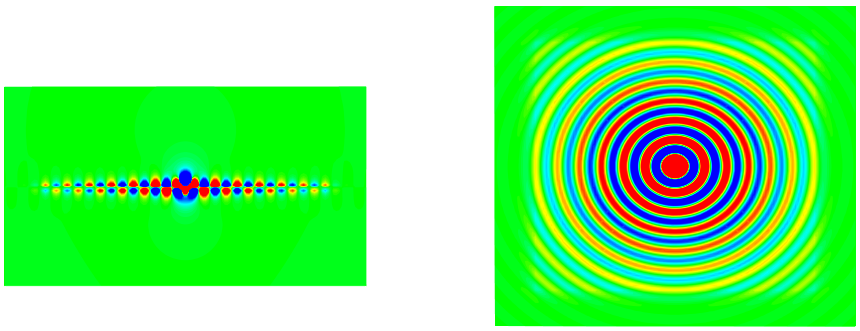
III. Numerical Results and Discussion

The efficient absorption of graphene surface waves through the proposed modified PML is explored in detail by measuring its global error throughout the computational domain. For this reason, a 2D 100×50 and a 3D $100 \times 50 \times 100$ grid is implemented, which have graphene surface placed perpendicular to $y-$axis, whereas the spatial increments is $\Delta x = \Delta y = \Delta z = 3.5\,\mu$m and time-steps are $\Delta t = 8.2\,$fs and $\Delta t = 6.2\,$fs, respectively.



(a) (b)

Fig. 2: Temporal evolution of the relative global error of the proposed PML condition (squared electric field values summed throughout the entire domain) for (a) a 2D and (b) a 3D lattice.



(a) (b)

Fig. 3: Distribution of the normal-to-graphene electric field component for (a) a 2D and (b) a 3D lattice.

Moreover, two PML regions are realized for each lattice, consisting of 16 and 32 cells, with the reflection required to be less than 10^{-5} for a quadratically graded loss with respect to depth. Observe that both computational domains, considered to provide the exact solution when compared the featured PML scheme, are large enough to avoid the reflection from their outer boundaries. Also, graphene's chemical potential is chosen as 0.1 eV and the scattering rate 0.11 meV, i.e. appropriately low to decrease the losses of the surface wave due to graphene's finite conductivity. Numerical results, illustrated in Fig 2, indicate that the global is kept at extremely low levels, thus verifying the remarkable performance of the proposed method. However, a large number of PML cells is needed to minimize the overall reflections, mainly owing to the nature of graphene surface waves. Also, Fig. 3 depicts the distribution of the normal-to-graphene, electric field component, where the efficiency of the modified PML is clearly confirmed.

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