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FDTD modeling of graphene-based materials and its application in sensing devices

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***Abstract*—This manuscript presents, an implementation for the modeling of graphene-based frequency-dispersive materials based on piecewise linear recursive convolution scheme is proposed. Moreover, the time-varying character of graphene's conductivity is exploited for its application in sensing. A graphene oxide sensing antenna operating at 6 GHz is presented and a time analysis of detection mechanism is conducted.**

***Index Terms*—FDTD methods, gas sensing, graphene, transient phenomena**

I. Introduction

The promising thermal, optical, and mechanical properties of graphene [1], [2] has caught the eye of the research community in the last years. Recently, many applications of graphene-enhanced devices has been proposed, including antennas, attenuators or absorbers [3], [4], among others. Several of these devices utilize the electrically adjustable conductivity of graphene to facilitate various features, such as radio-frequency identification (RFID), absorption of terahertz and microwave frequencies, beam manipulation, or interference mitigation [5], [6].

Top-down methods, in which layers of graphene derivates are extracted from a carbon source (typically graphite), have gained attention among researchers, since they are proven to be less time-consuming and more flexible than bottom-up techniques like chemical vapour deposition (CVD). Among them, graphene oxide (GO) and reduced graphene oxide (rGO) have shown a number of attractive mechanical, thermal, and electrical properties that make them a good alternative for industrial applications [7]. This includes the utilization of graphene-oxide for the design of sensors [8]. One the one hand, the variation of graphene's conductivity when exposed to a gas or a vapor is exploited as detection mechanism. On the other hand, the mechanical and electronic behaviour of graphene facilitates the transduction of the signal that is being sensed [9]–[11].

The efficient and precise modeling of graphene-based dispersive media is crucial for the viability of the aforementioned applications. The Debye model can be used to represent rGO, since it can be consider a planar material with negligible electrical thickness up to terahertz frequencies [7]. However, in order to perform an efficient analysis of modern devices, numerical algorithms are often needed, making it necessary to incorporate the surface conductivity into these methods. Among them, the transient nature of the finite difference time-domain (FDTD) method [12] allows for the broadband simulation of time-varying phenomena. Various investigations have been made on the inclusion of frequency dispersive planar materials into the FDTD, with an special focus on graphene materials [13], [14]. For certain applications, the recursive convolution method (RCM) has demonstrated some advantages [15]. It is of particular interest to exploit the piecewise linear recursive convolution (PLRC) technique, since it allows for a higher order accuracy like other popular methods such as the auxiliary differential evolution (ADE), while mantaining the advantages of the RCM method.

On the following, an implementation of graphene-like planar conductive materials using the PLRC method is proposed and applied to the design of a sensor antenna. The transient features of the method are exploited to conduct a study of the sensing capabilities of the device and their dependance with the material recovery times.

The rest of the paper is organized as follows: Section II introduces the proposed FDTD modeling for frequency-dispersive planar conductive materials. Then, in Section III the developed implementation is applied to the design of an rGO sensor implemented on a patch antenna. Finally, the last section contains some concluding remarks.

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II. Proposed FDTD modeling

We consider any planar material to be infinitesimally thin and characterized by its surface conductivity $\sigma_p(\omega)$. Then, the dispersive media is represented in the FDTD scheme as the equivalent surface $\mathbf{J}_p$, defined as

$$\mathbf{J}_p(\omega) = \sigma_p(\omega)\mathbf{E}(\omega), \tag{1}$$

where $\mathbf{E}$ is the electric field at the same region. Figure 1 illustrates the placement of the conductive layer, which is orientated at the xz-plane.

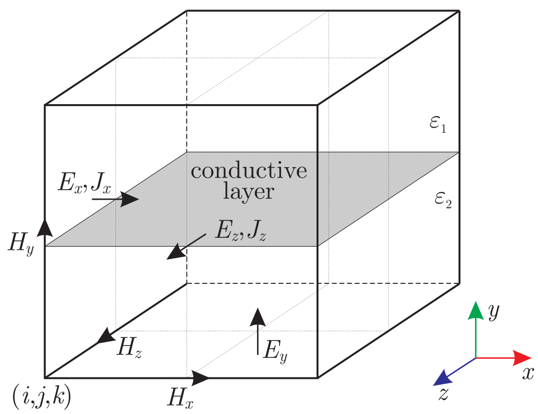

Fig. 1. Yee cell architecture including the modeling of the conductive layer as a surface current density.

More details about the incorporation of the planar material contribution into the electric field update equation can be found in [16]. To model the dispersion of the conductive layer, the second-order accurate PLRC method is appropriately adjusted. At a first instance, Equation (1) is transformed into the time-domain, resulting in

$$\mathbf{J}_p(t) = \sigma_p(t) * \mathbf{E}(t), \tag{2}$$

Equation (2) can be discretized, resulting in the following expression:

$$\mathbf{J}_p|^n = \int_{\zeta=0}^{n\Delta t} \sigma_p(\zeta)\mathbf{E}(n\Delta t - \zeta)\mathrm{d}\zeta. \tag{3}$$

with Δt being the time-step considered for discretization, and ζ being connected to the integration depth towards the previous electric field values. The continuous integration can be calculated at each time-step, assuming that the electric field follows a linear progression. Then, the surface current update equation can be formulated as

$$\mathbf{J}_p|^n = \sum_{i=0}^{n-1} \left[\mathbf{E}|^{n-i}\chi^i + (\mathbf{E}|^{n-i-1} - \mathbf{E}|^{n-i})\xi^i\right]. \tag{4}$$

being χ^i and ξ^i integration terms, defined as

$$\chi^i = \int_{\zeta=i\Delta t}^{(i+1)\Delta t} \sigma_p(\zeta)\mathrm{d}\zeta, \quad \xi^i = \int_{\zeta=i\Delta t}^{(i+1)\Delta t} \sigma_p(\zeta)(\zeta - i\Delta t)\mathrm{d}\zeta \tag{5}$$

In Equation (4), all the previously stored electric field values are required, which affects considerably the performance of the FDTD algorithm. To tackle this, a recursive computation scheme is adopted for the time-domain conductivity functions. This can be combined with some well-known dispersion models, such as the Drude, Lorentz or Debye functions. Equation (4) can be then expressed for this kind of functions as

$$\mathbf{J}_p|^n = \mathbf{E}|^n\chi^0 + (\mathbf{E}|^{n-1} - \mathbf{E}|^n)\xi^0 + C_{\mathrm{rec}}\mathbf{J}_p|^{n-1}, \tag{6}$$

where $C_{\mathrm{rec}} = \chi^{i+1}/\chi^i = \xi^{i+1}/\xi^i$ is a recursion constant and

$$\mathbf{J}_p|^{n-1} = \sum_{i=0}^{n-2} \left[\mathbf{E}|^{n-i-1}\chi^i + (\mathbf{E}|^{n-i-2} - \mathbf{E}|^{n-i-1})\xi^i\right]. \tag{7}$$

Subsequently, the proposed approach is employed to simulate an rGO layer, and the conductivity of the layer is assessed using the Debye function as shown in [17]:

$$\sigma_{\mathrm{rGO}}(t) = \varepsilon_0\omega_p^2 \mathrm{e}^{-\frac{t}{\tau}}u(t), \tag{8}$$

where $u(t)$ is the unit step-function. The continuous integration terms χ^i and ξ^i, and the recursion constant C_{rec} are calculated from Equation (5), whereas χ^0 and ξ^0 are obtained as indicated in [12].

One of the main advantages of the proposed FDTD implementation is the exploitation of the time-domain nature of the method, which allows the alteration of the transient conductivity. This can be used to emulate real conductivity changes, that can be induced by an electrostatic bias or an humidity change in the case of graphene derivates [9]. For instance, the conductivity can be modulated as

$$\sigma_{\mathrm{rGO}}(t) = \varepsilon_0\omega_p^2 \mathrm{e}^{-\frac{t}{\tau}}u(t)\left[1 + m_0\sin(\omega_m t)\right], \tag{9}$$

where m_0 and ω_m are the modulation strength and frequency, respectively. Then, χ^0 and ξ^0 can be reformulated as

$$\chi^0 = \varepsilon_0\omega_p^2\tau\left(1 - C_{\mathrm{rec}}\right)\left[1 + m_0\sin(\omega_m n\Delta t)\right], \tag{10a}$$

$$\xi^0 = \frac{\varepsilon_0(\omega_p\tau)^2}{\Delta t}\left[1 - \left(\frac{\Delta t}{\tau} + 1\right)C_{\mathrm{rec}}\right]\left[1 + m_0\sin(\omega_m n\Delta t)\right]. \tag{10b}$$

This scheme is verifying hereafter by the comparison with the results provided by a well-established full-wave simulator, CST Studio Suite [18], modeling the conductive layer as a surface impedance. Two $50 \times 50\,\mathrm{mm}^2$ rGO sheets are placed at the distance of $d = 7.6\,\mathrm{mm}$, as depicted in the illustration included in Figure 2. The source is tangential to both layers, and the electrical field is captured with a monitor placed after the second layer.

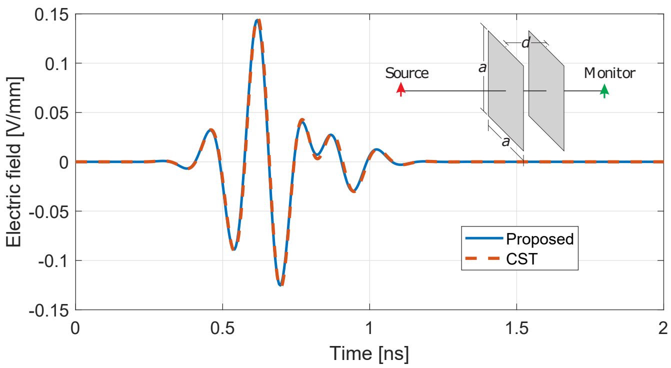

Fig. 2. Comparison of the electric field between the proposed scheme and the CST commercial software.

Figure 2 illustrates a comparison between the proposed implementation of the PRLC method and a simulation conducted in the CST commercial software. An almost full agreement between the two curves can be observed, presenting both some reflections between both rGO layers after 0.8 ns.

III. Application: Graphene-based sensor

The proposed sensor consist on a rGO-antenna, depicted in Figure 3. It is a patch antenna presenting its main resonance around 6 GHz. A 2 mm-thick Teflon substrate (with an electric permittivity of $\varepsilon = 2.33$) is used as a base for the metal patch and the rGO layer. The 3D computation domain is composed of $56 \times 56 \times 56$ cells, with $\Delta x = \Delta y = 2.5$ mm, $\Delta z = 2$ mm, and a time-step of $\Delta t = 4.4$ ps. Moreover, perfect match layer (PML) [12], [15], [19] with a thickness of 8 cells are employed.

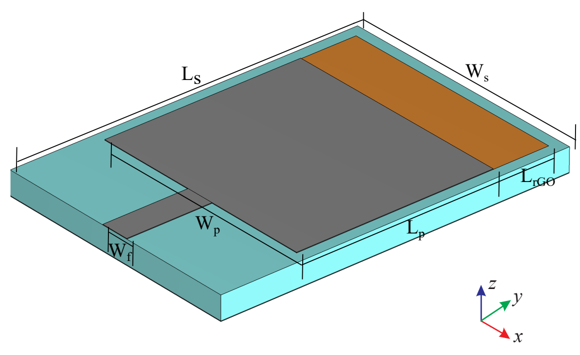

Fig. 3. Reduced graphene oxide patch antenna. Geometrical parameters: $L_p = 17.5$ mm, $L_{\mathrm{rGO}} = 5$ mm, $L_s = 28.5$ mm, $W_f = 2.5$ mm, $W_p = 15$, mm and $W_s = 19.5$ mm.

When the conductivity of rGO is altered, it can result in a shift in the resonant frequency. This discovery can be utilized as a detection method for different applications such as gas or humidity sensing. To demonstrate how a modification in the rGO properties affects the antenna response, a voltage monitor is positioned at the antenna source and the voltage changes are displayed over time in Figure 4.

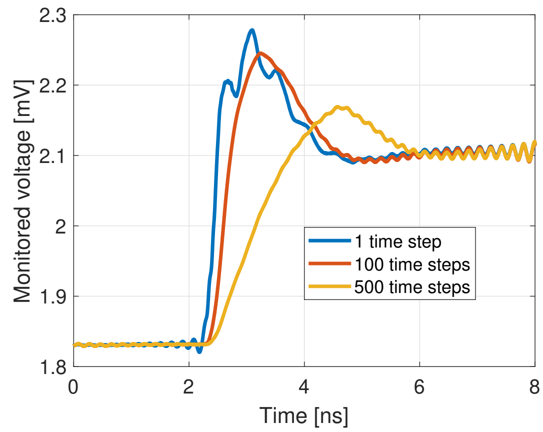

Fig. 4. Voltage at the antenna source before and after a variation of σ_{rGO} from 2 to 1 mS.

As it can be clearly appreciable in the Figure, the change of conductivity provokes an augmentation of the monitored voltage of about 0.4V, which can serve as a valid detection mechanism for sensing. Looking at the results, there are three different graphs displayed. The blue graph represents the scenario where σ_{rGO} undergoes an abrupt change within one time step. On the other hand, the red and yellow curves correspond to the case where the conductivity changes linearly over 100 and 500 time-steps respectively. Despite the gradual change in σ_{rGO} over multiple time-steps, we can still observe a significant oscillation in the voltage. This simulation closely mimics a realistic situation compared to the one with abrupt conductivity changes, making it suitable for detecting materials with a wide range of recovery times.

IV. Conclusions

A new FDTD-based scheme for the modeling of dispersive graphene-based materials has been presented in this paper. Moreover, this scheme is used for the design of a sensor antenna operating at 6 GHz. The sensing mechanism exploits the conductivity changes of the graphene material. Future research lines include the application of the proposed method for the modeling of more complex structures of a transient nature.

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