



GLOBAL JOURNAL OF RESEARCHES IN ENGINEERING: F
ELECTRICAL AND ELECTRONICS ENGINEERING

Volume 17 Issue 4 Version 1.0 Year 2017

Type: Double Blind Peer Reviewed International Research Journal

Publisher: Global Journals Inc. (USA)

Online ISSN: 2249-4596 & Print ISSN: 0975-5861

Simulating Framework for Graphene based Devices using Finite Difference Time Domain Method

By Abdullah Al Hadi & Syed Rafiee Abied

Islamic University of Technology

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GJRE-F Classification: FOR Code: 090699



SIMULATINGFRAMEWORKFORGRAPHENEBASEDDEVICESUSINGFINITEDIFFERENCECTIMEDOMAINMETHOD

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Simulating Framework for Graphene based Devices using Finite Difference Time Domain Method

Abdullah Al Hadi ^α & Syed Rafiee Abied ^σ

Abstract- This paper focuses on studying a simulating framework for graphene based devices using finite-difference time-domain (FDTD) method. Conventional FDTD is modified for graphene material using Surface Boundary Condition (SBC) where graphene is considered as a two dimensional ultra-thin conductive sheet. Then a Perfectly Matched Layer (PML) technique is implemented to terminate the computational grids. Using the surface boundary condition technique to model the graphene thin layer significantly reduces the computational cost compared to using the conventional FDTD. The given formulation is accompanied by required validation.

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I. INTRODUCTION

Graphite materials come in a variety of forms. The 3-D graphite is the most commonly seen form, and the 1-D carbon nanotube (CNT) has been another recent research interest, especially in composite materials. The newly discovered graphene is the 2-D graphitic material, and is essentially the building block of the other forms. A 2-D crystal is in general hard to grow because as the lateral size of the crystal grows, the thermal vibration also rapidly grows and diverges on a macroscopic scale, which forces the 2-D crystallites to morph into a stable 3-D structure [1]. Graphene has many outstanding properties. Its electrical properties include its high carrier mobility, which is measured in various devices as $8000-10000 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ and could reach $200000 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ in suspended graphene [2]. Graphene's non-electronic properties bring a new dimension to graphene research. It was found to have a breaking strength of 40 N/m, reaching the theoretical limit, as well as a Young's modulus of 1.0 TPa, which is a record value [3]. Graphene field-effect transistors (FET) and graphene wafer scale integrated circuits have been fabricated and versatile graphene applications in EM and transformation optics has been developed in recent years.

Author α: Department of Electrical and Electronic Engineering, Bangladesh University of Engineering and Technology, Dhaka 1000.

Author σ: Department Electrical and Electronic Engineering, Islamic University of Technology, Board Bazar, Gazipur 1704, Bangladesh.
e-mails: alhadi@bubt.edu.bd, rafiee.abied@gmail.com

The nanopatch antenna simulation has been done using FEKO and is discussed in [4]. The graphene transformation optics structures are discussed in [5] and simulation process has been done using CST Microwave Studio. In both studies, the simulations are in the frequency domain, where the graphene conductivity is a complex number at a particular frequency. One can enter the conductivity value into the commercial software and run the simulation without making further modification to the software. Simulating graphene-based devices in time domain has several advantages. In this paper, the transient behavior of the device can be observed and studied and the result for a wide frequency band can be obtained from a single simulation in time domain.

The remainder of the paper is organized as follows: Section II introduces graphene transformation Optics. FDTD Modeling for graphene is discussed in section III. Implementation of SBC in 2-D FDTD for Graphene are provided in section IV. PML loss parameters in discrete space are given in section V. Finally conclusion and future work is described in section VI.

II. GRAPHENE TRANSFORMATION OPTICS

Graphene has been investigated for its potential in material and transformation optics recently [5]. Graphene's conductivity is a function of the chemical potential, which depends on gate voltage, and/or chemical doping [6]. Its tunable conductivity allows it to shape electro-magnetic field into desired spatial patterns which is a great advantage over the noble material.

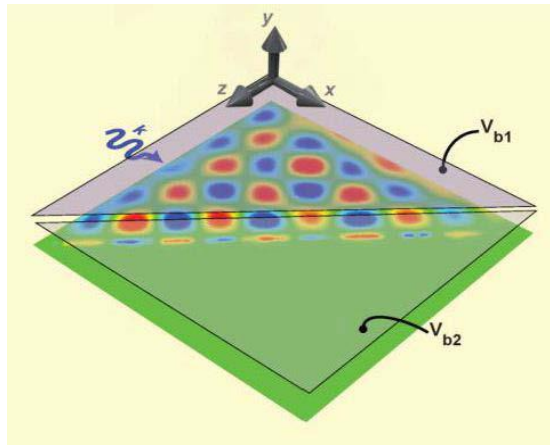


Figure 1: Graphene controlled by bias voltage

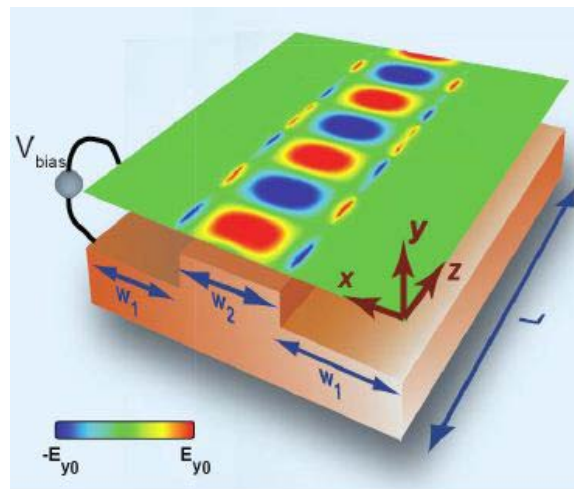


Figure 2: Graphene conductivity controlled by uneven ground plane

Figure 1 shows it is possible to have part of the graphene sheet supporting a surface Plasmon Polariton (SPP) wave while not on the other part, and this can be done by varying the sign of the imaginary part of the conductivity by varying the gate voltage [7]. The tuning can be done in real time by varying the gate voltages. Figure 2 shows alternatively; an uneven ground plane underneath the graphene can be implemented to design the conductivity profile on the graphene.

III. FDTD MODELING FOR GRAPHENE

Finite-Difference Time-Domain (FDTD) is a popular electromagnetic modeling technique. It is easy to understand, easy to implement in software, and since it is a time-domain technique it can cover a wide

frequency range with a single simulation run. The FDTD method belongs in the general class of differential time domain numerical modeling methods. Maxwell's (differential form) equations are simply modified to central-difference equations, discretized and implemented in software. The equations are solved in a leap-frog manner; that is, the electric field is solved at a given instant in time, then the magnetic field are solved at the next instant in time, and the process is repeated over and over again.

a) Graphene Conductivity Model

The graphene conductivity (in unit of [S]) is given by the Kubo formula,

$$\sigma(\omega, \mu_c, \gamma, T) = \frac{je^2(\omega - j2\gamma)}{\pi\hbar^2} \left[\frac{1}{(\omega - j2\gamma)^2} \int_0^\infty \epsilon \left(\frac{\partial f_d(\epsilon)}{\partial \epsilon} - \frac{\partial f_d(-\epsilon)}{\partial \epsilon} \right) d\epsilon - \int_0^\infty \frac{f_d(-\epsilon) - f_d(\epsilon)}{(\omega - j2\gamma)^2 - 4(\epsilon/\hbar)^2} d\epsilon \right] \quad (1)$$

In equation (1), $f_d(\epsilon) = (e^{(\epsilon - \mu_c)/k_B T} + 1)^{-1}$ is the Fermi Dirac distribution, ω is the angular frequency

in radians, γ is the scattering rate is per sec, T is the temperature in Kelvin, $-e$ is the electron charge, $\hbar$ is the

reduced Planck's constant, k_B is the Boltzmann constant, μ_c is the chemical potential in eV which can be controlled by chemical doping or by applying a bias

The Kubo formula can be simplified and the intra-band conductivity is,

$$\sigma_{intra}(\omega, \mu_c, \gamma, T) = \frac{j e^2 k_B T}{\pi \hbar^2} \left(\frac{\mu_c}{k_B T} + 2 \ln \left(e^{(-\mu_c/k_B T)} + 1 \right) \right) \frac{1}{\omega - j 2 \gamma} \quad (2)$$

and the inter-band conductivity is as follows,

$$\sigma_{inter}(\omega, \mu_c, \gamma, 0) = \frac{-j e^2}{4 \pi \hbar} \ln \left(\frac{2|\mu_c| - (\omega - j 2 \gamma) \hbar}{2|\mu_c| + (\omega - j 2 \gamma) \hbar} \right) \quad (3)$$

The intra-band conductivity is mainly account for the low frequency electrical transport and inter-band

conductivity is for the optical excitations [8]. Taking the parameters used in graphene parallel plate waveguide, $\mu_c = 0.5eV$, $\gamma = 10^{12}$ and $T = 300K$, the corresponding conductivity values are plotted in the figure given below.

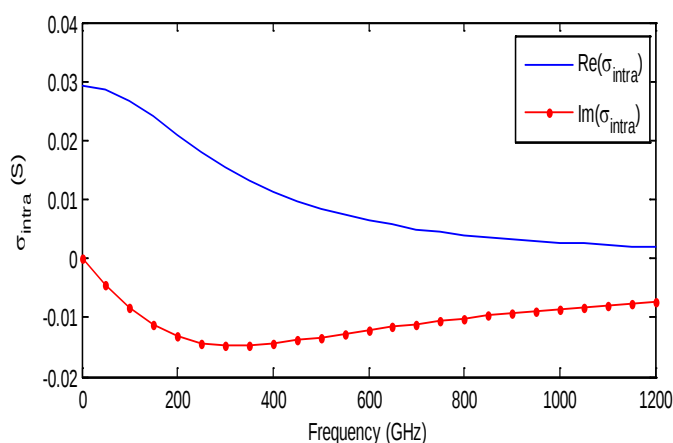


Figure 3: Graphene surface intra-band conductivity for $\mu_c = 0.5eV$, $\gamma = 10^{12}$ and $T = 300K$.

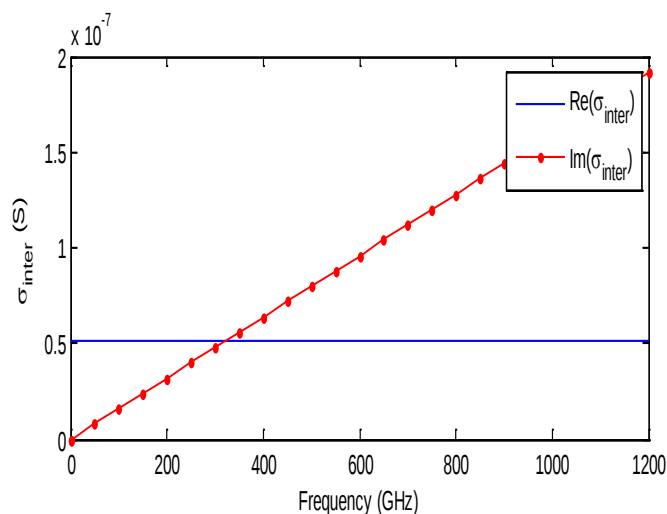


Figure 4: Graphene surface inter-band conductivity for $\mu_c = 0.5eV$, $\gamma = 10^{12}$ and $T = 300K$.

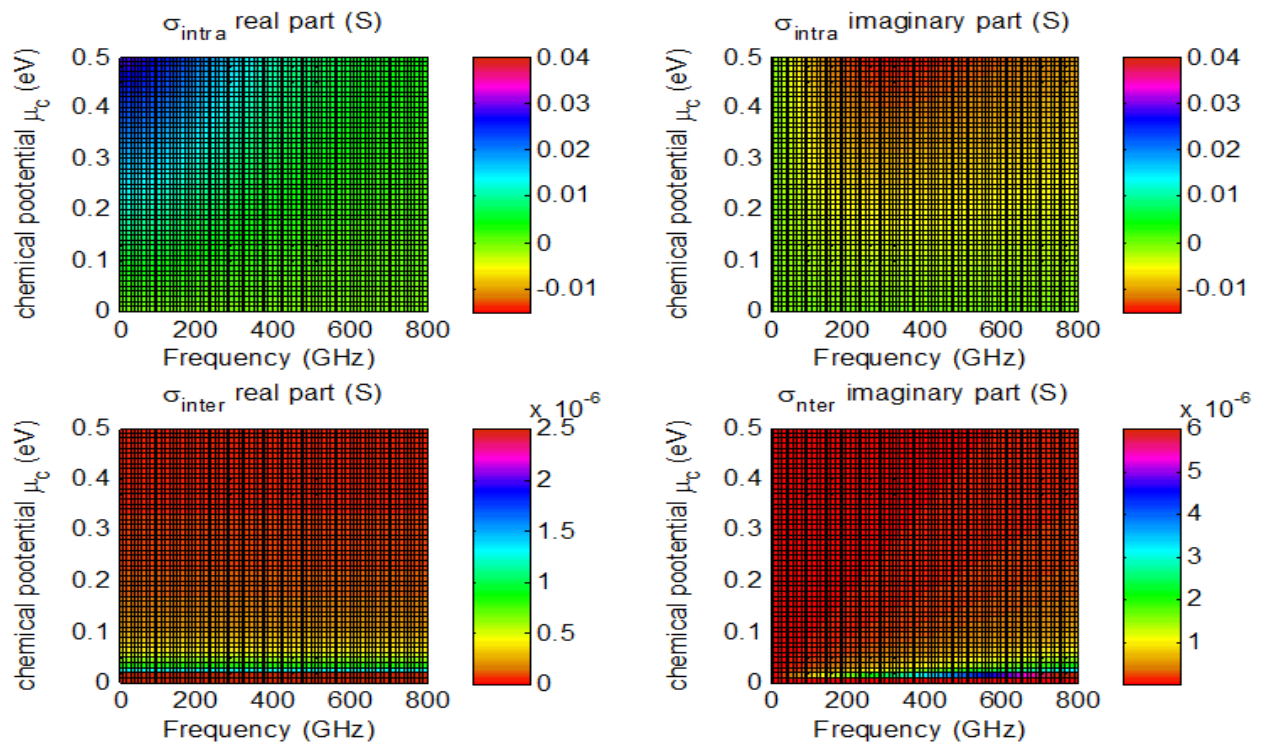


Figure 5: Graphene surface conductivity for $\mu_c = 0.5\text{eV}$, $\gamma = 10^{12}$ and $T = 300\text{K}$.

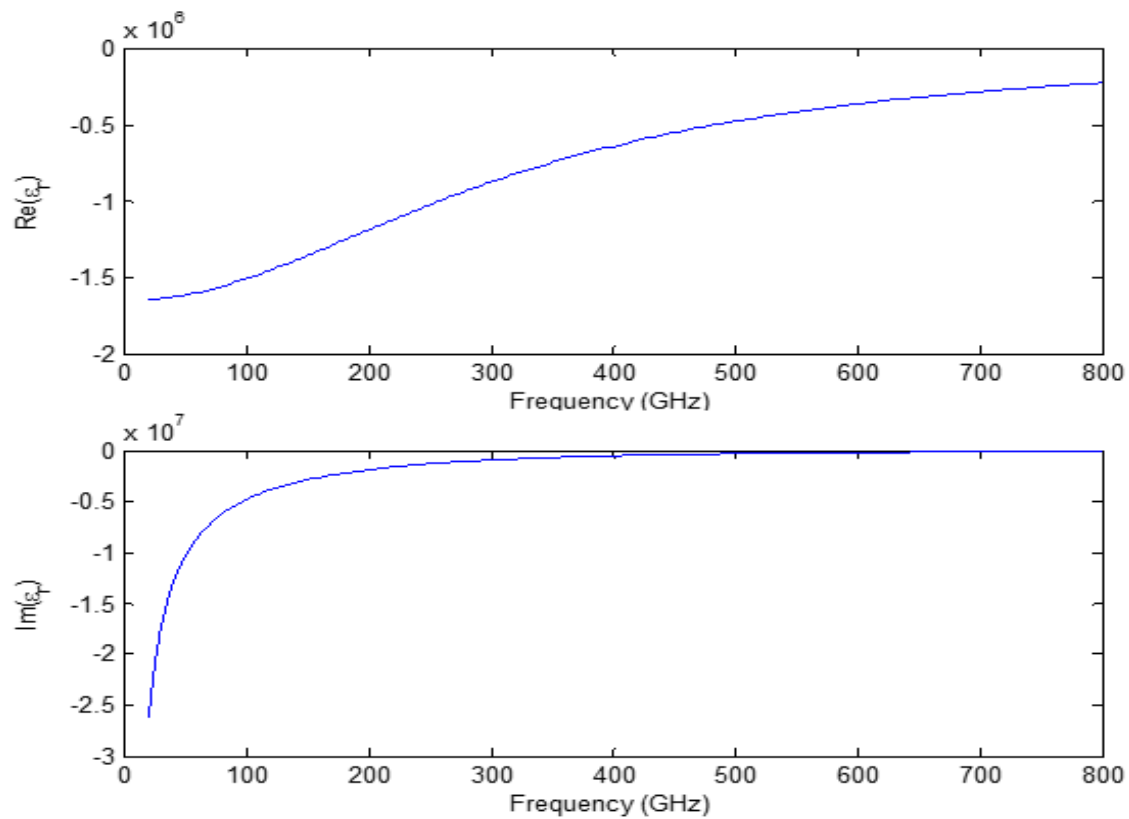


Figure 6: Graphene relative permittivity for $\mu_c = 0.5\text{eV}$, $\gamma = 10^{12}$ and $T = 300\text{K}$.

We can see from Figure 5 that in the frequency up to 800 GHz, the value of σ_{intra} dominates over that of σ_{inter} . Therefore σ_{inter} can be ignored for most simulations below optical range.

The expression of σ_{intra} is in fact a Drude model and can be expressed as,

$$\sigma_{intra,s} = \frac{Q'}{j\omega + 2\gamma} \quad (4)$$

where,

$$Q' = \frac{e^2 k_B T}{\pi \hbar^2} \left(\frac{\mu_c}{k_B T} + 2 \ln \left(e^{\left(-\mu_c / k_B T \right)} + 1 \right) \right) \quad (5)$$

The surface conductivity can be converted as to the volumetric conductivity (in unit of [S/m]) by dividing $\sigma_{intra,s}$ by the thickness of graphene, which is assumed to be 1nm or 10^{-9} m.

$$\sigma_{intra,v} = \frac{\sigma_{intra,s}}{10^{-9}} \quad (6)$$

$$\sigma_{intra,v} = \frac{Q}{j\omega + 2\gamma} \quad (7)$$

where,

$$Q(\mu_c, T) = \frac{Q'}{10^{-9}} = \frac{\left[\frac{e^2 k_B T}{\pi \hbar^2} \left(\frac{\mu_c}{k_B T} + 2 \ln \left(e^{\left(-\mu_c / k_B T \right)} + 1 \right) \right) \right]}{10^{-9}} \quad (8)$$

$$\mathbf{H}_x^{n+0.5}(i, j) = \mathbf{H}_x^{n-0.5}(i, j) - \frac{\Delta t}{\Delta y \mu_0} \{ \mathbf{E}_z^n(i, j+1) - \mathbf{E}_z^n(i, j) \} \quad (13)$$

The $\mathbf{H}_y$ field update equation for all other nodes is,

$$\mathbf{H}_y^{n+0.5}(i, j) = \mathbf{H}_y^{n-0.5}(i, j) + \frac{\Delta t}{\Delta y \mu_0} \{ \mathbf{E}_z^n(i+1, j) - \mathbf{E}_z^n(i, j) \} \quad (14)$$

And the $\mathbf{E}_z$ field update equation for all other nodes is,

$$\mathbf{E}_z^{n+1}(i, j) = \mathbf{E}_z^n(i, j) + \frac{\Delta t}{\epsilon_0} \left\{ \frac{\mathbf{H}_y^{n-0.5}(i, j) - \mathbf{H}_y^{n-0.5}(i-1, j)}{\Delta x} - \frac{\mathbf{H}_x^{n-0.5}(i, j) - \mathbf{H}_x^{n-0.5}(i, j-1)}{\Delta y} \right\} \quad (15)$$

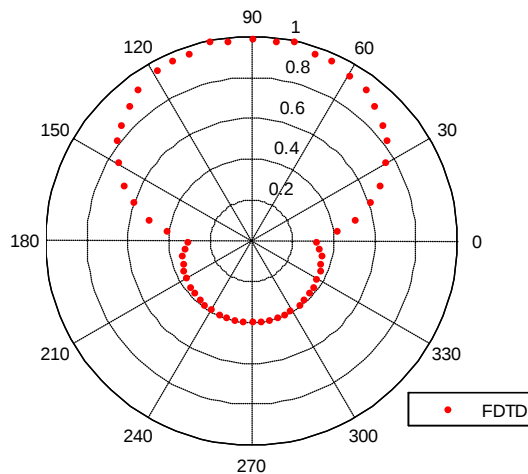


Figure 7: Normalized pattern of E_z at the wavelength of 100 μm .

To find the relative permittivity (ϵ_r) from the conductivity, the following equations are used. The results of the simulation curve are shown in figure 6.

$$\epsilon_r = \epsilon' - j\epsilon'' \quad (9)$$

$$\epsilon'' = \frac{\sigma}{\omega \epsilon_0} \quad (10)$$

$$\epsilon_r = 1 - j \frac{\sigma}{\omega \epsilon_0} \quad (11)$$

$$\epsilon_r = 1 + \frac{Q}{j\omega \epsilon_0 (j\omega + 2\gamma)} = 1 + \frac{Q/\epsilon_0}{-\omega^2 + 2\gamma j\omega} \quad (12)$$

IV. IMPLEMENTATION OF SBC IN 2-D FDTD FOR GRAPHENE

Let, the 2D computational domain is located in xy plane. So for TM mode, the fields components of electric and magnetic field are E_z , H_x and H_y .

The $\mathbf{H}_x$ field update equation for all other nodes is,

V. PML LOSS PARAMETERS IN DISCRETE SPACE

The PML is usually backed by a PEC wall. The transmitted signal through the PML undergoes significant attenuation by the PML layer [9]. Again the reflected signal from the PEC wall also attenuated by the PML. In a PML, reflection coefficient ($R(\phi)$) is a function of the incident angle (ϕ) of the wave incidence on the PML. The reflection coefficient can be expressed as,

$$R(\phi) = \exp(-2\sigma_D \eta d \cos\phi) \quad (16)$$

Here, η = wave impedance for free space

ϕ = wave incident angle

d = depth of PML layer

σ_D = conductivity of PML layer

$R(\phi)$ is PML reflection error. It gives the relative magnitude of the spurious reflected wave, which enter back into the computational domain. The larger the d and σ_D , the lesser the reflection.

VI. CONCLUSION AND FUTURE WORK

The simulated results matched with the analytical results. The given modified FDTD algorithm is able to simulate graphene based microwave problems where graphene is considered as very thin conductor. In order to extend the existing framework to model devices up to optical frequency, the inter band conductivity need to be taken into consideration. This can be done by applying the Padé approximation for graphene inter-band conductivity [10]. For devices operating at the high terahertz frequency range, where the intra-band conductivity and the inter-band conductivity have comparable magnitudes, both models are needed for accurate simulation results.

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