Simulation of high-frequency carrier dynamics in graphene

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INTRODUCTION

Since the discovery of graphene and its unique properties [1], considerable amount of research has been done on its fundamental electronic properties [2] and low-field, *dc* transport [3]. One of the motivations is the prospect of using graphene in electronic devices [4], [5], [6]. However, graphene has also been used as a novel material for interconnects, transparent conductors, photodetectors and in other photonic and optoelectronic applications including metamaterials [7]. These photonic and optoelectronic applications require a deeper understanding of the interaction of high-frequency electromagnetic radiation with the carriers in two-dimensional graphene. Here we present a numerical simulation of two-dimensional carrier transport in monolayer graphene coupled with an electromagnetics solver, focusing on the calculation and characterization of the *ac* conductivity of graphene.

NUMERICAL MODEL

The numerical simulation uses a 3D finite-difference time-domain (FDTD) solver of Maxwell's equations combined with an ensemble Monte Carlo (EMC) simulation of carrier transport. The EMC and FDTD solvers are coupled in each time step, with the FDTD fields accelerating carriers and the EMC motion in turn resulting in a sourcing current density. This technique coupled with molecular dynamics for short-range Coulomb fields has been used to accurately calculate the *ac* conductivity of doped silicon [8], [9]. In this work, we apply the 3D EMC-FDTD technique to graphene and simulate carrier dynamics for different modes of high frequency excitation.

The simulation domain consists of a monolayer graphene sheet with a silicon dioxide substrate at the bottom and air on the top as shown in Fig. 1. The dielectric constants of the graphene, silicon dioxide and air regions are $\epsilon_{\mathrm{g}} = 2.5$, $\epsilon_{\mathrm{SiO_2}} = 3.9$ and $\epsilon_{\mathrm{air}} = 1$, respectively. The boundaries in the direction of transport are periodic in order to simulate bulk material, whereas the other boundaries can be terminated by a perfectly matched absorbing layer for the FDTD and reflecting boundaries with roughness for the EMC. The carrier density in graphene including both electrons and holes is calculated from a given Fermi level and temperature. The two-dimensional carrier transport is limited by the long-range Coulomb fields of remote impurities in the substrate in addition to electron-phonon scattering in the graphene layer. Here we use electron-phonon scattering rates calculated using the plane wave method [10] with a range of deformation potentials.

Ensemble averages of drift velocity, current density and energy are calculated at each time step for evaluating time evolution. Fig. 2 shows the time evolution of carrier velocity for a 13 THz plane wave excitation, with electric field along the y-direction. Phasor current density and electric fields are computed after reaching steady state using fast Fourier transform. The complex conductivity is then calculated from these phasor quantities. We calculate the conductivity as a function of the frequency and carrier density with and without the effect of substrate impurities. Fig. 3 shows a plot of the real part of the *ac* conductivity for two different carrier densities, without substrate impurities.

CONCLUSION

In conclusion, we present a coupled 3D EMC-FDTD simulation of high-frequency carrier dynamics in graphene. The calculated *ac* conductivity shows a strong variation with frequency of excitation. As expected from the simple Drude model, the effect of carrier density on the conductivity diminishes as frequency increases. We expect the characterization of *ac* conductivity to be useful for a better utilization of graphene in photonic and optoelectronic applications.

ACKNOWLEDGMENT

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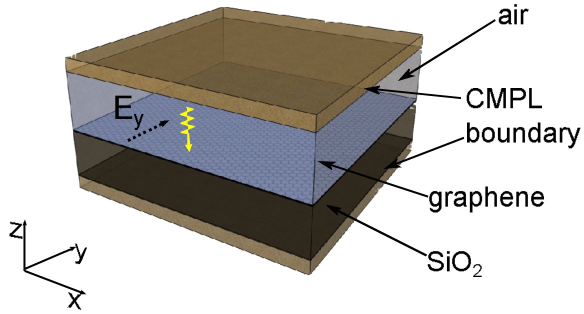

Fig. 1. 3D EMC-FDTD model geometry. Yellow arrows denote direction of propagation and the direction of the electric field is shown by the dotted arrows. The x and y perpendicular planes are terminated by periodic boundary conditions in this case.

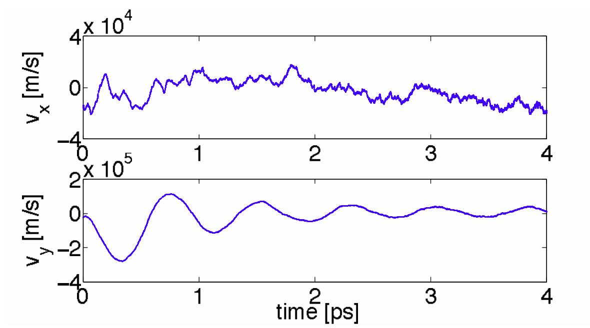

Fig. 2. Time evolution of average carrier velocity for a 13 THz plane wave excitation with electric field along y-direction as shown in Fig. 1.

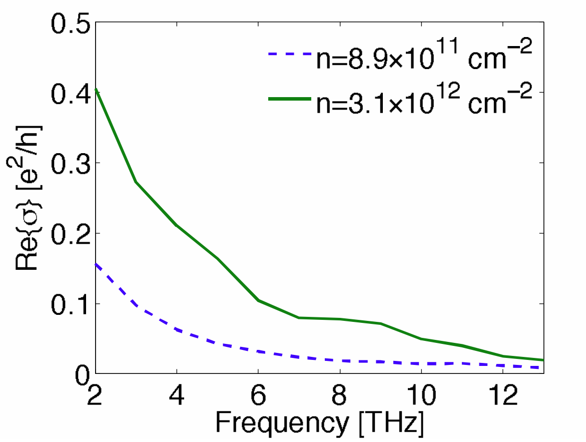

Fig. 3. Real part of the complex *ac* conductivity without the effect of substrate impurities.