Substrate-dependent THz conductivity and Drude weight in graphene

N. Sule, S. C. Hagness, and I. Knezevic*
University of Wisconsin-Madison, Madison, WI 53706
*e-mail: knezevic@engr.wisc.edu

The optoelectronic properties of graphene [1] make it a promising material for terahertz (THz) applications [2]. The frequency-dependent conductivity, $\sigma(\omega)$, of graphene in the THz range (100 GHz–10 THz) is dominated by intraband transitions and is well described by the Drude model [3], [4]. Moreover, in the THz range, the conductivity of graphene can be modulated by tuning the Fermi level via a back-gate voltage, leading to applications such as THz modulators [2]. The Drude weight, D, is often obtained by fitting the THz-range conductivity [3], [4] with the Drude-form expression,

$$\sigma(\omega) = \frac{iD}{\pi(\omega + i\Gamma)}, \qquad (1)$$

where D is the Drude weight, ω is the frequency, and Γ is the scattering rate. Theoretically, with electron-electron interactions neglected, the Drude weight in graphene is given by random phase approximation (RPA) [5] to be $D_0 = 2\pi E_{\mathrm{F}}/\hbar$ [in the units of $(\mathrm{e}^2/\mathrm{h}) \cdot 1/\mathrm{s}$]. Recent experiments have revealed the value of D to be lower than D_0 [3], [4]. At the same time, theoretical studies that include electron-electron interactions predict an enhancement [5] of D as compared to the non-interacting value, D_0. Although this discrepancy is believed to be due to extrinsic factors such as charged impurities, there is no clear evidence on how charged impurities affect the Drude weight.

We have calculated $\sigma(\omega)$ in the THz range (see Fig. 1–3) by simulating carrier dynamics in graphene using the coupled EMC/FDTD/MD method [6], [7], which combines the ensemble Monte-Carlo (EMC) method for solving the Boltzmann transport equation with the finite-difference time-domain (FDTD) method for solving Maxwell's curl equations and molecular dynamics (MD) for real-space particle-particle short-range interactions. By fitting Eq. (1) to the numerically calculated $\sigma(\omega)$, we extract effective values of D and Γ. We compare $\sigma(\omega)$ for graphene on $\mathrm{SiO_2}$ and hexagonal-BN with suspended graphene and investigate the role of charged impurities (see Fig. 4) and electron-electron interactions on $\sigma(\omega)$ and D. We show, in agreement with experiments [3], that D is significantly lower than the value of the RPA result (D_0). We attribute the lower values of D in comparison to D_0 to electron-charged impurity interactions. We show that intraband electron-electron interactions would be important only at high carrier densities ($> 6 \times 10^{12}\,\mathrm{cm}^{-2}$) in extremely clean samples and would result in reduced Drude weights. Finally, we show that graphene on h-BN is better suited for application in THz modulators [2] than both graphene on $\mathrm{SiO_2}$ or suspended graphene (see Fig. 5). This is due to a combination of (1) higher carrier density in graphene on h-BN than on $\mathrm{SiO_2}$ for the same gate bias (or Fermi level) and (2) higher total scattering rate compared to suspended graphene resulting in a smaller slope of frequency-dependent conductivity in the THz range.

ACKNOWLEDGMENT

This work was supported by the AFOSR, grant FA9550-11-1-0299 (primary support), and by the NSF, grant 1201311 (partial support).

REFERENCES

[1] F. Bonaccorso, Z. Sun, T. Hasan and A. C. Ferrari, *Graphene photonics and optoelectronics*, Nat. Photon. **4**, 611–622 (2010).

[2] B. Sensale-Rodriguez, R. Yan, M. M. Kelly, T. Fang, K. Tahy, W. S. Hwang, D. Jena, L. Liu, H. G. Xing, *Broadband graphene terahertz modulators enabled by intraband transitions*, Nat. Commun. **3** 780–787 (2012).

[3] J. Horng, Chi-Fan Chen, B. Geng, C. Girit, Y. Zhang, Z. Hao, H. A. Bechtel, M. Martin, A. Zettl, M. F. Crommie, Y. Ron Shen and F. Wang, *Drude conductivity of Dirac fermions in graphene*, Phys. Rev. B **83**, 165113 (2011).

[4] H. Yan, F. Xia, W. Zhu, M. Freitag, C. Dimitrakopoulos, A. A. Bol, G. Tulevski and P. Avouris, *Infrared Spectroscopy of Wafer-Scale Graphene*, ACS Nano **5**, 9854–9860 (2011).

[5] S. H. Abedinpour, G. Vignale, A. Principi, M. Polini, Wang-Kong Tse and A. H. MacDonald, *Drude weight, plasmon dispersion, and ac conductivity in doped graphene sheets*, Phys. Rev. B **84**, 045429 (2011).

[6] K. J. Willis, S. C. Hagness, I. Knezevic, *Multiphysics simulation of high-frequency carrier dynamics in conductive materials*, J. Appl. Phys. **110** (2011).

[7] N. Sule, K. J. Willis, S. C. Hagness and I. Knezevic, *EMC/FDTD/MD simulation of carrier transport and electrodynamics in two-dimensional electron systems*, J. Comput. Electron. **12** 563–571 (2013).

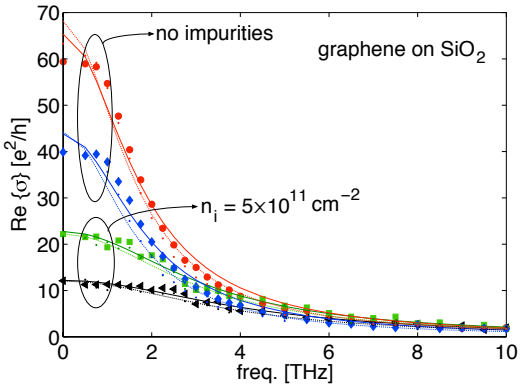

Fig. 1. Real part of the complex $\sigma(\omega)$ for graphene on SiO_2 calculated for two different carrier densities (n) and charged impurity densities (n_i): $n = 3\times10^{12}\,\mathrm{cm}^{-2}$ (black/blue symbols), $n = 6\times10^{12}\,\mathrm{cm}^{-2}$ (green/red symbols), and $n_i = 5\times10^{11}\,\mathrm{cm}^{-2}$ (green/black symbols), $n_i = 0$ (red/blue symbols). The dot-symbols represent simulation results when electron-electron interactions are not considered. The solid/dotted lines are fits using Eq. (1) with the Drude weight, D, and effective scattering rate, Γ, as fitting parameters.

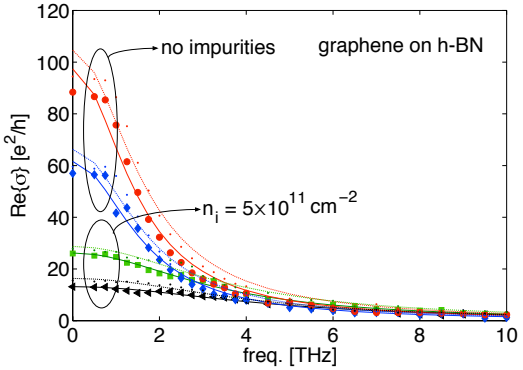

Fig. 2. Real part of $\sigma(\omega)$ calculated for graphene on hexagonal-BN. The symbols here correspond to the same parameters as described in Fig. 1.

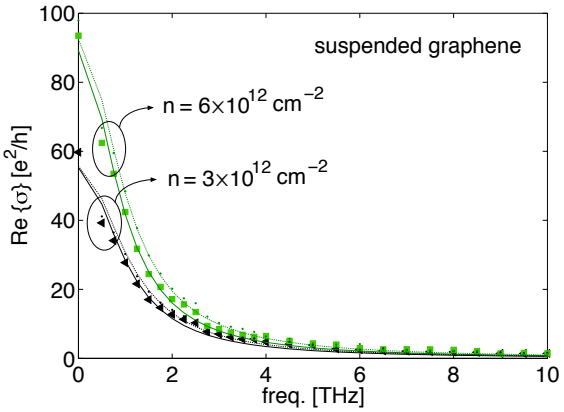

Fig. 3. Real part of $\sigma(\omega)$ for calculated suspended graphene without charged impurities. Here, again the solid/dotted lines are fits using Eq. (1).

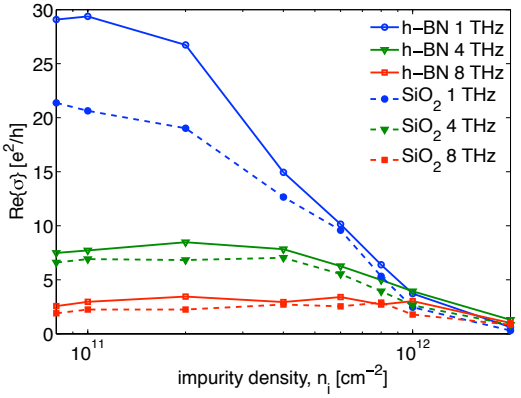

Fig. 4. Real part of $\sigma(\omega)$ calculated for $n = 3\times10^{12}\,\mathrm{cm}^{-2}$ in graphene on SiO_2 (dashed lines) and h-BN (solid lines) at different THz frequencies.

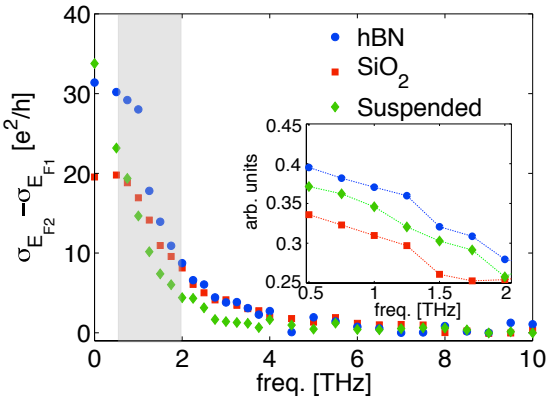

Fig. 5. The change in THz conductivity by modulating the Fermi level in graphene is shown as a function of frequency for graphene on h-BN (blue circles), graphene on SiO_2 (red squares) and suspended graphene (green diamonds). Inset shows the normalized change in conductivity $[(\sigma_{E_{F2}} - \sigma_{E_{F1}})/\sigma_{E_{F2}}]$ in the range 500 GHz–2 THz (shaded in grey) where graphene on h-BN exhibits better modulation.