Simulation of Single and Multi-Layer Graphene Field-Effect Devices

M.G. Ancona
Naval Research Laboratory
Washington, DC, USA

Abstract—**Building on previous work, we discuss a diffusion-drift description of electron and hole transport in both single and multi-layer graphene that includes the possibility of a small bandgap. To illustrate the theory, the effects of these new features on field-effect device characteristics are exhibited.**

Keywords: Graphene; diffusion-drift; bandgap; multi-layers.

I. INTRODUCTION

The burgeoning field of graphene research has been powered by a combination of exciting experiments [1] and intriguing theory [2]. Among other things, the former has indicated the possibility of excellent bipolar transport characteristics in a practical planar geometry, as well as the potential for unique device applications. From the experimental side a key discovery has been that graphene is a robust material that can be formed in single or multiple layers, and can be contacted and tested electrically. Perhaps most interesting from a device perspective is recent evidence for the existence of a bandgap of ~0.26eV in single-layer graphene formed epitaxially on SiC by sublimation of silicon [3-5] at high temperature. Although it remains far from clear whether graphene (in any form) will ever lead to a practical electronics technology, the rapid progress that has been made is here taken as motivation for developing device-oriented theory that may one day serve as a toolbox for electronic device design and optimization.

Most theoretical work on graphene to date has centered on its ideal characteristics and on the exotic physical properties that it can exhibit, including when restricted in dimension as in carbon nanoribbons [2]. However, apart from the technologically uninteresting case of suspended exfoliated graphene [6], the mobilities seen experimentally are generally far from ideal [7], apparently because of strong scattering by nearby charges and/or localized "midgap" states [8]. The presence of this strong scattering, while clearly not beneficial from a device perspective, constitutes the main basis for believing a diffusion-drift (DD) description can be reasonable. Beyond this, there is also the well-known simplicity and robustness of the DD approach that has led to its continued utility in electronics even when its foundational assumptions no longer seem to hold. With these attributes in mind, in previous work we developed a DD theory of single-layer graphene [9]. The present paper extends this line of research by generalizing the earlier theory to allow for the existence of a bandgap and for the possibility of multi-layer transport. These aspects should make the theory discussed herein especially applicable to the situation of epitaxial graphene on silicon carbide [3-5].

II. DD THEORY OF GRAPHENE

A. Foundations

As discussed in [9], because of the 2-D nature of graphene, the differential equations of DD theory must be a hybrid of 2-D and 3-D equations. The DD transport equations for electrons and holes in the graphene are in 2-D and may be written as

$$\nabla\cdot\mathbf{J}_n = -R \quad \text{and} \quad \mathbf{J}_n = qn\mu_n\nabla\left(\varphi_n - \psi\right) \tag{1a}$$

$$\nabla\cdot\mathbf{J}_p = -R \quad \text{and} \quad \mathbf{J}_p = -qn\mu_p\nabla\left(\varphi_p + \psi\right) \tag{1b}$$

where n and p are areal densities in cm^{-2}, the current densities $\mathbf{J}_n$ and $\mathbf{J}_p$ are in A/cm, the recombination/generation rate R is in Coul/(cm^2-sec), and the derivatives are surface gradients/divergences within the graphene layer. Having the usual units, μ_n and μ_p, and φ_n and φ_p are the mobilities and chemical potenials of the electron and hole gases, respectively. When more than a single layer of graphene is present, each additional layer would be described by additional equations analogous to those in (1) and the rate R would then also incorporate interlayer transfer/recombination processes (which are believed to be weak [10]). Because the graphene layer is embedded within a larger device structure that includes insulators and metal contacts, the 2-D equations describing transport in the graphene must be coupled to a 3-D electrostatic equation

$$\nabla\cdot\left(\varepsilon_d\nabla\psi\right) = qN_{fixed} \tag{2}$$

where N_{fixed} is the net fixed volumetric charge density and ε_d is the permittivity in the surrounding materials. (If the device also included bulk semiconductors, then 3-D DD transport equations would also have to be considered).

In addition to the differential equations one must also provide a consistent set of boundary conditions to be applied at interfaces. All of these are standard and so we note only that among these conditions is an electrostatic one across the graphene layer, namely,

978-1-4244-1753-7/08/$25.00 ©2008 IEEE

$$\mathbf{n}\cdot\left(\varepsilon_{d2}\mathbf{E}_2-\varepsilon_{d1}\mathbf{E}_1\right)=q\left(n-p-N\right) \tag{3}$$

where the subscripts indicate values on either side of the graphene layer and N is the net surface charge (due to dopants and fixed charge) at the insulator-graphene-insulator interface.

To complete the DD theory one must specify the various material response functions appearing in the foregoing equations. Of these equations, those present at equilibrium — namely, φ_n and φ_p — are most easily developed since the powerful tools of statistical mechanics can be brought to bear. The functions $\varphi_n(n,T)$ and $\varphi_p(p,T)$ are the equations of state for the electron and hole gases in the graphene, and to derive expressions we assert that the conduction band in graphene having bandgap E_G is well described by

$$E(k)=\frac{E_G}{2}+\frac{\hbar^2k^2c^2}{\hbar|k|c+E_G/2} \tag{4}$$

where $c\cong10^8 cm/s$ and the energy is measured from midgap. It is then readily shown that the density of states is given by

$$g(E)=\frac{1}{2\pi\hbar^2c^2}\left[E+\sqrt{\frac{E-E_G/2}{E+3E_G/2}}\left(E+E_G\right)\right],\quad E>\frac{E_G}{2} \tag{5}$$

which reduces to that of ideal graphene [1,4] when E_G vanishes. The expression for the valence band is entirely analogous. Employing the standard expression of statistical mechanics for the electron and hole densities in thermal equilibrium, one can readily show that the densities, doping and Fermi level are interrelated as shown in Fig. 1 for E_G = 0 and 0.26eV. Of course, having a bandgap is desirable from a device perspective, and this may be seen in the reduction in the density at the neutral point in Fig. 1 and more fully in Fig. 2. Finally, for use in the DD theory one can obtain approximations for the chemical potentials using numerical inversion. An expression for the electron gas is

$$\varphi_n\left(n,T\right)\cong k_BT\left\{\ln\left(\frac{n/N_{gr}}{1+\gamma E_G/k_BT}\right)+\beta\left(\frac{n/N_{gr}}{1+N_0/n}\right)^{\alpha}\right\} \tag{6}$$

where $\gamma=0.3$, $\alpha=0.58$, β and N_0 are slowly varying functions of E_G, and $N_{gr}\equiv k_BT/\hbar^2c^2\pi$ which at room temperature equals $4.9\text{x}10^{10}\text{cm}^{-2}$. As seen in Fig. 3, (6) accurately describes the electron gas for E_G = 0.26eV for $n<5\text{x}10^{13}\text{cm}^{-2}$.

Unlike in [9] where field-dependent mobility models were introduced, here we simply assume constant mobilities of 500cm^2/V-s in all layers so that the effects of the multilayers and bandgaps are not obscured in our results. And with respect to the generation/recombination terms in $(1a)_1$ and $(1b)_1$, having a narrow bandgap (and in the limit no bandgap [9]) means that it is important to include the possibility of band-to-band tunneling. For this paper, we utilize a local model similar to that introduced in [10].

Finally, in order to match the graphene situation, the DD theory of [9] treated the electron and hole transport in 2-D (or in 1-D if one assumes infinite width) and the electrostatics in

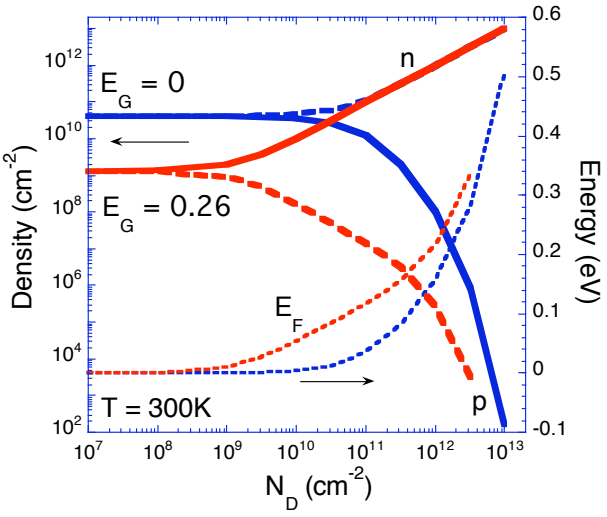

Fig. 1. Electron chemical potential versus electron density for single-layer in the ideal band structure.

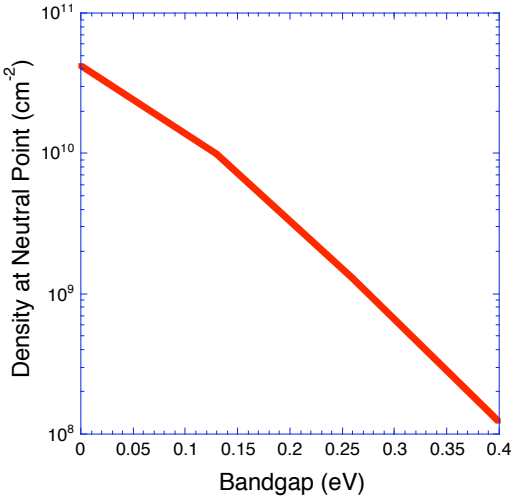

Fig. 2. Electron chemical potential versus electron density for single-layer in the ideal band structure.

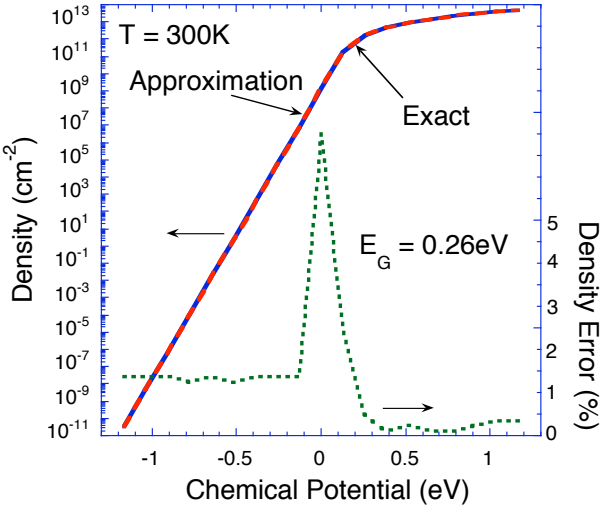

Fig. 3. Electron chemical potential versus electron density for single-layer in the ideal band structure.

3-D (or 2-D). The present work generalizes the earlier approach to allow for multiple layers by assuming that the transport in each layer acts independent of the others apart from the electrostatic interaction [10]. The electron and hole gas responses in each layer are given by the foregoing equations of state in which, according to [3], the first four graphene sheets have bandgaps of 0.26, 0.13, 0.07 and 0.02eV, respectively. As far as the electrostatics is concerned, we treat these sheets as distinct layers separated by very thin insulators so that the electrostatic interactions between carriers in each layer are incorporated explicitly.

III. Results and Discussion

For this paper, we model graphene field-effect transistors with the geometry shown in Fig. 4. For simplicity these FETs are assumed to be depletion-mode so that at zero bias the entire region between source and drain is electron-rich. For such a device to be useful, it obviously needs to turn off when a sufficiently negative bias is applied to the gate electrode. In discussing our DD simulations of these devices it is important to emphasize that the theory in its present state of development contains a number of uncertainties (primarily in the mobility and G-R models) that make results only semi-quantitative at best. Consequently, their value is primarily in illustrating the DD approach, and in exhibiting certain qualitative effects that may be seen in such devices.

A. Effect of bandgap

As is well known, ideal graphene field effect devices have small on/off current ratios because of their lack of a bandgap, and it is therefore not surprising that the introduction of a bandgap will lead to better performance. That graphene can have a bandgap as large as 0.26eV [3] seems especially interesting in that this is similar to the bandgap of InSb, a material currently considered a legitimate candidate for a future low-power digital technology [11].

The effect of the bandgap on the transfer characteristics is illustrated in the set of DD simulations plotted in Fig. 5. The off-state current (at large negative gate voltage) is largely associated with band-to-band tunneling in these simulations. The effect of thermal generation/recombination is less important, apparently because of the very small collection volume. According to our calculation, a bandgap of as little as 0.1eV can produce an on/off ratio ~100. The simulations with bandgaps of greater than 0.2eV did not converge beyond the values shown, an effect most likely due to the fact that the channel region was not otherwise contacted and so constituted a "floating body". Lastly, it should be noted that the bandgap had little effect on the on-state current.

B. Effect of mulitlayers

To illustrate the DD simulation of multi-layer graphene transport, we again assume the mobilities are constant and equal, and focus on the effects of geometry, bandstructure, and electrostatics on the transport in each layer. The results for a structure composed of 4 layers of ideal (zero gap) graphene are shown in Fig. 6. In this figure, we plot the percentage of

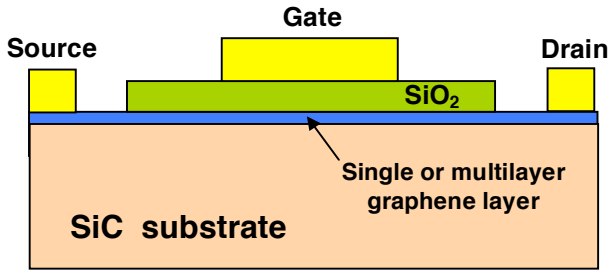

Fig. 4. Schematic of depletion-mode graphene field effect transistor as modeled in this work.

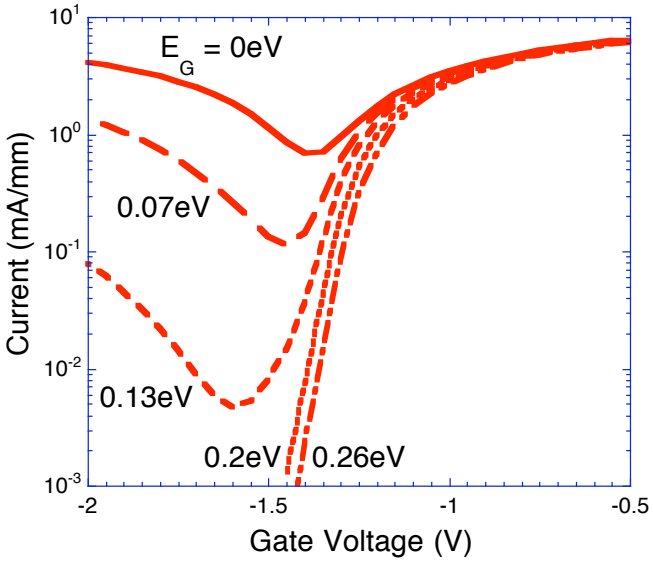

Fig. 5. DD simulation of the effect of a bandgap on the I-V characteristics of a single-layer graphene FET with $L = 0.5\mu m$ and $V_D = 50mV$.

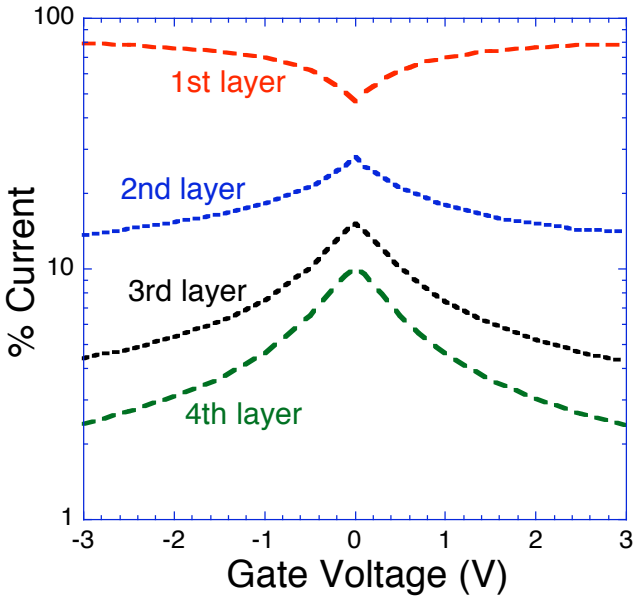

Fig. 6. DD simulation of the urrent contributions in a 4-layer zero-gap graphene FET as a function of gate voltage.

the total current carried in each layer in order to highlight the effect of the multiple layers. The behavior is readily understood. At low gate voltage, the intrinsic density in each layer leads each to contribute significantly, while at higher bias the accumulation of electrons or holes in the layer closest to the gate screens the other layers and leads to it being increasingly dominant.

IV. SUMMARY

The DD theory of electron and hole transport in graphene is extended to treat the case of epitaxial graphene on SiC, which often consists of more than a single layer and which may have a small substrate-induced bandgap. The theory for these situations is illustrated with some simple device examples. This theory should be useful in interpreting experimental measurements on such material. And if material properties continue to improve, then the graphene-on-SiC approach could well lead to a low-power electronics technology for which the DD theory would be of value for design and optimization.

ACKNOWLEDGMENT

The author thanks Dr. Chagaan Baatar and the Office of Naval Research for funding support.

REFERENCES

[1] B. Ozyilmaz et al, "Electronic transport in locally gated graphene nanoconstrictions," Appl. Phys. Lett. 91, 192107 (2007).

[2] D.A. Areshkin, D. Gunlycke and C.T. White, "Ballistic transport in graphene nanostrips in the presence of disorder: Importance of edge effects," *Nano Letts*. **7**, 204 (2007).

[3] S.Y. Zhou et al., "Substrate-induced bandgap opening in epitaxial graphene," *Nature Mat.* **6**, 770 (2007).

[4] S. Kim, J. Ihm, H.J. Choi and Y.-W. Son, "Origin of anomalous electronic structures of epitaxial graphene on silicon carbide," *Phys. Rev. Lett.* **100**, 176802 (2008).

[5] For a dissenting view see E. Rotenberg, A. Bostwick, T. Ohta, J.L. McChesney, T. Seyller and K. Horn, "Origin of the energy bandgap in epitaxial graphene," *Nature Mat.* **7**, 258 (2008).

[6] K.I. Bolotin *et al.*, "Ultrahigh electron mobility in suspended graphene," *Solid-St. Comm*. **46**, 351 (2008).

[7] T. Stauber, N. Peres and F. Guinea, "Electronic transport in graphene: A semiclassical approach including midgap states," *Phys. Rev. B* **76**, 205423 (2007).

[8] M. Lemme, T. Echtermeyer, M. Baus & H. Kurz, *IEEE Elect. Dev. Lett*. **28**, 282 (2007).

[9] M.G. Ancona, "Graphene field-effect devices from a diffusion-drift perspective," to be published, *J. Comp. Elect.* (2008).

[10] G. Hurkx, H. de Graaff, W. Kloosterman and M. Knuvers, "A new analytical diode model including tunneling and avalanche breakdown," *IEEE Trans. Elect. Dev.* **39**, 2090 (1992).

[11] T. Ashley *et al.,* "Heterogeneous InSb quantum well transistors on silicon for ultra-high speed, low power logic applications," *Elect. Letts*. **43**, 777 (2007).