Modeling electrostatic doping and series resistance in Graphene-FETs

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Abstract—We model the source/drain series resistance and the electrostatic doping effects associated to the source and drain metals in graphene FETs using a Monte Carlo transport simulator. We compare the new model to simulations assuming chemical doping in the source/drain regions. A procedure to include the series resistance as part of the self-consistent Monte Carlo loop is proposed and verified against the widely employed method based on look-up tables.

Index Terms—Graphene FET (GFET), Monte Carlo, electrostatic doping, series resistances.

I. INTRODUCTION

Graphene FETs (GFET) have a great potential as high cutoff frequency devices [1]. However, far from ideal metal/graphene contacts and series resistances reduce the extrinsic transconductance and limit the GFET performance [1]. Since it is difficult to chemically dope graphene [2], metals are used to induce an electrostatic doping and to control the polarity of the source/drain (S/D) regions [3], [4]. Clearly, it is fundamental to account for these effects in GFET simulation tools in order to reliably assess the RF performance of GFETs. The Monte Carlo (MC) method has been used in [5], [6] to describe quasi-ballistic transport in short channel GFETs. Here, we extend the MC transport model of [6] to include the S/D contacts. In addition, the contribution of the series resistances is directly accounted for by dynamically adjusting the terminal voltages in the self-consistent loop for the calculation of device electrostatics as opposed to the time consuming generation of a look-up table based post-processing of the MC transport simulations [6], [7].

II. MODELING ELECTROSTATIC DOPING

The MC simulator for GFET devices developed in [6] couples, in a self-consistent loop, the Boltzmann transport equation for electrons and holes in the graphene sheet to the non-linear Poisson equation. A gapless energy dispersion relationship in the graphene is assumed and scattering with acoustic and optical phonons in the graphene as well as with remote phonons in the top-oxide and back-oxide (Fig. 1) are considered. A local model for the band-to-band tunneling (BBT) in graphene (generation–recombination based on the local electric field and occupation function) is also included.

Fig. 1 sketches GFETs with chemical doping (CD, a) and electrostatic doping (ED, b) in the S/D regions. The dashed box is the domain of the MC transport simulation. For the case of chemical doping, S/D regions are part of the domain and Neumann boundary conditions are used in the Poisson equation [6].

For the case of electrostatic doping, instead, S/D regions are external, but coupled to the MC domain as follows. First, the electrostatics of the vertical metal/graphene stack is solved (see section AA' in Fig. 1(b)), assuming the presence of an insulating layer (IL, by default 0.2 nm of vacuum, consistently with [8], [9]) between metal and graphene, acting as a tunnel barrier [10].

Fig. 2 shows the band diagram of the stack at the source.
\[
\phi_M - \frac{Q_{GR}}{C_{IL}} = \chi_{GR} - E_D
\]

(1)

\[
Q_{GR} = q \int_{-\infty}^{0} DoS(E) \cdot [1 - f(E, E_D)] \, dE - \int_{0}^{\infty} DoS(E) \cdot f(E, E_D) \, dE
\]

(2)

Fig. 3. Energy displacement $E_D$ vs. the work-function of the S/D metal contact considering (dashed line) or neglecting (solid line) the presence of 20 nm of SiO$_2$ as back-oxide. The source to back-gate voltage is null.

Fig. 5. $I_{DS}$ vs. $V_{DS}$ for GFETs with chemical (dashed) and electrostatic (solid) doping. Results including BBT according to the model in [6] are reported at $V_{TG} = 0.3$ V for the case with CD. BBT model for the ED is under development.

Fig. 3 shows the energy displacement $E_D$ vs. the work-function $\phi_M$ of the metal contact for a few values of the IL thickness $t_{IL}$ in the metal/IL/graphene stack (solid lines) and in the metal/IL/graphene/insulator/metal structure (dashed lines). As expected, $E_D$ is null when the metal work–function equals the graphene affinity ($\chi_{GR} = 4.6$ eV) and, the thinner the IL, the larger the charge induced in the graphene is, since $C_{IL}$ increases. We see that the presence of the back–oxide (here 20 nm of SiO$_2$, consistently with what simulated in the following of this work) does not change significantly the amount of the induced charge in the graphene and finally, the value of $E_D$ is almost the same of the previous structure (compare solid and dashed lines).

Concerning the transport simulations of complete GFETs, in both CD and ED cases, carriers are injected at the S/D ends of the MC simulation domain according to a Fermi–Dirac distribution with $E_F^S = 0$ and $E_F^D = -qV_{DS}$, respectively, similarly to what was done for MOSFETs in [11]. For the sake of a fair comparison between the devices in Fig. 1, we set a work–function of the S/D metal ($\phi_M = 2.061$ eV) that induces in the ED case a $Q_{GR}/q = 5 \times 10^{13}$ cm$^{-2}$, that is, exactly the same value of the doping in the CD case. Unless otherwise stated, we simulated report calculations on n-GFETs with channel length $L_{GH} = 30$ nm, 2 nm underlap, 2 nm SiO$_2$ top–oxide ($t_{BG}$) and 20 nm SiO$_2$ back–oxide ($t_{BG}$).

Fig. 4 compares the average electron density under the top–gate vs. $V_{TG}$ in the case of CD and ED for $V_{DS} = 0$ V. The mutual agreement between curves is good, as expected, since the electrostatics is controlled by the gate, while the S/D regions only set the electron Fermi level. This results proves the correct implementation of the model.
Fig. 6. Electron velocity (a), density (b) and potential energy (c) along the channel for GFETs with chemical (black–dashed) and electrostatic (solid–red) doping for $V_{TG}=0.3$ V and $V_{DS}=0.05$ V. Device parameters: $L_{CH}=30$ nm, 2 nm underlap, $t_{RG}=2$ nm (SiO$_2$) and $t_{BG}=20$ nm (SiO$_2$).

Fig. 7. The same as in Fig. 6 with $V_{DS}=0.5$ V.

Fig. 8. $I_{DS}$ evolution during the MC simulation of a GFET with series resistance. Without damping procedure, the simulation does not converge (solid line). The damping algorithm solves the problem (dashed line). The dash–dotted line is the current value used in the algorithm to calculate the Fermi-level drop across the series resistances at each iteration.

Fig. 9. Potential energy profile along the GFET (CD) without (dashed black) and with (solid red) the series resistances. The Fermi levels in the S/D regions ($E_F^S$, $E_F^D$) are reported (dashed black: no R, solid red: with R). The shift of the Fermi levels in the source and in the drain regions reduces the intrinsic $V_{DS}$.

Fig. 5 compares the output characteristics for GFETs with CD or ED in the source and drain. The motivation for the observed differences are investigated with the help of Figs. 6 and 7 showing the electron velocity (a), concentration (b) as well as the potential energy (c) profiles at $V_{DS}=0.05$ V and $V_{DS}=0.5$ V, respectively. At high $V_{DS}$ the agreement between these profiles in the CD and ED cases is worse than at low $V_{DS}$, explaining the small differences in the resulting output characteristics of Fig. 5. For the CD case, simulations including the contribution of BBT are also reported in Fig. 5, showing the typical non–saturated behavior [6]. The BBT model for the ED case is under development, since the determination of the BBT rate requires a careful estimation of the carrier fluxes in the high electric field regions [6] that feature significant differences in the ED and CD cases.

III. MODELING SERIES RESISTANCES

So far we have included the effect of the metal contact on the electrostatics. The non–negligible tunneling resistance of the IL translates into a significant series resistance [12], [13]. In order to have a comprehensive GFET simulation tool, we include directly in the self–consistent MC loop the series resistances ($R$) at each side, inclusive of contributions from tunneling resistance, graphene sheet resistance in S/D, etc. At each iteration, the electrons' Fermi levels of the source and drain are shifted by $qRI_{DS}$. The instantaneous current ($I_{DS}$, estimated as an average along the channel of the product between the carrier concentration and the average carrier velocity) requires a proper estimation. In fact, Fig. 8 shows that, without introducing some damping, the simulation does not converge (solid line). To overcome this difficulty, we limit the variations of the $R_{DS}$ value to less than 1% between two MC iterations. The dash–dotted line in Fig. 8 shows the current value used to calculate $R_{DS}$, while the dashed line is the $I_{DS}$ obtained at the given iteration, that converges thanks to the proposed damping scheme.

Fig. 9 shows the potential energy profile for the CD GFET w/o and with $R=100$ $\Omega$ $\mu$m. For $R>0$, $E_F^*$ is reduced, while $E_F^D$ is increased, thus reducing the intrinsic voltage drop across the channel ($V_{DS}=V_{DS}-2RI_{DS}$). In addition, the
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Fig. 10. Potential energy profile along the GFET (CD). Solid red: simulation with \( V_{DS}, V_{TG} \) and the series resistance. Dashed black: simulation with the intrinsic biases \( V_{TG}^i = V_{TG} - RI_{DS}, V_{DS}^i = V_{DS} - 2RI_{DS} \) and without the series resistance. \( \Delta S = \Delta_{CH} \) demonstrates that it is present only a pure shift between the two potential energy profiles, since \( E_B^p \) and \( E_B^D \) are shifted of \( qRI_{DS} \) in the two simulations.

Fig. 11. \( I_{DS} \) as a function of \( V_{DS} \) for a GFET with chemical doping without (left) and with (right) the contribution of BBT. Results without (dashed lines) and with the series resistance (solid lines) are compared. Symbols are the data without \( R \) after the transformation of the plane \( (V_{DS}, V_{TG}) \) to include the series resistance potential drop (as proposed in [7]).

REFERENCES


