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Interpretation of graphene mobility data by means of a semiclassical Monte Carlo transport model

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ABSTRACT

In this paper we compare experimental data and simulations based on a semiclassical model in order to investigate the relative importance of a several scattering mechanisms on the mobility of graphene nano-ribbons. Furthermore, some new experimental results complementing the range of ribbon widths available in the literature are also reported.

We show that scattering with remote phonons originating in the substrate insulator can appreciably reduce the mobility of graphene and it should not be neglected in the interpretation of graphene mobility data. In fact by accounting for remote phonon scattering we could reproduce fairly well the experimentally observed dependence of the mobility on the ribbon width, the temperature and the inversion density, whereas the agreement with experiments is much worse when remote phonons are not included in the calculations.

1. Introduction

Due to its high carrier mobility [1,2], graphene is being widely investigated as an alternative channel material for future MOSFETs. The absence of an energy gap and the consequent high band-to-band tunneling (BBT) rate result in graphene MOSFETs (GFETs) with large off currents and undesirable ambipolar behavior, which seriously limit the use of GFETs for digital circuit applications. Patterning graphene into nano-ribbons (GNRs) opens a gap, but this is associated to a much lower mobility compared to large area monolayer flakes, as predicted by the modeling results in [3] and then confirmed by experiments [4]. In [3], the ribbon width (W) dependence of the mobility is explained based on the modification of the band structure with the GNR width. Only phonons originating in the GNR were included in the model of [3]. Ref. [5] instead shows that edge roughness scattering becomes the dominant collision mechanism for W below approximately 4 nm. Combining the phonon-limited mobility (computed based on a simple analytical band structure) with the edge roughness, defects and impurity limited mobility given by the Non-Equilibrium Green's Function calculations of the transmittance of randomly generated GNRs, it was concluded in [6,7] that phonons, edge-roughness and defects jointly contribute to reducing the mobility as the GNRs get narrow.

The models in [3,5,6,8] describe electrons in the GNR as a 1D gas and are thus expected to be accurate for narrow ribbons but also difficult to calibrate with experimental data, because all the model parameters have to be simultaneously adjusted on the few and disperse measurements available for $W < 10$ nm. To overcome this limitation, in this paper we employ an energy model [9] where quantum corrections to the 2D dispersion relationship of graphene sheets are introduced in order to cover a wide range of W spanning from few nanometers to microns. Different scattering mechanisms have been calibrated on independent experiments. Our model includes the scattering due to the remote phonons originating in the polar substrate, and extends the work presented in [10] by comparing the simulation results with a much broader set of experimental data as a function of ribbon width, inversion density and temperature.

2. Simulation model

The simulation model employed in this work is based on the semi-classical approach. The Boltzmann–Transport–Equation is solved using the Monte Carlo method. The dispersion relationship is given by the analytical expression [9]:

$$E = \hbar v_F \sqrt{k_x^2 + k_y^2 + \left(\frac{\pi}{W}\right)^2} \quad (1)$$

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which has been validated by direct comparison against tight-binding calculations of GNRs with various widths including edge disorder [9,11]. The density of states corresponding to the energy relation of Eq. (1) is in much better agreement with the tight-binding calculations mentioned above than the one derived from a 1D representation of the carrier gas. A more detailed discussion about the differences in using a 1D or a 2D carrier gas description in GNRs can be found in [9].

In this paper we consider uniform situations where a constant electric field F_x is applied in the x direction, so the solution of the Boltzmann–Transport–Equation with the Monte–Carlo technique consists in free-flights during which k_x is varied by $eF_x t_{FF}/\hbar$, where t_{FF} is the free-flight duration, stochastically selected using the self-scattering technique. The position along x of the particle does not matter, since we assume uniformity along the device length. On the other hand, we keep trace of the y position in order to account for edge roughness (ER), that is treated as a diffusive reflection at the edges, similarly to [12]. This is a worst case scenario compared to silicon inversion layers, where only a fraction of the reflections at the interface are diffusive, whereas the others are specular. The y position is modified during the free-flight by $v_y t_{FF}$, where the group velocity v_y along y is obtained deriving Eq. (1) over k_y (dividing by $\hbar$).

Free-flights are interrupted by scattering events. We include scattering with: phonons (elastic and inelastic) originating in the GNR (labeled as PH) and remote phonons originating in the polar dielectric (RP). The expressions for the scattering rate with elastic and inelastic phonons originating in the GNR can be found in [9].

As for RP scattering, we have extended the model in [13] to the dispersion relationship given by Eq. (1). The scattering rate is given by:

$$S_{RP}(E) = \frac{1}{\pi\hbar} k(E \pm E_{RP}) \left.\frac{dk}{dE}\right|_{E\pm E_{RP}} \times \int_0^{\pi} \frac{1+\cos\theta}{2} S_{VV} \times \left(\sqrt{k^2(E) + k^2(E \pm E_{RP}) - 2k(E)k(E \pm E_{RP})\cos\theta}\right) d\theta \quad (2)$$

where the E–k, k–E and dk/dE relationships are easily derived from Eq. (1) and θ is the angle between the initial and final wave-vector. Since we consider extended states with a density of states similar to the one of a 2D carrier gas [9], the wave-functions are assumed to be the same as in a large graphene layer and the spinor overlap factor is $(1+\cos\theta)/2$. The term S_{VV} is given by:

$$S_{VV}(Q) = e^2 \left(n_{RP} + \frac{1}{2} \mp \frac{1}{2}\right) \frac{\hbar\omega_{SO}}{2Q} \left(\frac{1}{\varepsilon_1 + \varepsilon_2^i} - \frac{1}{\varepsilon_1 + \varepsilon_2^0}\right) e^{-2Qd} \quad (3)$$

where ε_1 is the permittivity of the top material (vacuum in the cases considered in this paper where no top-gate is present), ε_2^0 and ε_2^i are the low frequency and intermediate frequency permittivity of the SiO_2 substrate (bottom material). Note that Eq. (3) has no singularities because, due to the finite energy difference between the initial and final state, the magnitude Q of the scattering induced change in the carrier wave-vector is always non null.

The remote phonon energy $E_{RP} = \hbar\omega_{SO}$ is related to the energy of the lowest TO mode in the substrate $\hbar\omega_{TO}$ by

$$\omega_{SO} = \omega_{TO}\sqrt{\frac{\varepsilon_1 + \varepsilon_2^0}{\varepsilon_1 + \varepsilon_2^i}} \quad (4)$$

The distance d between the GNR and the substrate is not precisely known and is assumed to be zero in the following (perfect adhesion). In fact we verified that d values up to a few Angstroms do not appreciably change the results, essentially because the term $\exp(-2Qd)$ is close to 1.0 for the average values of the scattering induced exchange wave-vector Q. It should be noted that the model for RP scattering does not contain any adjustable parameter.

In the Monte–Carlo algorithm, RP scattering is implemented as follows. The total scattering rate $S_{RP}(E)$ (Eq. (2)) is used to determine the free-flight duration (summed to the scattering rate for the local phonons). When RP is selected as the scattering mechanism responsible for the interruption of the free-flight, the deflection angle θ is selected based on the relative contribution to the integral in Eq. (2). To enforce the Pauli exclusion principle, scattering events (RP and PH) are rejected based on the occupation of the final state.

Our treatment of the scattering with remote phonons does not account for a possible coupling between the lattice polarization of the back oxide and the electronic polarization of the graphene, in other words we do not include coupling between phonon and plasmon modes [14]. The phonon–plasmon coupling is a delicate matter, whose conclusive assessment is beyond the scope of the present work and whose quantitative investigation demands an accurate determination of both the real and the imaginary part of the graphene polarizability. In this respect, the analytical results for the graphene polarizability reported in [15,16] (and derived for $T = 0$ K) show that the imaginary part of the polarizability is *non* null in a wide region of the energy versus wave-vector plane. This implies that a large part of the coupled phonon–plasmon modes undergo strong Landau damping and cease to be collective excitations [17,18]. In the region of Landau damping not only the phonon–plasmon coupling is suppressed but also the screening of the RP modes due to the electronic polarizability of the graphene layer should not be included in the calculation, so that it is questionable to describe the screening by simply dividing the RP matrix elements by the graphene static dielectric function [16,8]. Given the very complicated and still debated theoretical framework, we embraced a relatively simple picture and did not include the graphene polarization in our calculations, thus neglecting the phonon–plasmon coupling. A recent publication [18] has shown that phonon–plasmon coupling is essentially negligible in silicon devices with SiO_2 or high-k dielectrics in all cases of practical interest. While the same conclusion is not granted for graphene devices, the analysis in [18] suggests that using the static dielectric function for the screening of RP most likely leads to a significant overestimation of the screening effect.

3. Device fabrication and mobility measurements

Low-field mobility was measured on samples fabricated by the exfoliation method and deposited on a silicon substrate with 90 nm thermally grown SiO_2. The contacts were fabricated by structuring a poly methyl methacrylate (PMMA), lift off mask with ebeam lithography and subsequent deposition of 50 nm of nickel. After lifting off the residual nickel the GNRs were defined in hydrogen silsesquioxane (HSQ) resist with e-beam. Then the uncovered graphene was etched in a reactive ion etch oxygen plasma. The GNR width is approximately 150 nm. The mobility has been extracted in four terminal devices according to:

$$\mu = \frac{I_{DS} L_{\text{int}}}{W Q_S V_{DS,\text{int}}} \quad (5)$$

where L_{int} is the length of the internal probes; the inversion charge Q_S has been estimated considering the capacitance of the back-gate contact, neglecting the contribution of the quantum capacitance that is not expected to be critical due to the large thickness of the back-oxide. Describing the capacitance of the back-gate as simply $C_{OX}WL_{\text{int}}$ may introduce a small error in the determination of Q_S, since the formula applies to a plate capacitor, whereas in our case W is only approximately 150 nm implying that the fringing capacitance is not negligible (since the back oxide is 90 nm thick). So, the capacitance should be larger in the GNR case resulting in lower