Drift velocity peak and negative differential mobility in high field transport in graphene nanoribbons explained by numerical simulations

Alessandro Betti, Gianluca Fiori, and Giuseppe Iannaccone

Dipartimento di Ingegneria dell’Informazione: Elettronica, Informatica, Telecomunicazioni,
Università di Pisa, Via Caruso 16, 56122 Pisa, Italy.

We present numerical simulations of high field transport in both suspended and deposited armchair graphene nanoribbon (A-GNR) on HfO$_2$ substrate. Drift velocity in suspended GNR does not saturate at high electric field ($F$), but rather decreases, showing a maximum for $F \approx 10$ kV/cm. Deposition on HfO$_2$ strongly degrades the drift velocity by up to a factor of $\approx 10$ with respect to suspended GNRs in the low-field regime, whereas at high fields drift velocity approaches the intrinsic value expected in suspended GNRs. Even in the assumption of perfect edges, the obtained mobility is far behind what expected in two-dimensional graphene, and is further reduced by surface optical phonons.

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Assessing the potential of Graphene Nanoribbons (GNRs) for future electronic applications requires full understanding of both quasi-equilibrium and far-from-equilibrium transport mechanisms [1, 2]. However experimental low-field (LF) mobility in 1 nm-wide GNRs can be as low as 100 cm$^2$/Vs and is limited by edge disorder [1, 3]. Furthermore, we know that achieving ideally smooth edges is not enough: full-band (FB) modeling shows that LF mobility due to only acoustic (AC) phonon scattering at low fields is close to 500 cm$^2$/Vs for 1 nm-wide GNRs [4]. Most importantly, nanoscale transistors do not operate in the LF mobility limit. Therefore, simulation of far-from-the-equilibrium transport conditions is required to understand achievable device performance. Whereas at low field carrier scattering is mainly due to low-energy intravalley acoustic phonons [4], at high electric field scattering is dominated by optical phonon emission (EM), which becomes relevant when electrons gain enough energy to emit optical phonons. High-field steady-state transport can be simulated by solving the Boltzmann transport equation (BTE) through the single-particle Monte Carlo (MC) method. When dealing with 1D systems, however, particular attention has to be paid in accurately describing the energy dispersion relation due to quantum lateral confinement: for each GNR subband there is a parabolic behavior close the subband minimum, and then the typical graphene quasi-linear behavior already for relatively small wavevector values, corresponding to a velocity $\approx 8 \times 10^6$ m/s. Some authors have considered phonon confinement and multisubband transport, focusing on quantum wires with the effective mass approximation [5, 6]. For GNRs, a multisubband MC approach has been followed in [7] and BTE has been solved in a deterministic way at criogenic temperatures in [8]. Bresciani et al. [8] have used a 2D model, which is not fully adequate for sub-10 nm GNRs, where size effects are indeed relevant.

In this work, we adopt a steady-state single-particle full band MC approach accounting for carrier degeneracy [10], which has a significant effect for materials with a small density of states as graphene. Scattering rates are obtained within the Deformation Potential Approximation (DPA) from phonon dispersions described by means of the fourth-nearest-neighbour force-constant approach (4NNFC) [11] and a $p_z$ tight-binding Hamiltonian for the electronic structure. We consider in-plane longitudinal acoustic and optical (LA and LO), transversal optical (TO) and surface optical (SO) phonons. In each subband, the rates are computed on a 2000-point grid in the $k_x$-space (due to symmetry only longitudinal electron wavevectors $k_x > 0$ have been taken into account), considering energy up to 1.5 eV above the bottom of the first subband and including up to 18 subbands: this ensures accurate results even for strong longitudinal electric field $F \leq 3 \times 10^2$ kV/m and for all the considered GNR widths ($W \leq 10$ nm). Due to Van Hove singularities in the 1D rates, the self-scattering method [12] is inefficient, so that we have adopted the MC procedure described in Ref. [12] and extended to quasi-1D systems [13]. The whole story of an electron has a duration $T = \sum_i \Delta t_i$ ($T \leq (10 - 100) \mu s$ depending on $W$ and $F$), where $\Delta t_i = t_{i+1} - t_i$ is the $i$-th time step and $t_i$ is the $i$-th sampled time. At each $t_i$, the wavevector $\mathbf{k} = (k_x, k_{y\parallel})$, where $k_{y\parallel}$ is the transverse quantized electron wavevector [4], is computed and the average value of quantity $X$ (either the drift velocity $v(\mathbf{k}) = 1/\hbar \cdot \partial E(\mathbf{k})/\partial k_x$ or the energy $E(\mathbf{k})$) is evaluated according to [12]: $\langle X \rangle_t = \frac{1}{\Delta t} \int_0^{\Delta t} X [k_x(t')] dt' = \frac{1}{\Delta t} \sum_i \int_{t_i}^{t_{i+1}} X [k_x(t')] dt'$. The electronic temperature $T_e$ under an applied homogeneous field $F$ is computed by equating $\langle v(k_x)^2 \rangle$ with the mean squared velocity at equilibrium $T_{lat}$. For $F = 0$, $T_{el}$ is equal to the lattice room temperature $T_{lat}$, whereas for $F > 0$, $T_{el} > T_{lat}$. Once obtained $T_{el}$, the distribution function is updated accordingly at each $t_i$ and final states for scattering are filled obeying to the Pauli exclusion principle (PEP).

The computed average drift velocity $\langle v_d \rangle$ limited by intrinsic phonons is plotted in Fig. 1 as a function of $F$ for suspended sub-10 nm GNRs and for a carrier density $n_{2D} = 10^{12}$ cm$^{-2}$. $\langle v_d \rangle$ strongly varies within the
considered $F$ interval and a maximum appears at high electric field ($F = F_{th}$). For $F < F_{th}$, $\langle v_d \rangle$ can be fitted by means of the Caughey-Thomas model, i.e. $\langle v_d(F) \rangle = (\mu_{in,0}/F)^{1/(1+\mu_{in,0}/v_p))^{\gamma}$, where $\gamma \approx (1.3 \div 2)$; $\mu_{in,0}$ is the intrinsic LF mobility and $v_p$ is the peak velocity, which ranges from $2 \times 10^5$ to $4 \times 10^5$ m/s, depending on $W$ (Table I). $\langle v_d \rangle$ does not saturate with $W$, analogously to what has been observed in the case of zigzag CNTs\cite{14}. As shown in Fig. 1, $\langle v_d \rangle$ slightly decreases for increasing $F$\cite{14}. However, in contrast to\cite{14}, the negative differential mobility (NDM) cannot be explained by the increased number of populated states in the second subband with smaller $v(k)$. Indeed, as in\cite{15}, we have verified for $W = 10$ nm that such effect is much more pronounced if we fictitiously limit transport to only one subband (red dashed line in Fig. 1). The velocity peak can be explained by the combined effect of the quasi-linear dispersion relation in GNRs and the strong increase of optical EM at high $F$, which increases the occurrence of backscattering events therefore reducing the average velocity. If we follow the story of a single electron, we can see that as $F$ increases, instantaneous electron velocity cannot increase beyond the limit imposed by the dispersion relation: any backscattering event will invert the instantaneous velocity sign and therefore reduce the average velocity. Therefore, in the absence of optical phonon EM, the drift velocity $\langle v_d \rangle$ would saturate to about $8 \times 10^5$ m/s. The onset of optical phonon EM makes $\langle v_d \rangle$ peak at a fraction of that value and then decrease with $F$. We believe that the very same mechanism explains also the NDM in zigzag CNTs, as well as in graphene\cite{16}, even if it has not been proposed before\cite{14,15}. One can also see that the peak velocity $v_p$ increases with $W$. Indeed, if $\hbar \omega$ is the optical phonon energy ($\approx 160$ meV for LA mode), the current $J$ can be estimated as $J = \frac{e\omega}{\hbar} \frac{\mu}{\kappa} \frac{\hbar}{\omega} \frac{\hbar}{\gamma} \hbar \omega \approx \hbar \omega \hbar \omega$, where $v_p$ is the Fermi velocity. Since $v_p = J/(\omega \omega)$ and the Fermi wavevector $k_F = \pi n_{2D} W/\omega^2$, we obtain $v_p = \omega W/\pi \propto W$.

The threshold field $F_{th}$ strongly decreases with $W$, because of the increased mean free path ($L_k$), which allows electrons to gain energy required to emit optical phonons at lower $F$. $F_{th}$ can be roughly estimated by imposing the cutoff energy $\hbar \omega_{EM}$ for optical EM equal to the mean kinetic energy gained between two scattering events, i.e. $qF_{th}(L_k)$. Since by increasing $W$ from 1 to 10 nm, $L_k$ increases from $\approx 6$ nm to 1 $\mu$m\cite{3}, $F_{th}$ decreases from $\approx 2.7 \times 10^5$ kV/cm to $\approx 1.6$ kV/cm. We remark also that the obtained values for $\langle v_{in} \rangle$ are in agreement with those found for zigzag CNTs with a circumference comparable with the considered $W$, both in linear and in non-linear regimes\cite{14}. In Fig. 2b, $\langle v_d \rangle$ is plotted as a function of $n_{2D}$ for $F = 10$ kV/cm: $\langle v_d \rangle$ does not depend on $n_{2D}$ even in the degenerate regime ($n_{2D} = 10^{12}$ cm$^{-2}$), where PEP limits up to the 50% of the scattering events. In Fig. 2 we show the intrinsic mobility $\mu_{in} \equiv \langle v_d \rangle/F$ as a function of $F$ for $n_{2D} = 10^{12}$ cm$^{-2}$. Since in the linear transport regime $v_d \propto F$, $\mu_{in}$ is constant for $F \leq F_{th}$ and decreases above $F_{th}$ as $\mu_{in} \propto 1/F^\alpha$ with $\alpha > 1$. In addition, the narrower the ribbons, the stronger the suppression due to lateral confinement. Results are in good agreement with a multi-subband model for $W \approx 5$ nm\cite{7}.

In the inset of Fig. 2 the average kinetic electron energy $\langle E_k \rangle$ in units of $k_B T_{lat}$ is shown as a function of $F$ for $n_{2D} = 10^{12}$ cm$^{-2}$. While for low $F \approx 0.1$ kV/cm electrons tend to remain near the first conduction subband edge and $\langle E_k \rangle \approx 1/2k_B T_{lat}$ for the narrowest ribbons,
for high field $F \geq 10^2 \text{kV/m}$, $\langle E_k \rangle \approx kT_{\text{sat}}$ and higher energy states are occupied. Note also that $\langle E_k \rangle$ increases with $W$, since subbands become closer, allowing electrons to populate higher subbands.

In Fig. 3a and 3b, the average drift velocity $\langle v_d \rangle$ and the mobility $\mu_{\text{ex}} = \langle v_d \rangle / F$ are shown, respectively, as a function of $F$ for GNRs deposited on HfO$_2$. Including the effect of SO phonons ($n_{2D} = 10^{12} \text{cm}^{-2}$), through the first SO(1) and second SO(2) modes ($\hbar \omega_{SO} = 12.4 \text{meV}$ for SO(1) mode). With respect to the suspended GNR case, $\langle v_d \rangle$, as well as mobility in GNR on HfO$_2$ are almost one order of magnitude smaller in the LF regime, while similar values are obtained for high field, as already noted for graphene on HfO$_2$ [10]. As in graphene [10], deposition on HfO$_2$ leads to an extension of the linear region to fields up to a factor 10 larger than those corresponding to suspended GNRs. For narrow ribbons, $\langle v_d \rangle$ does not saturate even for $F = 3 \times 10^2 \text{kV/cm}$.

In order to understand the different behaviour in suspended and deposited GNR on HfO$_2$, in Fig. 3a, we show the distribution function $G$ as a function of $(E_k - E_{C1})$, where $E_{C1}$ is the first subband edge, for $F = 1$ and $10 \text{kV/cm}$ ($W = 4.86 \text{nm}$) for GNRs, both suspended and deposited on HfO$_2$. At low fields, $G$ decreases rapidly with energy in both cases, showing, unlike graphene, sharp peaks due to intersubband scattering. At high fields instead, electrons are excited up to energies close or above $1 \text{eV}$, increasing $T_{\text{el}}$ (inset of Fig. 2). As expected, deposition on HfO$_2$ leads to a shorter high energy tail compared to that in intrinsic GNR (Fig. 3b) due to the introduction of an additional channel for energy and momentum relaxation which increases total scattering rate and pushes electrons down to lower average electron energy. As for graphene on HfO$_2$ [10], the rough absence of degradation of $\langle v_d \rangle$ at high $F$ can be explained by the reduced population in the high energy tail, i.e. by a smaller amount of electrons in the nonlinear dispersion energy region where the band velocity is smaller, which more than counterbalances the decrease of $\langle v_d \rangle$ resulting from the increased total scattering rate when depositing GNR on substrate. In order to explain the increase of the $F$ interval where $\langle v_d \rangle$ shows a linear behavior in the GNR on HfO$_2$ case, in Fig. 3 and 4, we show the relative ratio of scattering events for the different mechanisms as a function of $F$ for 5 nm-wide suspended GNR and GNR on HfO$_2$, respectively. For intrinsic GNR and $F \leq 1 \text{kV/cm}$, the main scattering events involve absorption (ABS) and EM of LA phonons (Fig. 4b). For $F \geq 10 \text{kV/cm}$, optical phonon EM (of both LO and TO phonons) becomes predominant, increasing up to 30% of the total number of events. For GNR on HfO$_2$ instead, scattering involving SO(1) phonons happens very often already for $F = 1 \text{kV/cm}$ whereas rates of LA, LO and TO phonons are limited to few percents even for high fields, as can be seen in Fig. 4c. In particular, the observed large absorption rate of SO(1) phonons (Fig. 4c), which is associated to the high Bose-Einstein occupation factor, appears to counterbalance SO(1) emission even at high $F$, and is the responsible of the extension of the linear region up to fields of $10 \text{kV/cm}$ or above, depending on $W$. In conclusion, we have performed a FB investigation of the dependence of drift velocity and mobility on the electric fields in GNRs. Suspended GNRs exhibit a drift velocity peak and then a NDM for large electric field, as also observed in zigzag CNTs. This property is due to the combined effect of quasi-linear dispersion relation and the emission of optical phonons. In particular, the maxima occur for a threshold field $F_{\text{th}} \propto 1/(L_k) \propto 1/W$. Depositing GNR on HfO$_2$ substrate strongly degrades $\langle v_d \rangle$ at low field by a factor $\approx 10$, whereas at high fields no degradation is observed [10]. Furthermore, in deposited GNRs velocity saturation and peak are shifted at higher $F$, due to the compensation of SO absorption and EM mechanisms.
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