Carrier scattering in graphene nanoribbon field-effect transistors

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The strong interest in graphene electronics was driven by its high mobility for quasiballistic transport, high carrier velocity for fast switching, and monolayer thin body for optimum electrostatic scaling and full planar processing. Although a two-dimensional (2D) graphene is a semimetal with no bandgap, a bandgap is opened by building a field-effect transistor (FET) on a nanometer-wide graphene nanoribbon (GNR) channel. The high mobility of graphene is characterized in 2D samples under low-field transport conditions. A nanoscale GNR-FET, however, has a quasi-one-dimensional (quasi-1D) channel with high-field carrier transport, which makes it necessary to understand the carrier scattering in a GNR-FET.

A recent experiment revealed that a 236 nm channel length GNR-FET delivers about 20% of the ballistic on current in the presence of strong elastic scattering and optical phonon (OP) scattering. While the small direct effect of OP scattering on the on current can be explained similarly as in carbon nanotube (CNT) FETs by an energy relaxation mechanism, the ballisticity of the GNR-FET at on state is still puzzling because the elastic scattering mean free path (mfp) of the GNR (~10 nm) was characterized to be much shorter than the channel length. The simulation study in this letter indicates that the short-mfp elastic scattering has a large effect on the source-drain dc of a GNR-FET due to its quasi-1D channel. In contrast to the intuition that an additional scattering mechanism lowers the current by increasing the scattering rate, the coupling of OP scattering to elastic scattering in a GNR-FET increases rather than decreases the current, compared to the value if there were only elastic scattering. Improving the GNR edge quality plays an important role in further increasing the ballisticity of a nanoscale GNR-FET.

The structure of the modeled p-type GNR-FET is shown in Fig. 1(a) which is similar to the experimental device. The Schottky barrier (SB) height for holes between the contacts and the channel is assumed to be $\phi_{SB} = 0$, which is close to the experimental value of the SB height between Pd contacts and a CNT channel with a similar bandgap.

A quantum treatment is used to capture quantum tunneling through SB. Ballistic simulations have been previously reported, and here we model quantum dissipative transport in GNR-FETs. The GNR-FET was simulated by self-consistently solving a transport equation in nonequilibrium Green’s function (NEGF) formalism and a three-dimensional Poisson equation. The Hamiltonian is described by a tight binding $p_z$ orbital model with nearest hopping. Scattering is treated in the NEGF formalism using Born approximation. The retarded Green’s function of the device is computed as

$$G(E) = [(E + i\delta I)I - H - \Sigma_1 - \Sigma_2 - \Sigma_3]^{-1},$$

where $\Sigma_1$ ($\Sigma_2$) is the self-energy of the source (drain) contact. $H$ is the channel Hamiltonian. $\Sigma_3$ is the self-energy of phonon scattering, which is computed from the in-scattering and out-scattering functions.

$$\Sigma_{in}^{\text{in}}(x, x'; E) = \sum_i D_{ii}(x, x'; \hbar \omega_i) [(N_{\text{in}} + 1) G^0(x, x'; E + \hbar \omega_i) + N_{\text{in}} G^0(x, x'; E - \hbar \omega_i)],$$

FIG. 1. (Color online) (a) The schematic plot of the modeled GNR-FET with 100 nm channel length and a bottom gate of 10 nm SiO$_2$. The thickness of the metal source/drain contact is 20 nm. The $n$=21 armchair edge-GNR channel has a width of 2.5 nm and a bandgap of $E_g$=0.49 eV. (b) The schematic sketch of edge scattering.
\[ \Sigma_{\text{out}}^{\text{el}}(x,x';E) = \sum_i D_0(x,x';\hbar \omega_i)[(N_{\omega_i} + 1)G^e(x,x';E - \hbar \omega_i) + N_{\omega_i}G^h(x,x';E + \hbar \omega_i)], \]

where \( \hbar \omega_i \) is the phonon energy and \( D_0 \) is the electron-phonon coupling strength of the \( i \)th phonon mode. \( G^e \) (\( G^h \)) is the electron (hole) correlation function, which is solved with \( \Sigma_{\text{el}} = \Sigma_{\text{el}}^{\text{out}} \) in a self-consistent Born loop to ensure current conservation. We assume that \( D_0 \) is nonzero only at \( x = x' \). Our phonon modes and electron-phonon coupling calculations for GNRs, following Refs. 11 and 12, respectively, indicate that the combined effect of acoustic phonon (AP) modes can be modeled as an elastic scattering mechanism, and the combined effect of the OP modes can be modeled as an inelastic scattering mechanism with an average energy of \( \hbar \omega_{\text{OP}} \approx 180 \text{ meV} \) for simplicity. The latter one is graphene-derivative and appears in CNT as well. Due to large OP energy, OP emission process is dominant at room temperature. The scattering mfps in a semiconducting GNR are energy dependent, and we cite the values at high carrier kinetic energy where the \( E-k \) is nearly linear. The mfp of AP scattering, predicted in the order of microns, is much longer than the channel length and has a small effect. The mfp of OP scattering takes the experimental fitting value, \( \lambda_{\text{OP}} \approx 15 \text{ nm} \), rather than the value inferred by electron-phonon coupling computation because the calculated \( \lambda_{\text{OP}} \) is several times larger than the experimental fitting value, similar to the case of CNTs. Although uncertainty of the OP scattering mfp exists, the qualitative conclusions are quite robust to variation of the OP scattering mfp by a factor of several. The phenomenological mfp determines \( D_0 \) in Eqs. (2) and (3). An elastic scattering mechanism with an experimentally characterized mfp was treated. To characterize the mfp, three GNR-FETs with channel lengths of \( L_{\text{ch}} = 110, 236, \) and 470 nm were fabricated on an individual GNR, and the measured channel resistances \( R_{\text{ch}} = \partial V_D/\partial \mu |_{V_D=0} \) were 165, 310, and 550 K\( \Omega \), respectively. At low source-drain bias (less than \( \hbar \omega_{\text{OP}} \)), OP scattering is negligible because OP emission is suppressed and elastic scattering dominates. The mfp of elastic scattering \( \lambda_{\text{el}} = 12 \text{ nm} \) is extracted from \( R_{\text{ch}} = R_t + R_d(L_{\text{ch}} + \lambda_{\text{el}})/\lambda_{\text{el}} \), where \( R_t \) is the series contact resistance and \( R_d = 13 \text{ K}\Omega \) is the quantum resistance. The short elastic scattering mfp was attributed to edge scattering, as schematically illustrated in Fig. 1(b). The edge scattering mfp increases as the quality of the GNR edges improves and the GNR width increases.

To explore the role of different scattering mechanisms, in Fig. 2 we simulated the \( I_D-V_D \) characteristics of the modeled GNR-FET in Fig. 1(a) (i) without scattering (ii) in the presence of only elastic scattering, and (iii) in the presence of both elastic and OP scattering. The following observations were made. First, under condition (ii) the current is significantly lowered, and the ballisticity slightly increases as \( |V_D| \) increases. Second, under condition (iii) the onset of an extra scattering process does not further increase the current. In contrast, OP scattering increases the on current (at \( V_D = -0.5 \text{ V} \) and \( |V_G-V_T| = 0.5 \text{ V} \) from 0.90 to 1.8 \text{ \mu A}. In addition, the \( I_D/V_D \) curve becomes more linear in the applied drain bias regime, and the ballisticity considerably increases as \( |V_D| \) increases.

In the presence of only elastic scattering, the short mfp due to edge scattering in a GNR-FET makes elastic scattering more important than in a quasiballistic CNTFET. In comparison, strong elastic scattering also exists in a nanoscale 2D Si metal-oxide-semiconductor (MOS)-FETs such as surface roughness scattering and ionized impurity scattering. However, a Si MOS-FET can deliver nearly 50\% of the ballistic on current even with a channel length of about 100 nm. Previous studies showed that if there were only elastic scatterings in a Si MOS-FET at high \( |V_D| \), only scattering in a so-called \( k_BT \) layer at the beginning of the channel has a direct effect on the current, and the rest of the channel essentially operates as a carrier absorber due to the following reason. In a 2D MOS-FET, the final states of elastic scattering distribute on a 2D \( k \)-space and a significant component of the carrier velocity is transferred from the transport direction to the transverse direction. At the drain end, most scattered carriers hence do not possess enough velocity along the transport direction to overcome the potential barrier at the source end. This argument does not hold for GNR-FETs. The effect of strong elastic scattering at high \( |V_D| \) is much more pronounced due to the quasi-1D channel geometry. As shown in Figs. 3(a) and 3(c), an elastic scattering event completely reverses the direction of the velocity and elastic scattering anywhere in the channel plays an important role. Edge scattering in a GNR-FET is analogous to surface roughness scattering in a Si MOS-FET in the sense that both of them are elastic scattering due to defects at the semiconducting channel surface or edge. With a similar mfp, edge scattering in a GNR-FET, however, has a larger direct effect on the on current than surface roughness scattering in a Si MOS-FET because the 1D channel leads the breakdown of \( k_BT \)-layer concept.

The increase in the on current after including OP scattering is explained next. Fig. 3(b) shows the local current spectrum in the presence of both OP and edge scattering at on state. As carriers travel through the channel, their energies are relaxed by emitting OPs, which is different from Fig. 3(a) in the presence of only elastic scattering. Due to large OP energy (~180 meV), a backscattered carrier after emitting an OP can hardly return to source. Any subsequent elastic scattering has a small direct effect on the current. Compared to that scattering in the entire 1D channel is important if only elastic scattering is present, now only the elastic scattering occurring at the beginning of the channel within a distance

![FIG. 2.](Color online) The \( I_D \) vs \( V_D \) characteristics at ballistic limit (solid line), with elastic scattering only (dashed line), and with both elastic scattering and OP scattering (dot-dash line). The elastic scattering mfp \( \lambda_{\text{el}} = 10 \text{ nm} \) and the OP scattering mfp \( \lambda_{\text{OP}} = 15 \text{ nm} \).
before carriers emit an OP plays a significant role. An additional scattering mechanism typically decreases the current by increasing the scattering rate. In contrast, coupling inelastic OP scattering to elastic scattering in GNR-FETs considerably increases the on current. We expect this effect is also valid in other 1D channel FETs if the effect of elastic scattering is considerable. The theory is in qualitative agreement with the experiments in terms of that the ballisticity increases as \( |V_D| \) increases and more linear \( I_D-V_D \) characteristics in the presence of both elastic and OP scatterings.

Finally, we examine the effect of improving the GNR edge quality, which is modeled by increasing the elastic scattering mfp. The mfp upper bound is set to 1 \( \mu \)m, which could be limited by AP scattering. As the elastic scattering mfp is varied from 10 nm to 1 \( \mu \)m, the ballisticity at \( V_D = -0.5 \) V increases from \( \sim 30\% \) to \( \sim 95\% \), as shown in Fig. 4, which indicates the imperative need for future experimental work to achieve longer elastic scattering mfp in GNRs. The ballisticity at high \( |V_D| \), where OP scattering is strong, is always larger than that at low \( |V_D| \), where OP scattering is negligible.

The model here is based on several assumptions. First, edge roughness not only results in edge scattering but also may modify the GNR electronic structure, which is not treated in this study. Second, only the results of one specific GNR width and SB height are presented here. Relaxing these assumptions adds perturbations to the simulation results but the qualitative conclusions of this study remain the same.

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\begin{figure}[h]
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\includegraphics[width=\textwidth]{fig3.png}
\caption{(Color online) The simulated local current spectrum as a function of channel position and energy in the presence of (a) only elastic scattering and (b) both elastic scattering and OP scattering at \( V_D = -0.5 \) V. The source Fermi level \( E_{FS} \) is chosen as zero. The conduction and valence subband edges are shown as \( E_C \) and \( E_V \), respectively. The schematic sketches (c) and (d) explain carrier (hole) scattering process in (a) and (b), respectively. \( \lambda_{el} = 10 \) nm and \( \lambda_{OP} = 15 \) nm.}
\end{figure}