Model of 1D Schottky Barrier Transistors Operating Far From Equilibrium

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***Abstract*— Nanotransistors typically operate in far-from-equilibrium (FFE) conditions, that cannot be described neither by drift-diffusion, nor by purely ballistic models. An analytical model capable to describe the operation of transistors in FFE conditions would then be required in order to swiftly assess their performance and limitations. In addition, in carbon-based nanotransistors, source and drain contacts are often characterized by the formation of Schottky Barriers (SBs), with strong influence on transport. Here we present a model for one-dimensional field-effect transistors (FETs), taking into account on equal footing both SB contacts and FFE transport regime. Our model represents a significant advancement with respect to the currently available ideal or semi-ideal transport models. We show that the interplay of SB and ambipolar FFE transport gives rise to a number of features in device characteristics, often detected in experiments.**

***Index Terms*— GNR, ballistic transport, compact model, drift-diffusion transport, Schottky barrier**

I. Introduction

Carbon nanotubes (CNTs), and single-layer or bi-layer graphene nanoribbons (GNRs), have lately attracted much interest for their possible application in nanoelectronic devices. In particular semiconducting carbon nanotubes (CNTs) [1], [2] and single-layer or bi-layer graphene nanoribbons (GNRs) [3], [4] have been successfully employed in quasi-1D nanotransistors. An important issue related to carbon-based channels is the nature of the metallic contact at source and drain, which can lead to different pinning of the Fermi level and consequently to the formation of ohmic or Schottky contacts [5].

Transport in nanotransistors is certainly far from of equilibrium, but is still not fully ballistic. As far as analytical models are concerned, transport in quasi-1D FETs is generally treated as purely ballistic or with a drift-diffusion assumption as in Refs. [6], [7], [8]. A largely invoked approach to treat partially ballistic transport including the effects of backscattering was proposed by Lundstrom *et al.* [9]. This approach, that is easily included as a correction to ballistic models, has the merit of offering a very simple and synthetic picture, but does not allow to describe the seamless transition from ballistic to quasi-equilibrium drift-diffusion transport conditions. Recently a rigorous semi-analytical model based on the Büttiker virtual probes approach [10], in which a non-ballistic transistor is seen as a suitable series of N ballistic channels, has been presented [11], [12], [13]. N is the ratio of the channel length to the mean free path.

In nanowire transistors, fully microscopic analysis of inelastic scattering due to phonon scattering, has also been addressed by adding a proper self energy correction on a site-representation propagating Hamiltonian by Jin *et al.* [14] and by M. Gilbert *et al.* [15], [16]. Preliminary studies of dissipative transport have been performed in CNT FET [17], and in GNR [18]. However numerical simulations with the inclusion of inelastic scattering remain complex and computationally expensive.

II. Model

In this work we propose a model based on the virtual probes approach capable to describe one-dimensional FETs, in which Schottky barriers are present at the contacts and transport occurs in FFE conditions. The charge injected in the channel and the current for a single

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ballistic transistor are calculated with the Landauer-Büttiker formalism, taking into account, when needed, the finite tunneling barriers with the assumption of loss of phase coherence in the channel [19] (see Fig 1). The potential at the center of a ballistic channel is self-consistently imposed by the vertical electrostatics, while at source and drain it is fixed by the SB heights. A transistor with SB contacts in the FFE transport regime is modeled as a series of N individually ballistic channels, spaced by a length corresponding to the mean free path, and connected by fully thermalizing virtual probes, with electrochemical potential μ_n ($n = 0, \ldots, N$). Head and tail of the series are connected to source and drain through SB contacts as sketched in Fig. 1(b), so that $\mu_0 = \mu_s$ and $\mu_N = \mu_d$. The self-consistent vertical electrostatics of the n-th channel, for which the $(n-1)$-*th* and the n-*th* contacts act respectively as source and drain, is described by the equation for the electrostatic charge induced by the gate-channel coupling

$$Q_n = -C_g \left(V_g - \phi_n\right). \tag{1}$$

The equation for the steady state mobile charge injected from the contacts in the α subband is

$$Q_n^{(\alpha)} = q \int \quad dE \quad D_\alpha(E) \left[\frac{T_S(2-T_D)}{T^*} f(x_{n-1}) + \right.$$
$$\left. + \quad \frac{T_D(2-T_S)}{T^*} f(x_n)\right] \tag{2}$$

with

$$x_n = \frac{E-\mu_n}{k_B T},$$

with T_S and T_D being the tunneling probabilities from source and drain to the channel, respectively, and $T^* \equiv T_S + T_D - T_s T_D$ and

$$D_\alpha(E) = \frac{2}{\pi\hbar}\sqrt{\frac{m_\alpha}{2(E-E_\alpha)}} \tag{3}$$

is the density of states of the channel in effective mass approximation. The two equations are simultaneously solved for the charge Q_n and the channel potential ϕ_n. All equation are summarized for brevity only for electrons, but the full model is ambipolar. The current in the n-th transistor in the α subband is instead calculated as

$$I_n^{(\alpha)} = \frac{q}{\pi\hbar}\int dE \frac{T_S T_D}{T^*}\left[f(x_{n-1}) - f(x_n)\right] \tag{4}$$

Exploiting current conservation we obtain a set of N equations, which have to be simultaneously solved in order to determine the $N-1$ unknown electrochemical potentials μ_n on each probe plus the drain-to-source current.

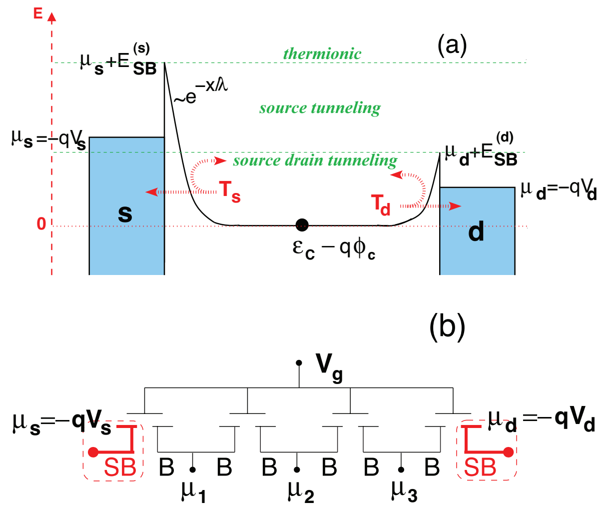

Fig. 1. (a)Conduction band edge profile of a SB nanoscale FET. The thermionic and tunneling energy ranges are shown. (b) Chain of N ballistic transistors with SB contacts at source and drain (first and last contact). ϕ_n is the self-consistent potential in the n-th channel.

The SBs have an exponential profile $V(x) \approx e^{-\frac{x}{\lambda}}$ (Fig.1(a)), with $\lambda = \sqrt{\epsilon \mathcal{A}/C^*}$. C^* and $\mathcal{A}$ are an effective capacitance and device cross section calculated through a model based on a fictitious separation of longitudinal and vertical electrical fluxes. In this model the longitudinal electrical flux is thought to be concentrated in an internal region of the device, in which we can neglect the variation of the potential in the vertical direction. The main potential variation along the vertical direction happens instead in the outer region, near the gate electrodes. The exploitation of the Gauss law directly leads to the aforementioned result. This approach finds a reasonable good agreement with both evanescent mode analysis [20] and numerical calculations [21]. Details of this model will be given elsewhere.

The tunneling coefficients $T_S(E)$ and $T_D(E)$ of the exponential SB are analytically calculated via WKB approximation. The integration of the imaginary part of the particle wavevector under the barrier, limited by its classical turning points, leads to the tunneling coefficient

$$T_i(\chi) = e^{-4\lambda\sqrt{\frac{2m}{\hbar^2}}\left[\sqrt{1-\chi} - \sqrt{\chi}\arctan\left(\sqrt{\frac{1-\chi}{\chi}}\right)\right]} \tag{5}$$

with $i = S, D$, and $\chi = \frac{\tilde{E}}{E_{SB}}$, where E_{SB} is the SB height and $\tilde{E}$ is the energy with respect to the i-th subband energy in the channel far away from source and drain contacts.

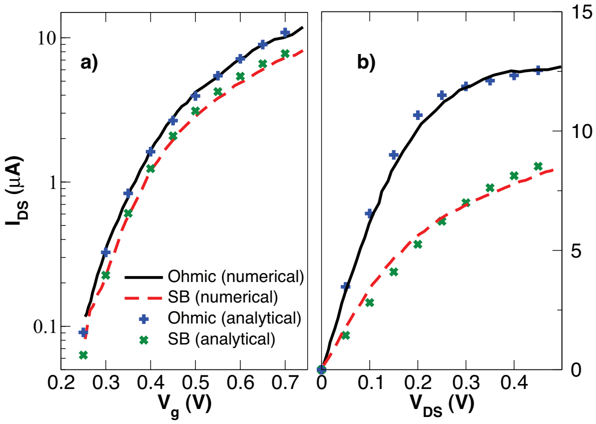

Fig. 2. Comparison between our model and numerical simulations from ref.[22]. The transfer characteristics (a) at $V_{ds} = 0.5$ V and characteristics (b) at $V_g = 0.75$ V of a ballistic double-gate armchair GNR FET, with Ohmic and SB contacts of height $E_g/2 \approx 0.3$ eV are shown. The SiO_2 gate oxide thickness is 1.5 nm and the GNR lattice has 12 dimer lines, which correspond to a width of 1.35 nm and a band gap of $E_g = 0.6$ eV. Assuming a GNR thickness of about 1 nm we obtain $\lambda \approx 1.3$ nm.

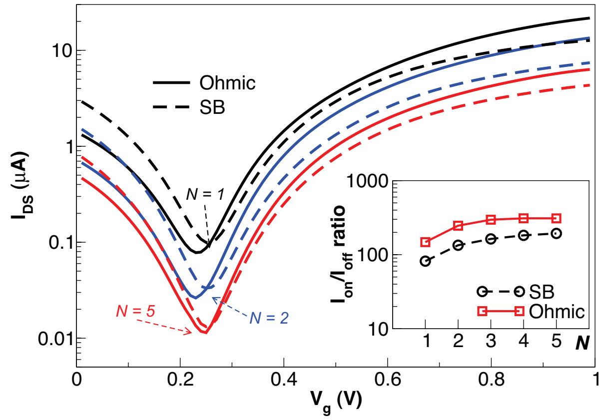

Fig. 3. Transfer characteristics of a ballistic chain of N double gate GNR FETs, with $N = 1, 2, 5$ and $V_{ds} = 0.5$ V, calculated with our model. In the inset the I_{on}/I_{off} ratio for $V_g^{(\mathrm{off})} = 0.25$ V, $V_g^{(\mathrm{on})} = 0.75$ V, and $V_{DS} = 0.5$ V, is plotted as a function of N.

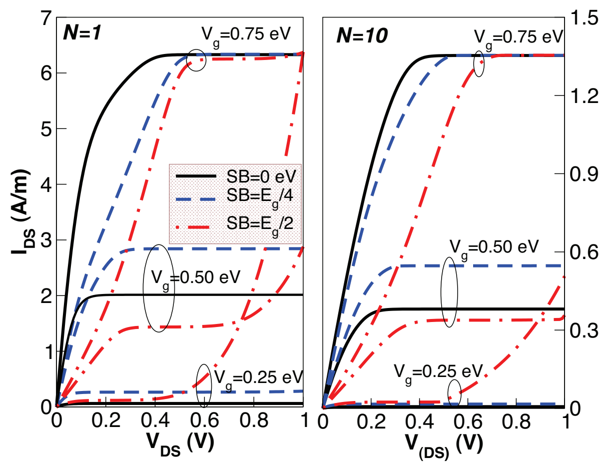

Fig. 4. Output characteristics of a ballistic chain made of a series of N double gate GNR FETs, with $N = 1$ and $N = 10$, with ohmic contacts (SB=0), with a Schottky barriers of height $E_g/2$ and $E_g/4$. The details of the device are the same as Fig.2, except $t_{ox} = 20$ nm.

III. Results and Discussion

In Fig.2 we compare the transfer characteristics (a) and the output characteristics (b) of a purely ballistic ($N = 1$) armchair GNR FET, as obtained with our model and with a numerical simulation based on the non-equilibrium Green's function formalism in [22]. We obtained the gate capacitance by fitting the characteristics of the transistor with ideal ohmic contacts, then included the SB contacts. The agreement between the numerical simulations and our compact model, for both curves (Fig. 2) with ohmic and SB contacts, demonstrating that the effects of SBs are well accounted for.

To analyze the effects of non-ballistic transport, we look for the case with for $N > 1$. For increasing N, we note that the transfer characteristics (Fig. 3) vertically shift in a semi-log plot, more significantly in the subthreshold region. Consequently, an increase of the I_{on}/I_{off} ratio as a function of N is observed as shown in the inset. This effect is related to the fact that in ballistic models, in subthreshold conditions, tunneling from the drain leads to hole accumulation under the channel, and consequently to large quantum capacitance and degradation of the subthreshold slope. This feature is partially resolved by the inclusion of a degree of inelastic relaxation in the non-ballistic cases, giving rise to larger I_{on}/I_{off} ratio.

With a thicker oxide ($t_{ox} = 20$ nm), corresponding to thicker tunneling barriers ($\lambda \approx 13$ nm), the output characteristics (Fig.4(a) and (b)) exhibit an "S" shape, typical for SB FETs [23]. For $N = 10$ all this features are less pronounced, but still the typical "S" shape associated with Schottky barrier contacts are easily recognized.

IV. Conclusion

In this work we presented a semi-analytical model able to tackle on equal footing the presence of tunneling contacts and far-from equilibrium transport for GNR transistors. The model provides significant improvements to typical compact models, which are restricted to a fully ballistic or to a drift-diffusion situation, by being able to smoothly reproduce the transition between the two limiting regimes. Results from our model are in good agreement with numerical simulations. We also show that accounting for partial thermalization of carriers in the channel, even with an energy relaxation time much larger than the average traversal times, our model predicts an increase of the I_{ON}/I_{OFF} ratio with respect to ideal ballistic compact models, which suffer from fictitious hole accumulation in the channel.

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