Monte Carlo study of ambipolar transport and quantum effects in carbon nanotube transistors

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***Abstract*—In this paper, we investigate the device operation of CNFETs using Monte Carlo simulation. Two types of contacts (ohmic and Schottky) are considered and the effect of ambipolar transport with Schottky barriers is analysed. We also discuss the actual influence of quantum effects on the basis of Wigner simulation results. The output and high-frequency characteristics of different structures are presented and discussed.**

Keywords-Monte Carlo simulation, carbon nanotube transistor, ambipolar, quantum effect.

I. INTRODUCTION

Exceptional transport properties of carbon nanotubes (CNTs), including very high carrier mobility [1] and mean free path [2], make these nanostructures very attractive for designing field-effect transistors (CNTFETs) likely to overcome the limits of Si transistors. Source and drain contacts in CNTFETs may be either Schottky- or ohmic-like, which may strongly influence their operation and performance. In particular, the ambipolar behaviour of Schottky transistors may lead to unacceptable leakage currents [3]. Furthermore, the possibly high ballisticity of such transistors can make the transport essentially coherent and one may wonder whether quantum transport effects have a strong impact or not on the device performance.

In this paper these questions are addressed by means of particle Monte Carlo (MC) simulation. Both semi-classical (Boltzmann) and quantum (Wigner) MC algorithms including phonon scattering are used. They are self-consistently coupled to 2D cylindrical Poisson's equation to simulate gate-all-around CNTFETs which have been shown to be optimal in ultimately scaled devices [4].

II. MODEL AND SIMULATED DEVICE

We have developed a model within the software MONACO to simulate the semi-classical transport in carbon nanotubes [2,5,6]. An analytical dispersion relation is used to describe the first three nanotube subbbands and electron-phonon scattering is included through acoustic, optical, and radial breathing phonon modes [2,5,7].

The two types of source-drain contacts are considered. Thermal equilibrium and local charge neutrality are used as boundary conditions at ohmic contacts. For Schottky-type source-drain contacts, the tunnelling transmission coefficient across the barrier at the metal-CNT interface is calculated according to the WKB approximation. The number of particles injected from metal at contacts is calculated by the Landauer formula [8]. The model of Schottky contact was initially developed for unipolar structures [9]. It is extended here to study ambipolar transport in CNTFETs.

For quantum transport simulation the Wigner MC algorithm initially developed for RTDs and MOSFETs [10] has been implemented for CNTFETs [11]. The 1D motion equation of the Wigner function f_w (Wigner Transport Equation, WTE) reads

$$\frac{\partial f_w}{\partial t} + \frac{\hbar k}{m^*}\frac{\partial f_w}{\partial x} = Q\,f_w + C\,f_w \qquad (1)$$

where Qf_W is the quantum evolution term resulting from the non-local effect of the potential $U(x)$, defined as

$$Q\,f_w(x,k) = \frac{1}{2\pi\hbar}\int dk'\,V_w(x,k')\,f_w(x,k+k') \qquad (2)$$

where the Wigner potential V_W is given by

$$V_w(x,k) = \int dx'\,\sin(kx')\left[U\left(x+\frac{x'}{2}\right)-U\left(x-\frac{x'}{2}\right)\right] \qquad (3)$$

The term Cf_W in (1), which encodes the effect of electron-phonon scattering on the Wigner function, is based on the same collision operator C as in the Boltzmann equation. In our model, the information on the quantum state of electrons is contained in a quantity called affinity assigned to each pseudo-particle, which evolves continuously according to the Wigner potential [10]. For a real semi-classical particle (Boltzmann) this affinity is just constant and equal to unity.

A semiconducting zigzag CNT (19, 0) is considered here with a band gap of 0.55 eV. The equivalent gate oxide thickness (EOT) is 5.3 nm. The gate length is either 100 nm or 25 nm. In ohmic transistors, source and drain access zones are 20 nm long and N-doped to 0.34 nm^{-1}. There is no access zone in Schottky-barrier (SB) transistors (see Fig. 1).

III. RESULTS AND DISCUSSION

For a gate length of 100 nm, Fig. 2 compares the transfer characteristics of a Schottky-barrier (SB) CNFET with that of an ohmic contact device (Boltzmann simulation). The SB height is mid-gap, i.e. $\Phi_B = 0.275$ eV, which leads to symmetric conditions of electron and hole injection. At high

V_{GS}, the current is mostly due to electrons going from source to drain. In contrast, at low gate voltage, holes injected at the drain barrier contribute mainly to the total current. The ambipolar transport makes SB-CNFET characteristics unconventional [12]. In particular, it degrades the subthreshold characteristics. For $V_{DS} = 0.3$ V the subthreshold slope is about 95 mV/dec instead of 70 mV/dec in the ohmic contact device. The Schottky contacts are also detrimental to the on-state current. The transconductance is limited to 20.5 µS in the SB device instead of 32 µS in the ohmic one.

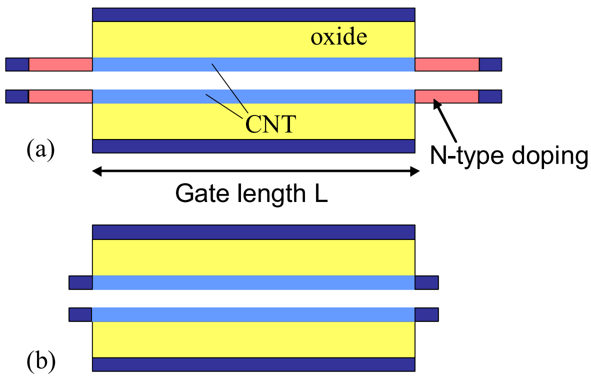

Figure 1. Schematic cross-section of simulated devices with (a) ohmic and (b) Schottky source and drain contacts.

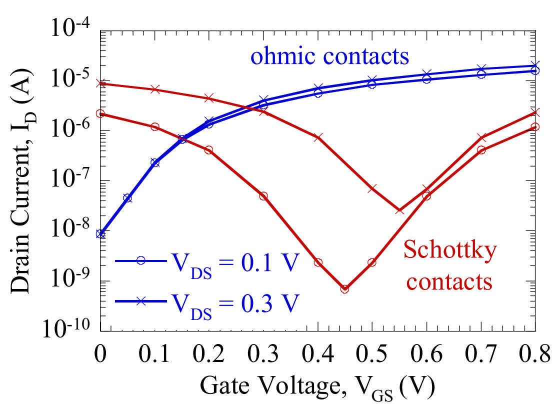

Figure 2. I_D-V_{GS} characteristics of ohmic and Schottky CNFETs for a channel length of 100 nm and an EOT of 5.3 nm. The S-D Schottky barrier height is $\Phi_B = 0.275$ eV.

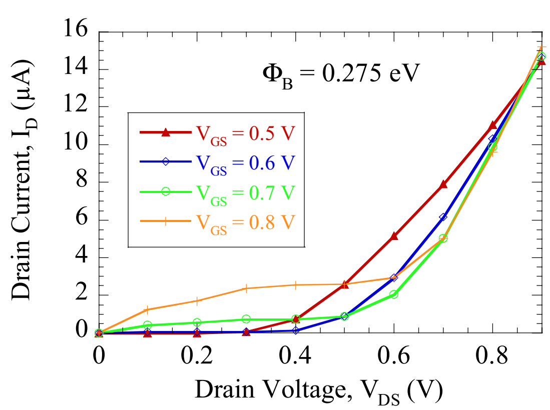

Figure 3. I_D-V_{DS} characteristics of SB-FET for different values of V_{GS} (L = 100 nm, EOT = 5.3 nm)

We observe in Fig. 3 that the I_{DS}-V_{DS} characteristics of the ambipolar transistor do not have the standard form. Due to the contribution of hole current injected at the drain contact, the current increases at high V_{DS} which degrades the current saturation or even makes it impossible. This behaviour has been observed experimentally in [3].

Fig. 4 shows the conduction band and electron velocity profiles in both devices at $V_{DS} = 0.1$ V for the same value $I_D \approx 1$ µA, i.e. for $V_{GS} = 0.8$ V and $V_{GS} = 0.1$ V in SB and ohmic devices, respectively. It should be noted that the electric field and maximum velocity reached in the channel are significantly higher in the latter device.

Actually, the height and form of Schottky barrier at contacts can be modified by interaction of metal or CNT with molecules of the environment or by the interface geometry [12]. To study the influence of the barrier height, we now consider two other barrier heights $\Phi_B = 0.1$ eV and 0 eV for electrons, which means it is $E_G - \Phi_B = 0.45$ eV and 0.55 eV for holes, respectively. In Fig. 5 two I_D-V_{GS} curves (at $V_{DS} = 0.1$ V) are compared to the previous case of mid-gap Schottky barrier. The electron injection at the source contact is enhanced to the detriment of hole injection at the drain, which typically increases the transconductance. These results are consistent with experimental ones [12]. The ambipolar transport can thus be reduced by adjusting parameters like the Schottky barrier height.

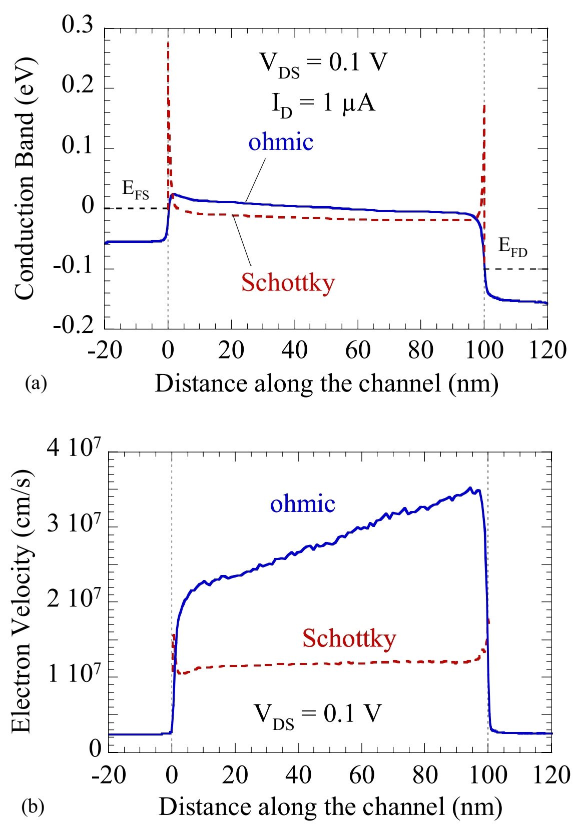

Figure 4. Conduction band and velocity profiles for SB and ohmic CNTFET at $V_{DS} = 0.1$ V and $I_D = 1$ µA

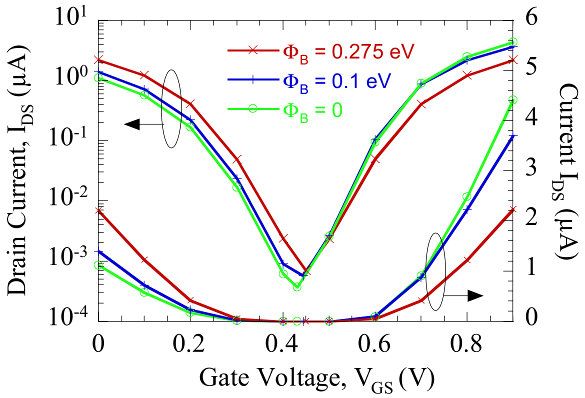

Figure 5. I_D-V_{GS} characteristics for two values of Schottky barrier height at source and drain contacts.

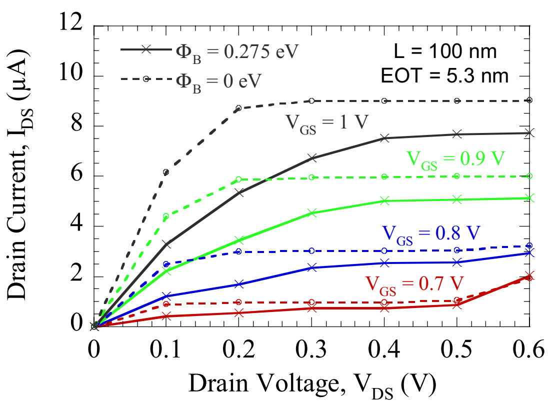

Figure 6. I_D-V_{DS} characteristics for different values of V_{GS} and two values of Schottky barrier height. L = 100 nm and EOT = 5.3 nm.

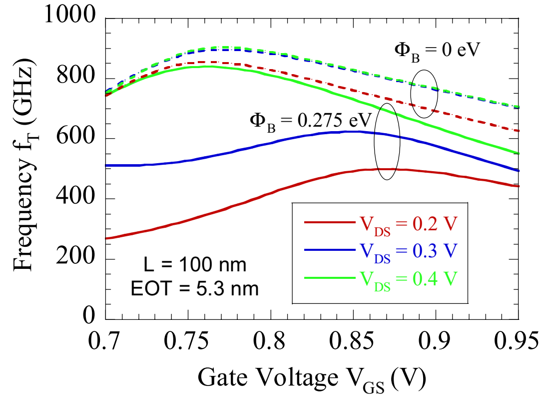

Figure 7. The frequency f_T as the function of the gate voltage V_{GS} for different drain voltages V_{DS}, considered for two values of Schottky barrier height Φ_B . The gate length is 100 nm.

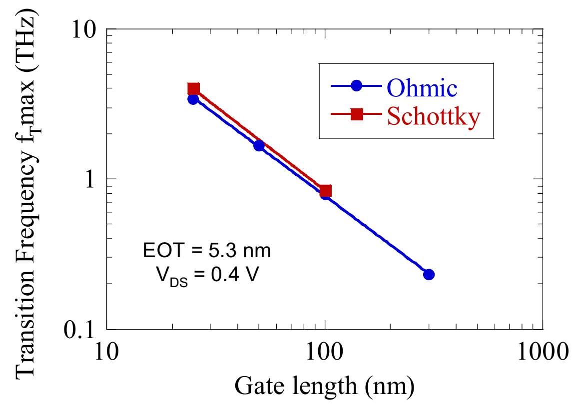

Figure 8. Maximum frequency f_T for ohmic contact and Schottky contact devices, with Φ_B = 0.275 eV for the Schottky contacts.

As shown in Fig. 6, the saturation behaviour of the drain current is significantly improved by reducing the SB height. Indeed, to get a clear drain current saturation, the drain voltage must be high enough to fully suppress the SB at the drain contact. For low Φ_B values the current saturation may thus occur for relatively small values of V_{DS}. For high SB an ohmic behaviour is observed over a large range of drain bias and the saturation is shifted to higher V_{DS} values, to such a point that, according to V_{GS}, an additional hole current strongly dependent on V_{DS} is likely to be injected at the drain contact. The current saturation is thus poor in transistors which exhibit a strong ambipolar behaviour.

To investigate the frequency performance of transistors we consider the transition frequency defined as $f_T = g_m / (2\pi\ C_{GS})$ where g_m and C_{GS} are the transconductance and the total gate capacitance, respectively. This figure of merit is plotted as a function of gate voltage in Fig. 7 for the same SB height as in Fig. 6. f_T is shown to depend strongly on the drain voltage in the case of high SB. It is a consequence of the poor saturation of the I_{DS}-V_{DS} characteristics and it makes the transistor difficult to use in analog applications. If the Schottky barrier height is reduced, the transition frequency becomes higher and much less dependent on the drain voltage in the range of current saturation, as in the case of ohmic contacts (not shown).

In Fig. 8 we compare the maximum transition frequency as a function of gate length for ohmic and Schottky contact devices at $V_{DS} = 0.4$ V, i.e. when the current saturation is nearly reached in both cases. In spite of drawbacks related to the ambipolar behaviour, SB-FET may provide performance similar to that of ohmic contact devices. It makes thus possible to envision the design of new multi-function logic circuits taking advantage of the ambipolar transport [13].

Now we consider quantum effects in ohmic contact CNFET with the gate length of 25 nm by using the Wigner's function formalism of quantum transport. The cartography of the Wigner function is compared to that of the Boltzmann function in Fig. 9. In the semi-classical case, the carriers are abruptly accelerated by the electric field at the drain-end of the channel. In contrast, in the quantum case, the acceleration seems much slower as if the carriers feel the potential fall in advance, which is consistent with the idea of delocalized electrons with finite extension of their wave function. Moreover, the positive-negative oscillations of the Wigner function at the drain-end of the gate are the signature of a strongly coherent transport with typical quantum effect as tunnelling and reflexion.

In spite of these strong differences observed at microscopic level, it is noticeable that the two types of simulation give quite close terminal currents (Fig. 10). In the case of quantum simulation, the electron reflexion related to the abrupt fall of potential at the drain-end of the channel is responsible for the slightly smaller total drain current than that obtained using Boltzmann simulation. In spite of the strongly coherent transport regime observed in this type of transistor [11], the semi-classical approach of transport is thus shown to be acceptable much beyond its theoretical domain of validity.

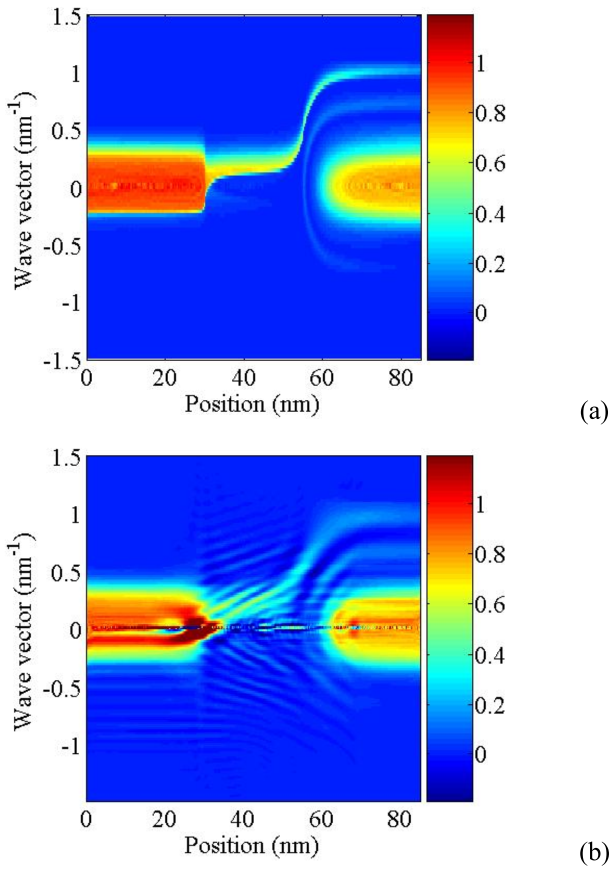

Figure 9. Cartography of Boltzmann (a) and Wigner functions (b) from semi-classical and Wigner MC simulation, for V_{GS} = 0.2 V, V_{DS} = 0.4 V. The access zones are here 30 nm long. The gate is located from x=30 to 55nm. The equivalent oxide thickness is here EOT = 0.4 nm.

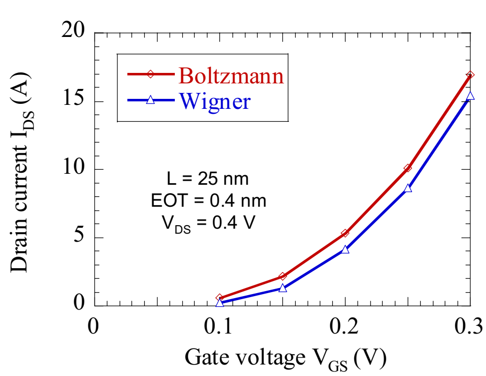

Figure 10. I_{DS}-V_{GS} Characteristics for the gate length of 25 nm, in the Boltzmann and Wigner formalisms.

IV. CONCLUSION

Boltzmann and Wigner MC simulations are proved to be efficient approaches to analyzing operation and performance of ohmic and Schottky contact CNTFET, including ambipolar transport and quantum effects. It is shown in particular that when band-to-band tunnelling can be neglected quantum transport effects have a strong influence at the microscopic level but do not change a lot the current voltage characteristics. The high-frequency performance of the CNTFET is less dependent on the drain voltage when the Schottky barrier height, i.e. the ambipolar behaviour is reduced.

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