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Self-consistent simulation of multi-walled CNT nanotransistors

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We present detailed results of the self-consistent analysis of carbon nanotube (CNT) field-effect transistors (FET), previously extended by us to the case of multi-walled/multi-band coherent carrier transport. The contribution to charge transport, due to different walls and sub-bands of a multi-walled CNT, is shown to be generally non-negligible. In order to prove the effectiveness of our simulation tool, we provide interesting examples about current–voltage characteristics of four-walled semiconducting nanotubes, including details of numerical convergence and contribution of sub-bands to the calculation.

Keywords: New and emerging technologies and materials, Modeling, Simulation and characterizations of devices and circuits

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I. INTRODUCTION

The extremely high carrier mobility, thermal conductivity, and ballisticity of charge transport make carbon nanotube (CNT) an excellent candidate for achieving the next generation of high-speed and high-performance RF electronics at the nanoscale, including field-effect transistors (FET), oscillators, frequency multipliers, sensors, and wireless devices.

The analysis of multichannel transport in CNT is usually carried out by "discrete" models, such as TB, and "continuous" models, such as effective mass and *kp* approximations, which stem from the approximation of TB around particular points of the dispersion curves. The reasons for the success of these models reside in that they make use of fairly good and verified assumptions, two in particular: transport is ballistic due to low dimensionality and high purity of carbon lattice and the energy interaction between electrons is weak because of the relatively long distances involved in charge displacement and is typically smaller than energy broadening due to temperature and contacts.

In this work, we exploit a multimode model of quantum transport that allows easy simulation of multi-walled CNT-FET, despite the possibly large number of walls. A general model is currently proposed in the literature in order to analyze the properties of carrier transport [1] of this kind of device [2–12].

This work summarizes and collects some of our recent achievements in the simulation and modeling of CNT devices. A self-consistent multi-mode approach to charge transport has been developed. Here we report some simulation results, considering the contribution of different walls to the total current driven by a four-walled CNT under externally applied voltage. Each wall includes, eventually, many electronic bands. The numerical convergence of the applied iterative scheme has also been explicitly shown.

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In a typical CNT-FET configuration, source and drain contacts are placed at the CNT terminations; we assumed that a cylindrical gate electrode completely surrounds the CNT. An insulator, of high relative permittivity ($\varepsilon = 25$), fills the space between the nanotube and the gate electrode. Perfect vacuum has been assumed within the CNT. The simulated structure is shown in Fig. 1.

We start by recalling the basic points of the approach already used in analyzing the behavior of a single-walled CNT in the configuration of Fig. 1 [6]. We will report the main results thus obtained, and compare these results with those obtained by extending the model to multi-walled and multi-band CNTs. A self-consistent solution of the system of Poisson and Schrödinger equations directly provides both the linear charge along the nanotube and the electrostatic potential along the CNT:

$$\left\{ \frac{d^2 V}{d\rho^2} + \frac{1}{\rho}\frac{dV}{d\rho} + \frac{dV}{dz^2} = -\frac{Q}{\varepsilon}, \right. \quad (1)$$

$$\left\{ \frac{d^2 \Psi_{h,e}}{dz^2} = -\frac{2m}{\hbar^2}(E - U_{h,e})\Psi_{h,e}. \right. \quad (2)$$

Following the notation of [2], V is the electrostatic potential within the outer cylinder, Ψ_h (Ψ_e) is the z-dependent wave function of a hole (electron) of energy E, traveling under the effect of a local potential energy U_h (U_e), and Q is the nanotube linear charge density, which is given by the difference between electron and hole charges, diffused from drain and source. We refer to the gate, source, and drain voltages as V_g, V_s, and V_d, respectively.

A self-consistent solution of equations (1) and (2) is achieved when

$$V(Q) = V, \quad Q(V) = Q. \quad (3)$$

Here the symbol " = " indicates the convergence of an iterative scheme, which is reached when the charge and potential differ from their values calculated at the previous step by less than a very small percentage. The Landauer–Büttiker

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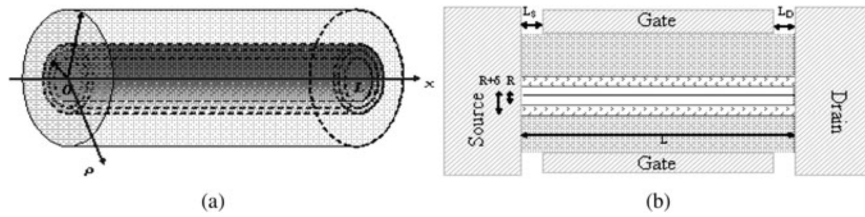

Fig. 1. (a) Geometry of a multi-walled CNT-FET. (b) Section of a double-walled CNT. L is the nanotube length, R and $R + \delta$ are the radii of the smaller and larger wall, respectively; we assume L_S and $L_D \to 0$.

formula [1] is used to calculate the total current flowing through the CNT:

$$I_{h,e} = -\frac{4e}{h} \int (f^s_{h,e} - f^d_{h,e})\, T_{h,e}\, dE. \qquad (4)$$

In (4), e is the electron (hole) unit charge for I_e (I_h), h is Plank's constant, T_e (T_h) is the transmission probability through the channel for the electrons (holes), and $f^{s,d}$ is the Fermi function at the source and drain.

Such a simplified model highlights the main characteristics of the transistor operation and provides the parameters of interest such as, for example, current–voltage curves, linear charge density, and transconductance [6]. In [2], the attention is focused, mainly, on the transmittance properties of the carriers through the channel: it is noted that the transmission probability of electrons and holes is a very highly peaked function. This is basically due to the abrupt discontinuities seen by the carriers along their path in the metal–CNT–metal structure. In other words, the resonance peaks are made so sharp by the band-offset of CNT and metal, as well as by the spatial modulation of the potential energy induced by the applied electrostatic voltage. For example, if the external potential is just enough to allow the electron wave function to propagate in the channel, the CNT becomes a resonant cavity very slightly coupled to the external electrodes.

In [13], the Poisson–Schrödinger model was improved in order to take an account of a more realistic geometry of the metal electrodes. Moreover, an analysis of the dependence of the device properties to variations of the geometric parameters was performed [3]. The model also lends itself to the analysis of the dynamic behavior of a CNT-FET: in [14] the unity-current-gain frequency f_T was estimated by means of an equivalent circuit, whose lumped elements are computed in the electrostatic limit.

This contribution is intended to provide further improvements to the models described above. In particular, the following items have been introduced. (i) The investigation of the effects of nanotube sub-bands, which are usually neglected, on the transistor device operation. (ii) The extension of the analysis to the case of multi-walled CNTs.

The improvement (i) is necessary as one may deal, in practice, with nanotubes of "large" diameters and/or with high applied voltages. In the former case, the dispersion curves may have many branches, i.e. sub-bands, very close to the fundamental one, so that their contribution to the total charge and current has to be included. Similarly, in the latter case, the high applied voltage may shift the local band structure to such an extent that some sub-bands carry a non-negligible contribution to charge transport. The improvement (ii) provides an important generalization to the analysis of nano-FET devices, as multi-walled CNTs may be easier to obtain and manipulate than single-walled CNTs.

II. MULTIPLE BAND TRANSPORT

In a multiple channel (band) simulation, equation (2) becomes

$$\frac{d^2\Psi^{n,m}_{h,e}}{dz^2} = -\frac{2m^{n,m}_{h,e}}{\hbar^2}(E - U^{n,m}_{h,e}(z))\Psi^{n,m}_{h,e}, \qquad (5)$$

where m indicates the mth wall and n indicates the nth sub-band. We still keep distinct all quantities related to electrons and holes. The potential energy appearing in (5) is defined as

$$\begin{cases} U^{n,m}_e(z) = \tilde{U}^{n,m}_e(z) - eV(R+\delta_m, z), \\ U^{n,m}_h(z) = \tilde{U}^{n,m}_h(z) + eV(R+\delta_m, z), \end{cases}$$
$$\begin{cases} \tilde{U}^{n,m}_e(z) = E_{vac} - e\chi^{n,m}_T, \\ \tilde{U}^{n,m}_h(z) = \tilde{U}^{n,m}_e(z) - E^{n,m}_g, \end{cases} \qquad (6)$$

where R is the radius of the smallest of the CNT walls, E_{vac} is the vacuum energy, $\chi^{n,m}_T$ is the electron affinity for the carriers of the (n,m)-channel, $E^{n,m}_g$ is the nth energy gap of the mth wall, and V is the electrostatic potential satisfying the Poisson equation, evaluated in correspondence of the radius

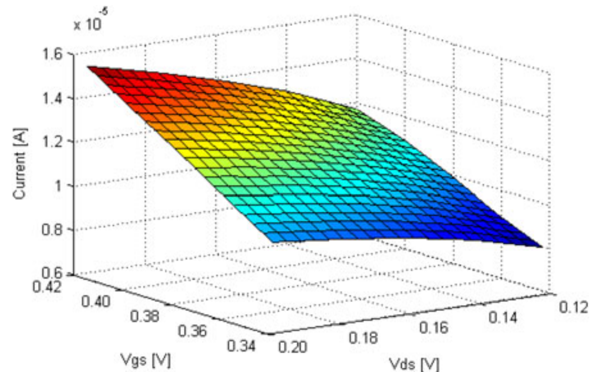

Fig. 2. Current of a four-walled CNT, 20 nm long, after numerical convergence of the iterative Schrodinger–Poisson scheme. The four CNT have the following chiralities: (10,0), (19,0), (28,0), and (37,0).

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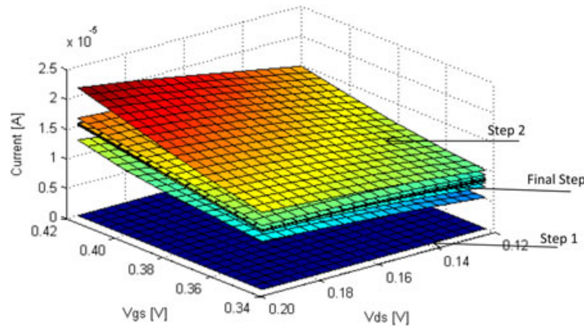

Fig. 3. Current of the four-walled CNT of Fig. 2: convergence is reached after a few iteration steps.

$(R+\delta_m)$ of the mth wall. The boundary conditions for V are given by

$$\begin{cases} V(R_G, z) = V_g - \Phi_g, \\ V(R+\delta_m, 0) = V_s - \Phi_s, \\ V(R+\delta_m, L) = V_d - \Phi_d, \end{cases} \quad (7)$$

where R_G is the radius of the gate electrode and Φ_g, Φ_d, Φ_s are the work functions of gate, drain, and source, respectively. The effective mass $m_e^{n,m}$ ($m_h^{n,m}$) is derived from the parabolic approximation of the nth branch above (below) the band gap of the dispersion curves of the mth wall.

The contributions of the (n,m)-channel to the linear charge and to the current are computed by solving separately the respective Schrödinger equations. However, even though the wave functions of different channels are not spatially coupled, they are coupled through the Poisson equation (1), because they all contribute to the source charge:

$$q_e^{n,m} = \int |\Psi_e^{n,m,D}(z)|^2 + |\Psi_e^{n,m,S}(z)|^2 dE,$$

$$q_h^{n,m} = \int |\Psi_h^{n,m,D}(z)|^2 + |\Psi_h^{n,m,S}(z)|^2 dE,$$

$$q^{n,m} = q_e^{n,m} - q_h^{n,m},\ Q = \frac{e}{2\pi}\frac{\delta(\rho - R - \delta_m)}{\rho}\sum_{n,m} q^{n,m}. \quad (8)$$

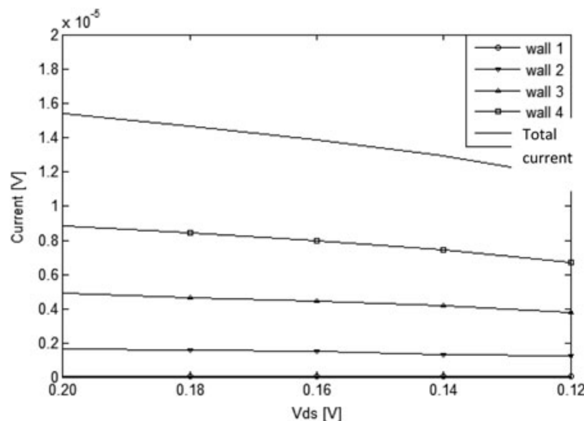

Fig. 4. Current of any of the four walls of the four-walled CNT of Fig. 2 after numerical convergence, as a function of V_d, with $V_g = 0.4$ V. The total current is also shown (no marker).

As for the charge, the total current is provided by the sum of the contributions of each wall with its own sub-bands

$$I = \sum_{n,m} (I_h^{n,m} + I_e^{n,m}). \quad (9)$$

In (9), $I_{h,e}^{n,m}$ is the current of the (n,m)-channel:

$$I_{h,e}^{n,m} = \frac{4e}{h}\int (f_{h,e}^S - f_{h,e}^D)\, T_{h,e}^{n,m}\, dE, \quad (10)$$

where $T_h^{n,m}$ ($T_e^{n,m}$) is the transmission probability through the (n,m)-channel for holes (electrons).

III. EXAMPLES

Figure 2 shows the total current, computed self-consistently with the electrostatic potential, for a four-walled CNT, 20 nm long. The current, obtained by an iterative computational scheme, as described above, is plotted as a function of drain and source voltages.

In Fig. 3, we show the numerical intermediate steps of this iterative scheme, which produce the current of Fig. 2 as final computational result.

In Fig. 4, we report, for completeness, the contributions of the walls of the considered four-walled CNT to the total current, as a function of the drain voltage for a fixed drain voltage, after numerical convergence.

IV. CONCLUSION

In this contribution, we report on numerical simulation of CNT-based transistors. In particular, we characterize the use of multi-walled CNT as channels for charge transport and evaluate the contribution to the electric current of individual walls, with emphasis on the numerical features of the implemented algorithm.

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