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Abstract:

A three-dimensional simulation approach for the investigation of Carbon NanoTube Field Effect Transistors (CNTFETs) is presented, based on the self-consistent solution of the 3D Poisson-Schrödinger equation with open boundary conditions, within the Non-Equilibrium Green's Function formalism. This approach enables accurate simulations of transport through ballistic CNTFETs for generic device structures, eliminating the use of ideal geometries, such as coaxial devices, often used in order to simplify the electrostatics of the device.

1. Introduction

Carbon NanoTubes (CNTs) represent a promising alternative to conventional silicon technology for future nano-electronics at the end of the roadmap. Since the first work on the topic by Iijima [1], significant improvements have been achieved, both from the point of view of technology and physical modeling.

In particular, Schottky Barrier CNT FETs have been demonstrated by Heinze et al. [2], where the modulation of the current is mainly determined by the field-induced modulation of the NanoTube band structure at the CNT ends. Such aspect can represent a limit for the performance of the CNT FET, because of the ambipolar behavior, and the possible degradation of electrical properties like I_{on}/I_{off} ratio, especially for NanoTubes with large diameters.

On the other end channel modulation of the barrier can be achieved by ohmic contacts at the source and drain ends, choosing a proper metal for the contacts [3] or inducing charge in the source and drain regions, by doping the reservoirs as reported in Ref. [4].

In this scenario, adequate physical models and simulation tools are necessary not only to provide explanations to the experimental results, but also to define device guidelines for the fabrication of CNT FETs, with performance comparable to their mainstream silicon counterpart.

A simplified approach is that in [5], where the potential profile of a three-dimensional structure is obtained by means of a two-dimensional simulator, and transport is computed through the Landauer formalism.

Gate-all-around CNT FETs have been studied instead in [6, 7] where the three-dimensional Poisson equation has

been reduced to two-dimensions because of the cylindrical symmetry of the electrostatic potential.

The same coaxial geometry has been adopted in [8], where the Poisson equation has been coupled with the Schrödinger equation with the Non-Equilibrium Green's Function (NEGF) formalism, with a mode space approach, which allows to limit the computation of transport properties to a small number of electron subbands.

However, typical experiments [9]-[10], focus on planar gate structures which are more attractive because of their simpler technological requirements.

To this purpose, a full three-dimensional approach has been followed in [11], where the Poisson equation has been solved using the method of moments. However, such a method, while requiring the computation of the Poisson equation only in regions where charge is not zero, has the drawback that is practically impossible to treat more than two different dielectric constants.

In this paper we present a three-dimensional approach, which is based on the self-consistent solution of the Poisson and full band Schrödinger equations with open boundary conditions, in the NEGF framework, which can deal with very general structures, since does not take advantage of particular symmetries, it is not limited by the number of materials it can consider at the same time, and it can consider mixed structure in which both CNTs and crystalline semiconductors can be present simultaneously.

2. Simulation Approach

The potential profile in the three-dimensional simulation domain obeys the Poisson equation

$$\nabla [\epsilon(\vec{r})\nabla\phi(\vec{r})] = -q [p(\vec{r}) - n(\vec{r}) + N_D^+(\vec{r}) - N_A^-(\vec{r}) + \rho_{fix}], \quad (1)$$

where ϕ is the electrostatic potential, ϵ is the dielectric constant, which can varies in the 3D domain, p and n are the hole and electron densities, respectively, N_D^+ is the concentration of ionized donors, N_A^- is the concentration of ionized acceptors, and ρ_{fix} is the fixed charge. Electron, hole, acceptor and donor densities are computed in the whole domain with the semiclassical approximation, while the electron and hole concentration in correspondence of the CNT are computed solving the Schrödinger equation with open boundary conditions.

In particular, the Schrödinger equation has been solved by means of the NEGF formalism [12], using a tight-binding Hamiltonian with an atomistic (p_z orbitals) real space basis [13].

The Green's function can then be expressed as

$$G(E) = [EI - H - \Sigma_S - \Sigma_D]^{-1}, \quad (2)$$

where E is the energy, I the identity matrix, H the Hamiltonian of the CNT, while Σ_S and Σ_D the self-energies of the source and drain, respectively.

The considered CNTs are all zig-zag Nanotubes, but the proposed approach can be easily generalized to armchair nanotubes or to nanotubes with a generic chirality, since the required changes involve only the Hamiltonian matrix. Once the length and the chirality of the nanotube are defined, the coordinates in the three-dimensional domain of each carbon atom are computed. After that, the three-dimensional domain is discretized so that a grid point is defined in correspondence of each atom, while a user specified grid is defined in regions not including the CNT.

A point charge approximation is assumed, i.e. all the free charge around each carbon atoms is condensed in the elementary cell including the atom. In particular, the electron and hole densities are computed from the Density of States (DOS), derived by the NEGF formalism. Assuming that the chemical potential of the reservoirs are aligned at the equilibrium with the flat Fermi level of the CNT, the electron concentration reads

$$n = \int_{E_i}^{+\infty} dE [\text{DOS}_S(E)f(E - E_{F_S}) + \text{DOS}_D(E)f(E - E_{F_D})], \quad (3)$$

while the hole concentration is

$$p = \int_{-\infty}^{E_i} dE \{ \text{DOS}_S(E) [1 - f(E - E_{F_S})] + \text{DOS}_D(E) [1 - f(E - E_{F_D})] \}, \quad (4)$$

where E_i is the Fermi level within the CNT, f is the Fermi-Dirac occupation factor, and DOS_S , DOS_D , E_{F_S} and E_{F_D} are the Density of States and the Fermi levels of the source and drain, respectively.

The current has been computed by means of the Landauer formula

$$I = \frac{2q}{h} \int_{-\infty}^{+\infty} dE T(E) [f(E - E_{F_S}) - f(E - E_{F_D})], \quad (5)$$

where q is the electron charge, h is Planck's constant and $T(E)$ is the trace of the transmission matrix.

We have to point out that, using a real space basis, the computed current takes into account intra- and inter-band tunneling, since, as compared to the mode space approach, all the bands of the nanotube are considered simultaneously.

From a numerical point of view, the non-linear system has been solved with the Newton/Raphson (NR) method with the Gummel iterative scheme.

In particular, the Schrödinger equation is solved at the beginning of each NR cycle of the Poisson equation, and

the charge density in the CNT is kept constant until the NR cycle converges (i.e. the correction on the potential is smaller than a predetermined value). The algorithm is then repeated cyclically until the norm of the difference between the potential computed at the beginning and at the end of the NR cycle is smaller than a predetermined value.

The Green's function is computed by means of the Recursive Green's Function (RGF) formalism.

A particular attention must be put in the definition of the self-energy, which can be interpreted as a boundary condition of the Schrödinger equation. In particular, we have considered two different kinds of self-energies : semi-infinite leads boundary conditions and Schottky Barrier boundary conditions.

The first kind of self-energy, enables to consider the CNT as connected to infinitely long CNTs at its end. This condition is particularly suitable for the study of infinitely long CNT-FET, or more likely, to study CNT with doped source and drain reservoirs.

Schottky Barrier (SB) is another important boundary condition to be taken into account. In particular, in order to mimic the metallic nanotube connected to the CNT in the channel, we have anti transformed in the real space the Hamiltonian expressed in the mode space approach in [13], which manages to reproduce on a wide energy interval, an almost constant DOS of a metallic nanotube.

We have to point out that the computation of the Self-Energy is quite demanding. In order to achieve faster results, we have followed the approach proposed in [14], which provides results four times faster as compared to a simple under-relaxation method.

3. Simulation examples

In this section we show some results in order to demonstrate that our approach can be used to study the impact of gate geometries on very general structures, which does not take advantage of particular symmetries. In particular, we have focused our attention on the Carbon NanoTube Field Effect Transistors, in which the channel is composed by a (7,0) zig-zag nanotube, whose diameter is about 0.6 nm and the energy gap E_{gap} is approximately 1.3 eV. Such nanotube is relatively small, but nanotubes with even smaller diameter ((5,0) zig-zag) have been demonstrated [15].

In particular, we will focus our attention on Schottky Barrier Nanotube FET (SB CNT FET), and on CNT FET with infinite long doped carbon nanotubes as reservoirs.

3.1 Schottky Barriers Carbon Nanotubes FETs

In Fig. 1 is shown the three-dimensional structure of the Schottky Barrier FET. For all the simulated devices, a Schottky barrier equal to $E_{gap}/2$ has been assumed at the source and drain terminals.

In Fig. 2, the transfer characteristics of devices embedded in a SiO_2 layer with $L=15$ nm, $t_{ox_1} = 1.7$ nm, and $t_{ox_2} = 50$ nm (we refer from here on as single-gate structure), and with $L=15$ nm, $t_{ox_1} = t_{ox_2} = 1.7$ nm (we refer from here on as double-gate structure) are shown for

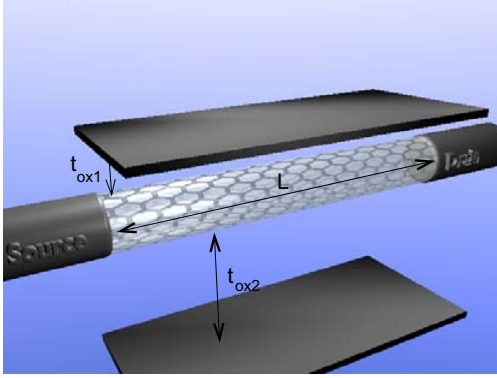


Figure 1: Three-dimensional structure of a Schottky Barrier CNT FET).

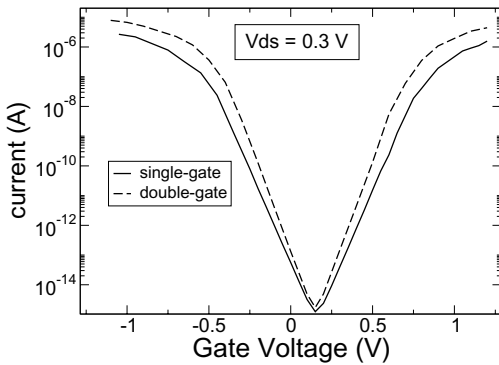


Figure 2: Transfer characteristics of Schottky Barrier FET with $L=15$ nm, $t_{ox1} = 1.7$ nm, $t_{ox2} = 50$ nm (solid line) and $t_{ox1} = t_{ox2} = 1.7$ nm (dashed line) defined in a SiO_2 substrate. The source-to-drain voltage is 0.3 V.

a source-to-drain voltage equal to 0.3 V. As can be seen, as expected for such kind of devices, the ambipolar behavior is reproduced [2], and the I_{off} current is in correspondence of $V_{GS} = V_{DS}/2$. Such device exhibits a good sub-threshold slope (78 mV/dec for the single-gate structure and 68 mV/dec for the double-gate structure), meaning that gate-all-around structures are not indispensable to achieve good voltage control over the channel.

We have to notice that, if we define the I_{on} current as the current at a gate voltage (V_{GS}) equal to 1.1 V, in both devices, the I_{on}/I_{off} ratio is larger than 10^9 . This is due to the large band gap of the considered nanotube, which prevent a significant leakage current at the ambipolar bias point (i.e. the point in correspondence of the minimum of the transfer characteristic).

3.2 Carbon Nanotubes FETs with infinite long doped carbon nanotube reservoirs

We now focus our attention on CNT FETs, whose reservoirs are composed by semi-infinite doped carbon nanotubes. In order to mimic the positive charge due to the ionized donors, we have imposed a positive fixed charge around the CNT so that the fraction of doping atoms on carbon atoms is about 10^{-3} .

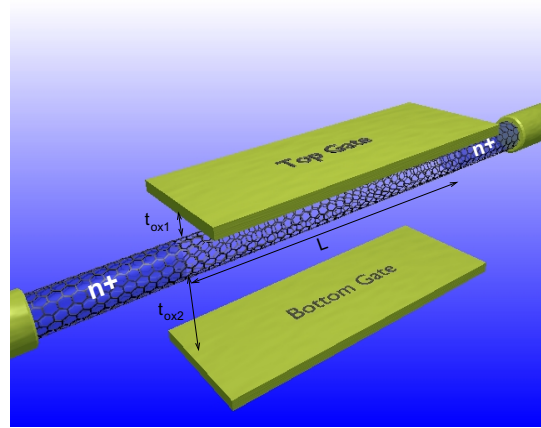


Figure 3: Three-dimensional structure of a CNT FET with doped reservoirs.

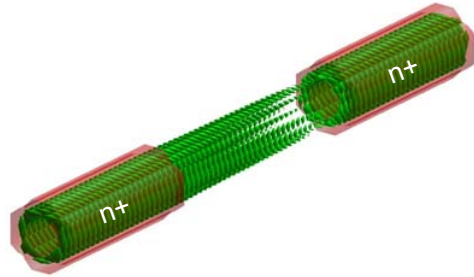


Figure 4: Electron density isosurface $n = 1 \times 10^{24} \text{ m}^{-3}$, for a gate voltage equal to 0.5 V and a source-to-drain voltage equal to 0.3 V.

Fig. 3 shows the three-dimensional structure of the simulated devices. In order to make a comparison with the previously considered SB CNT FETs, we have considered the same channel length, as well as the same oxide thickness for the double-gate and single-gate structures.

In Fig. 4 we show the electron density isosurface for $n = 1 \times 10^{24} \text{ m}^{-3}$, for a gate voltage equal to 0.5 V and a source-to-drain voltage equal to 0.3 V. Source and drain region are highlighted, while the charge depletion in correspondence of the drain end shows device saturation. Transfer characteristics for both devices are shown in Fig. 5. The sub-threshold slope for the single-gate device (dashed line) is equal to 72 mV/dec, and 60 mV/dec for the double-gate structure (solid line). As compared to the SB CNT FET, the CNTs with doped reservoirs exhibit a better gate control and an ideal sub-threshold slope (double-gate structure). As expected, [11] modulating the channel barrier is more effective in controlling the current flux, as compared to modulating the Schottky barrier at the channel ends.

Fig. 6 shows conduction bands for both CNT FET with Schottky barriers and doped reservoirs for both single and double gate structures. In both cases, double-gate structures exhibit less affection to short channel effects,

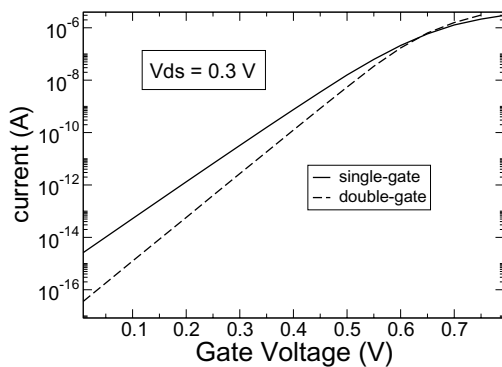


Figure 5: Transfer characteristics for CNT with doped source and drain regions defined in a SiO₂ substrate. $L=15$ nm, $t_{ox1} = 1.7$ nm, $t_{ox2} = 50$ nm (solid line) and $t_{ox1} = t_{ox2} = 1.7$ nm (dashed line), while the source-to-drain voltage is 0.3 V.

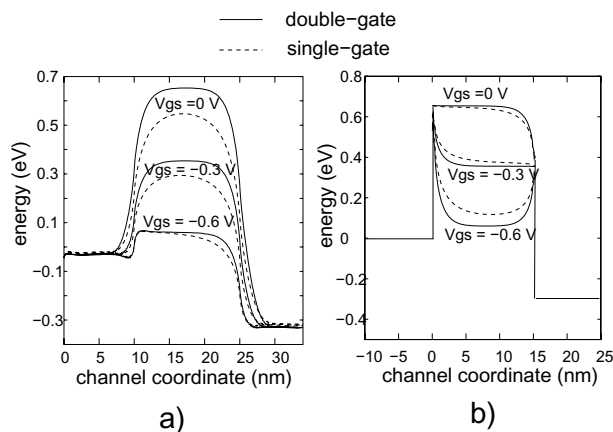


Figure 6: Conduction bands for single and double-gate structures as a function of the gate voltage for : a) CNT FET with doped reservoirs ; b) SB CNT FET.

as shown by the flatter band profiles as compared to the single-gate band profiles. In addition, double-gate structures show better control over the channel barrier, since same gate voltage variations, produce larger channel barrier lowering in double-gate than in single-gate structures.

4. Conclusions

We have developed a three-dimensional approach for the study of carbon nanotube FETs, based on the self-consistent solution of the 3D Poisson and Schrödinger equations, within the NEGF framework. In particular, an atomistic tight-binding Hamiltonian, within a real space approach, has been used, in order to take into account inter and intra band tunneling. As compared to others approach present in literature, it is able to consider very general structures, as, for example, single or double-gate structures, which do not take advantage of particular symmetries, and to consider structures formed by several different materials.

5. Acknowledgments

The authors would like to thanks Dr. Diego Kienle and Dr. Avik Ghosh for the useful discussions. This work has been partially supported by the EU NoE SINANO. Work at Purdue has been supported by NSF under Grant # EEC-0228390.

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