Atomistic Simulation of Carbon Nanotube Field-Effect Transistors Using Non-Equilibrium Green's Function Formalism

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In recent years, significant progress in understanding device physics and in identifying potential applications of carbon nanotube electronic devices has occurred [1, 2]. In a nanotube, low bias transport can be nearly ballistic across distances of several hundred nanometers. Deposition of high-κ gate insulators does not degrade the carrier mobility. Carbon nanotube field-effect transistors (CNTFETs) with near ballistic operation and excellent device performance have been recently demonstrated [3]. Developing physical simulation capabilities are important for understanding experiments and exploring device design issues. It has been previously shown that correct modeling of CNTFETs needs to incorporate quantum-mechanical tunneling at the metal/CNT interface, and unique transport properties of the one-dimensional nanotube channel [4].

In this work, we simulated ballistic CNTFETs by self-consistently solving the Poisson and Schrödinger equations using the non-equilibrium Green's function (NEGF) formalism. The NEGF transport equation is solved at two levels: i) an atomistic real space approach using the p_z orbitals of carbon atoms as the basis, and ii) an atomistic mode space approach, which only treats a few subbands in the tube's circumferential direction while retaining an atomistic grid along the carrier transport direction. The real space approach resolves the nanotube channel in an atomistic scale along both transport and circumference directions. The mode space approach is applicable when the potential variation around the tube is small compared to the subband spacing, and it is computationally more efficient than the real space approach. A phenomenological model is developed to treat metal/CNT junctions. The Schottky barrier height is an input parameter to the simulation rather than a computed one. Simulation examples show that these approaches describe quantum transport effects in CNTFETs. Analysis of a short-channel CNTFET using this simulator shows that the simulation agrees with the experimental measurement well [3].

We first simulate a MOSFET-like CNTFET as shown in Fig. 2a. The nanotube length is ~50nm, consisting of $\sim 1.2\times10^4$ carbon atoms. A self-consistent Poisson-NEGF simulation in the real space (using the recursive algorithm for computer the Green's function) is performed. The computed energy-resolved local-density-of-states (LDOS) plot (Fig. 2b) shows that the bandgap, quantum interference, quantum confinement, and higher subbands are correctly described. Next, we explore the validity of the mode space approach. Fig. 3 shows that the mode space approach exactly reproduces the I-V of the real space approach with much less computational cost when the potential is invariant around the tube. Finally, we treat a Schottky barrier CNTFET. The LDOS plot (Fig. 4b) shows that the metal-induced gap states (MIGS) near the metal/CNT interfaces are apparent and decay rapidly with a tail of a few nanometers inside the channel. The tunneling states under the Schottky barrier in the conduction band at the source end of the channel are clear.

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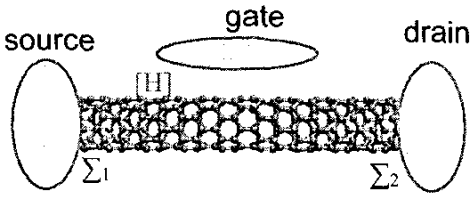


Fig. 1. The atomistic simulation of a CNTFET using NEGF formalism. An atomistic p_Z orbital description is used for the nanotube channel [H], the S/D contact self-energy, $\Sigma_{1,2}$, is obtained using a recursive algorithm for doped tube contacts and a phenomenological model for metal contacts. Poisson equation is self-consistently solved.

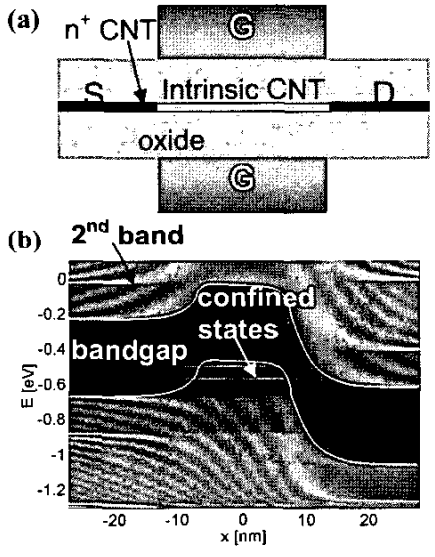


Fig. 2. (a) A coaxially gated CNTFET with heavily doped tubes as S/D extensions. (b) Local-density-of-states (LDOS) computed by the real space approach at V_G=0.25V and V_D=0.4V. The tube diameter d~2nm and bandgap Eg~0.4eV. The gate length is 15nm. The results describe quantum effects in the CNTFET.

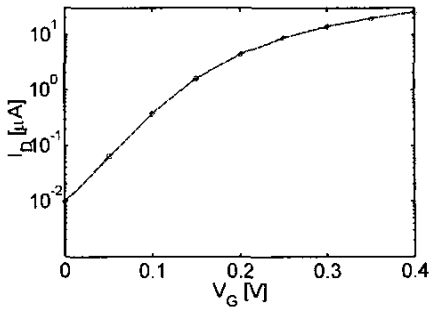


Fig. 3. The $I_D - V_G$ computed by the real space approach (line) and the mode space approach (circles) for a CNTFET as shown in Fig. 2a. The (13,0) nanotube channel length is 15nm. The mode space approach agrees with the real space approach.

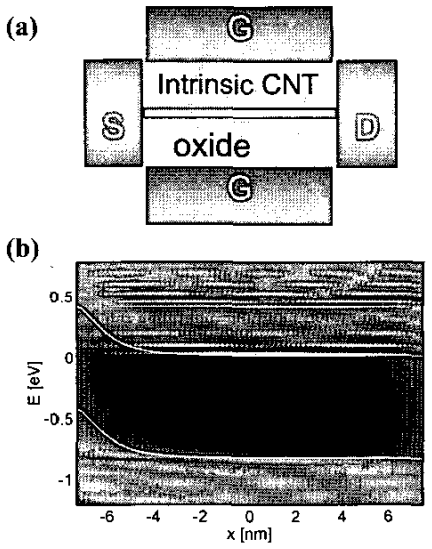


Fig. 4. (a) A coaxially gated Schottky barrier CNTFET with a CNT directly attached to metal S/D contacts. The channel is a (13,0) CNT with a diameter d~1nm and band gap Eg~0.83eV. (b) The local-density-of-states (LDOS) at $V_D = V_G = 0.4$ V, which clearly shows tunneling through the Schottky barrier at the source end of the channel, and metal induced gap states (MIGS) at the metal/CNT interfaces

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