Rigorous Modeling of Carbon Nanotube Field Effect Transistors

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Carbon nanotube field-effect transistors (CNTFETs) have been studied in recent years as a potential alternative to CMOS devices because of their capability of ballistic transport. While early devices have shown poor device characteristics, high performance devices were achieved recently [1–4]. To investigate the behavior of these devices we employ the Non-Equilibrium Green's Function (NEGF) formalism. Using this approach, both quantum interference effects and scattering processes can be rigorously considered. Recently a semiclassical Monte Carlo analysis [5] was performed to investigate the effect of scattering on CNTFET characteristics. However, even with quantum corrections included semiclassical methods cannot accurately predict the behavior of these devices because of the strong quantum effects. Based on the NEGF formalism we investigated transport phenomena in CNTFETs. The effects of acoustic phonon (AP) scattering and optical phonon scattering (OP) on the device performance were studied. Simulation results show that AP scattering has a more detrimental effect than OP scattering on the device characteristics. Only for very short devices, performance is not degraded because of the long mean free path (MFP) for AP scattering

Exceptional electronic and mechanical properties together with nanoscale diameter make carbon nanotubes (CNTs) candidates for nanoscale field effect transistors (FETs). Depending on the work function difference between the metal contact and the CNT, carriers at the metal-CNT interface encounter different barrier heights. Devices with positive (Schottky type) [6] and zero (ohmic) [7] barrier heights were fabricated. Devices with positive barrier heights have lower I_{on} and also suffer from ambipolar behavior [8], while devices with zero barrier height theoretically [9] and experimentally [3] show better performance. In this work we focus on devices with zero barrier height for electrons. The barrier height for holes is given by the band gap of the CNT. Using MINIMOS-NT [10], the Poisson equation is solved in three-dimensions. By assuming that carriers are distributed uniformly over the surface of the tube, which is a reasonable approximation for CNTs with a diameter of several nanometers, the transport equations need to be solved only in one-dimension.

$$G^r = [EI - H - \Sigma^r]^{-1} \quad (1)$$

$$G^{<,>} = G^r \Sigma^{<,>} G^a \quad (2)$$

$$\Sigma^{r,<,>} = \Sigma^{r,<,>}_{s,d} + \Sigma^{r,<,>}_{ph} \quad (3)$$

$$\Sigma^{r,<,>}_{ph} = \Sigma^{r,<,>}_{el} + \Sigma^{r,<,>}_{in} \quad (4)$$

$$n = -2i \int tr\{G^<(E)\} \frac{dE}{2\pi} \quad (5)$$

$$I = \frac{4\mathrm{q}}{\hbar} \int tr\{\Sigma^< G^> - \Sigma^> G^<\} \frac{dE}{2\pi} \quad (6)$$

In (1) an effective mass Hamiltonian is assumed. The total self-energy (3) consists of the self-energies due to the contacts and electron-phonon scattering. The coupled system of the transport and Poisson equations is solved iteratively. We used an adaptive method to discretize the transport equations in energy space. We have shown that by using this method the stability of the self-consistent loop increases and the simulation time decreases considerably [11]. For a fair comparison with experimental results, we used the same material and geometrical parameters as reported in [3]. All our calculations assume a CNT with 0.5 eV band gap, corresponding to a diameter of 1.7 nm [3]. The MFPs of semiconducting CNTs at high energies approach those of a metallic CNT [5]. Reference [12] reported $\lambda_{\mathrm{AP}} \approx 1.6\mu\mathrm{m}$ and $\lambda_{\mathrm{OP}} \approx 10\mathrm{nm}$ for a metallic CNT with a diameter of $1.8\mathrm{nm}$. AP scattering is due to zone boundary phonons and OP scattering is due to optical phonon modes with $\hbar\omega_{\mathrm{op}} = 160$ and $200\mathrm{meV}$ [12]. As a good approximation we used these parameters in our calculations.

Fig. 1a and Fig. 1b show the energy spectrum of the source and drain current for the given potential profile (Fig. 1c). Due to the conservation of energy in AP scattering the spectra of the source and the drain current are identical. By decreasing the MFP for AP scattering the resonances in the current spectrum smear out and the device current decreases considerably. Due to energy exchange in OP scattering the spectrum of the source and drain current are different. By decreasing the MFP for OP scattering more electrons scatter from high energies to lower energies, but interestingly the total current decreases only a little. For a better comparison the output characteristics of the device for AP and OP scattering with different MFPs are shown in Fig. 2a. The effect of AP scattering on the device

current can be more pronounced than that of than OP scattering. Because of the long MFP, AP scattering in CNTs has only little effect on the device current of short channel devices. Despite OP scattering does not decrease the device current, it strongly affects the carrier concentration and the current spectrum. Similar results were observed in Monte Carlo simulations [5]. OP scattering is expected to have an indirect effect [13] on the device characteristics by changing the carrier density spectrum and the self-consistent potential. Fig. 2b and Fig. 2c show the comparison between experimental data [4] and simulation results. Excellent agreement between simulation and experimental results confirms the validity of our approach. This detailed analysis allows the performance of CNTFETs [14] to be optimized.

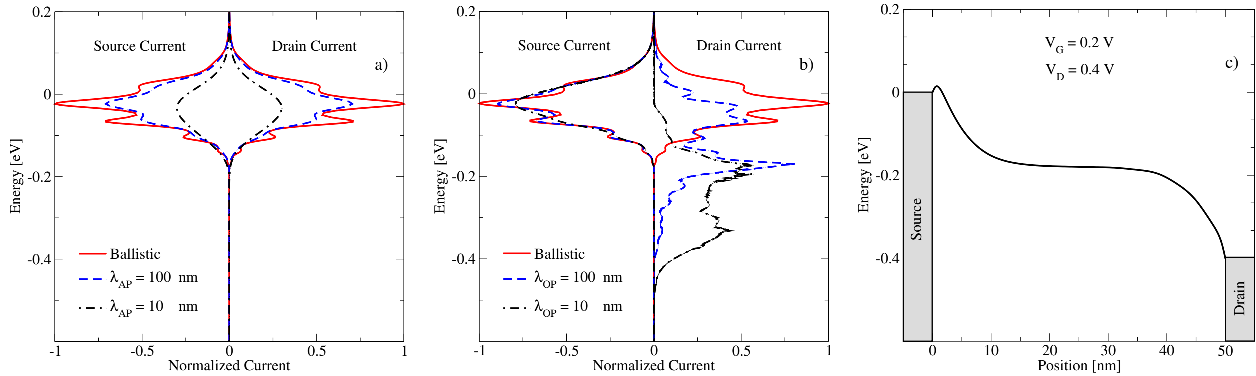

Figure 1: The effect of a) AP scattering and b) OP scattering on the energy spectrum of the source and drain currents. c) The conduction band-edge profile.

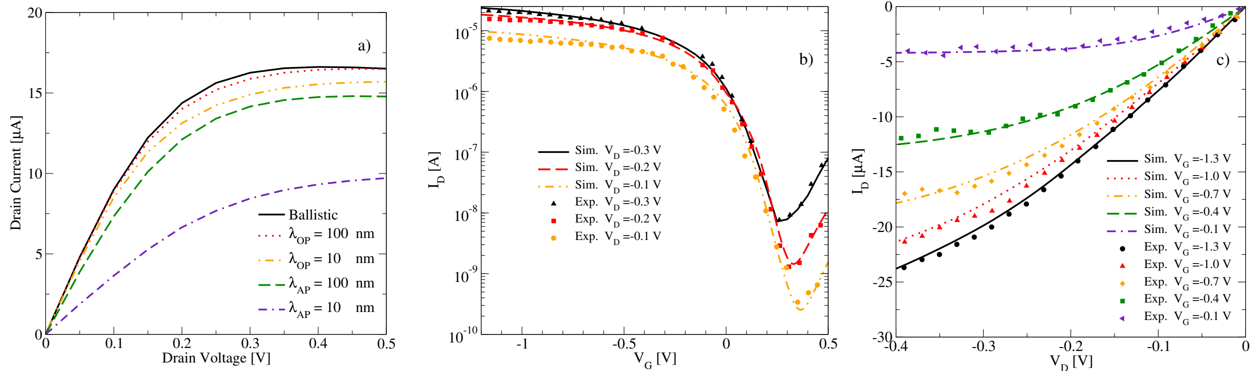

Figure 2: a) The effect of AP and OP scattering on the output characteristics. Comparison of the experimental and simulation results for the b) transfer characteristics and c) output characteristics.

Acknowledgment This work has partly been supported by the European Commission, IST-506844, NoE SINANO.

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