Institute of Physics Publishing Journal of Physics: Conference Series **38** (2006) 29–32
doi:10.1088/1742-6596/38/1/008 NPMS-7/SIMD-5 (Maui 2005)

Rigorous modeling of carbon nanotube transistors

Mahdi Pourfath, Hans Kosina, and Siegfried Selberherr
Institute for Microelectronics, Technische Universität Wien,
Gußhausstraße 27–29, A-1040 Wien, Austria
E-mail: {`pourfath|kosina|selberherr`}`@iue.tuwien.ac.at`

Abstract. Based on the non-equilibrium Green's function formalism the performance of carbon nanotube field-effect transistors has been studied. The effects of elastic and inelastic scattering on the device performance have been investigated. The results indicate that elastic scattering has a more detrimental effect on the device characteristics than inelastic scattering. Only for short devices the performance is not affected because of the long mean free path for elastic scattering.

1. Introduction

A carbon nanotube (CNT) can be viewed as a rolled-up sheet of graphite with a diameter of a few nano-meters. Depending on the chiral angle the CNT can be either metallic or semiconducting. Semiconducting CNTs can be used as channels for field-effect transistors (FETs). CNTFETs have been studied in recent years as potential alternatives 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, 2].

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) [3] and zero (ohmic) [4] barrier heights were fabricated. Devices with positive barrier heights have lower I_{on} and also suffer from ambipolar behavior [5], while devices with zero barrier height theoretically [6] and experimentally [2] 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 the non-equilibrium Green's function (NEGF) formalism quantum phenomena like tunneling, and scattering processes can be rigorously modeled. The NEGF formalism has been successfully used to investigate the characteristics of nano-scale transistors [7, 8], CNTFETs [6, 9], and molecular transistors [10]. Recently a semiclassical Monte Carlo analysis of the effect of scattering on CNTFET characteristics has been reported [11]. However, even with quantum corrections included, semiclassical methods cannot accurately predict the behavior of these devices because of the strong quantum effects. Therefore, in this work the NEGF formalism has been chosen to investigate transport phenomena in CNTFETs. The effect of elastic and inelastic scattering has been studied separately.

2. Approach

Due to quantum confinement along the tube circumference, the wave functions of carriers are bound around the CNT and can propagate along the tube axis. Assuming that the potential profile does not vary around the circumference of the CNT, sub-bands can be decoupled [8]. In this work we assume bias conditions in which the first sub-band contributes mostly to the total current. In the mode-space approach [8] the transport equations for each sub-band can be written as (1) and (2), see [12].

$$G^R = [EI - H - \Sigma^R_{\mathrm{el-ph}} - \Sigma^R_{\mathrm{s,d}}]^{-1} \tag{1}$$

$$G^{<,>} = G^R[\Sigma^{<,>}_{\mathrm{e-ph}}(E) + \Sigma^{<,>}_{\mathrm{s,d}}(E)][G^R]^{\dagger} \tag{2}$$

where $\Sigma^R_{\mathrm{e-ph}}$ is the self-energy due to electron-phonon interaction, $\Sigma^R_{\mathrm{s,d}}$ is the self-energy due to the coupling of the device to the source and drain contacts, which is only non-zero at the boundaries. A recursive Green's function method is used for solving (1) and (2), see [7]. In (1) an effective mass Hamiltonian is assumed, which is discretized using finite differences.

$$H = \begin{pmatrix} U_1 + 2t & -t & 0 & 0 & 0 & 0 & 0 \\ -t & U_2 + 2t & -t & 0 & 0 & 0 & 0 \\ 0 & \bullet & \bullet & \bullet & 0 & 0 & 0 \\ 0 & 0 & 0 & \bullet & \bullet & \bullet & 0 \\ 0 & 0 & 0 & 0 & -t & U_{n-1} + 2t & -t \\ 0 & 0 & 0 & 0 & 0 & -t & U_n + 2t \end{pmatrix} \tag{3}$$

Here U_j is the potential energy at the point j, $t = \frac{\hbar^2}{2m^* a^2}$, and a is the grid spacing. The self-energy due to electron-phonon interaction consists of the contribution of elastic and inelastic scattering mechanisms, $\Sigma^{<,>}_{\mathrm{e-ph}} = \Sigma^{<,>}_{\mathrm{el}} + \Sigma^{<,>}_{\mathrm{inel}}$. Assuming a single sub-band the electron-phonon self-energies are simplified as (4)-(8).

$$\Sigma^{<,>}_{\mathrm{el}}(E) = D_{\mathrm{el}} G^{<,>}(E) \tag{4}$$

$$\Sigma^{<}_{\mathrm{inel}}(E) = \sum_{\nu} D_{\mathrm{inel},\nu}[(n_B(\hbar\omega_\nu) + 1)G^<(E + \hbar\omega_\nu) + n_B(\hbar\omega_\nu)G^<(E - \hbar\omega_\nu)] \tag{5}$$

$$\Sigma^{>}_{\mathrm{inel}}(E) = \sum_{\nu} D_{\mathrm{inel},\nu}[(n_B(\hbar\omega_\nu) + 1)G^>(E - \hbar\omega_\nu) + n_B(\hbar\omega_\nu)G^>(E + \hbar\omega_\nu)] \tag{6}$$

$$\Im m[\Sigma^R_{\mathrm{e-ph}}(E)] = \frac{1}{2i}[\Sigma^>_{\mathrm{e-ph}} - \Sigma^<_{\mathrm{e-ph}}] \tag{7}$$

$$\Re e[\Sigma^R_{\mathrm{e-ph}}(E)] = \frac{1}{\pi}\mathbf{P}\int \frac{\Im m[\Sigma^R_{\mathrm{e-ph}}(E')]}{E' - E} dE' \tag{8}$$

where n_B is given by the Bose-Einstein distribution function. D_{el}, and D_{inel} are related to the mean free path of the corresponding scattering mechanisms [9]. The transport equations are iterated to achieve convergence of the electron-phonon self-energies, resulting in a self-consistent Born approximation. The carrier concentration and the current density at some point j of the device can be calculated as (9) and (10).

$$n_j = -2i \int G^<_{j,j}(E) \frac{dE}{2\pi} \tag{9}$$

$$j_j = \frac{4q}{\hbar} \int 2Re\{G^<_{j,j+1}(E) H_{j+1,j}\} \frac{dE}{2\pi} \tag{10}$$

Carriers are treated as a sheet charge distributed over the surface of the CNT [13]. After convergence of the scattering self energies, the coupled system of the transport and Poisson equations is solved iteratively. We use an adaptive method to discretize the transport equations in energy space. We have shown that this method increases the stability of iteration to obtain self consistency and decreases the simulation time considerably [14].

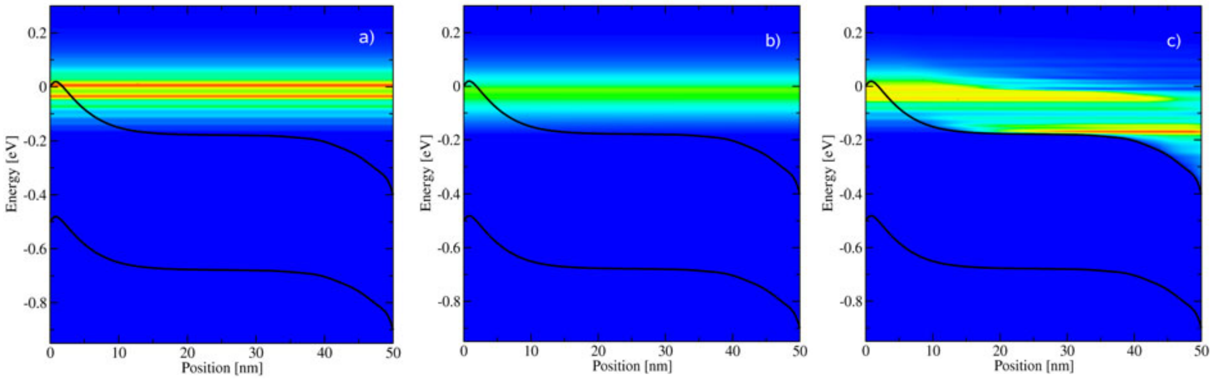

Figure 1. Current spectrum through the device for ballistic transport (a), with elastic scattering $\lambda_{\mathrm{el}} = 10$ nm (b), and with inelastic scattering $\lambda_{\mathrm{inel}} = 10$ nm (c).

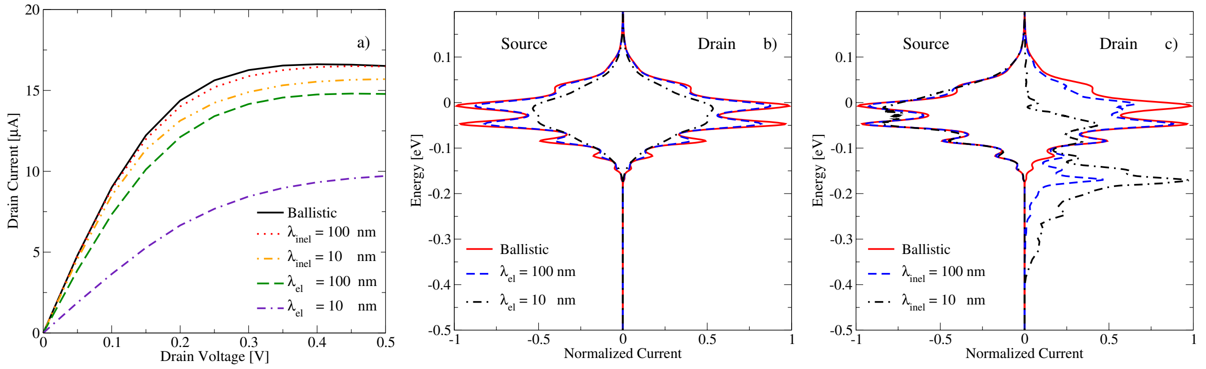

Figure 2. The effect of elastic and inelastic scattering on the output characteristic (a). The spectrum of the current by accounting for elastic (b), and inelastic scattering (c).

3. Simulation Results and Discussions

The mean free path of carriers in semiconducting CNTs at high energies approach those in metallic CNTs [11]. Reported values are $\lambda_{\mathrm{el}} \approx 1.6\ \mu$m and $\lambda_{\mathrm{inel}} \approx 10$ nm for a metallic CNT with a diameter of 1.8nm, [15]. Elastic scattering is due to acoustic phonons, and inelastic scattering is due to zone boundary and optical phonon modes with energies of $\hbar\omega_{\mathrm{op}} = 160$ meV and 200 meV, respectively [15]. First we investigate the effect of each scattering mechanism separately. Fig. 1 shows the normalized spectrum of the current for different conditions. In all cases a large amount of current is delivered by tunneling. Elastic scattering conserves the energy of carriers as in the ballistic case, but the current decreases considerably due to the elastic back-scattering of carriers. On the other hand, with inelastic scattering the energy of carriers is not conserved. Carriers which acquire enough kinetic energy can emit phonons and scatter into lower energy states. This process does not decrease the current as much as elastic scattering does, since scattered carriers lose their kinetic energy and the probability for back-scattering is low [11]. For a better comparison Fig. 2-b, and Fig. 2-c show the spectra of the source and drain currents for these scattering mechanisms. When the mean free path for elastic scattering is decreased, the resonances in the current spectrum vanish (due to broadening) and the total current decreases considerably. When the mean free path for inelastic scattering is decreased, more carriers scatter from high energy states into lower energy states, and the shape of the source and drain current spectrum becomes asymmetric. Fig. 2-a shows that elastic scattering, unlike inelastic scattering, can severely degrade the on-current of the device.

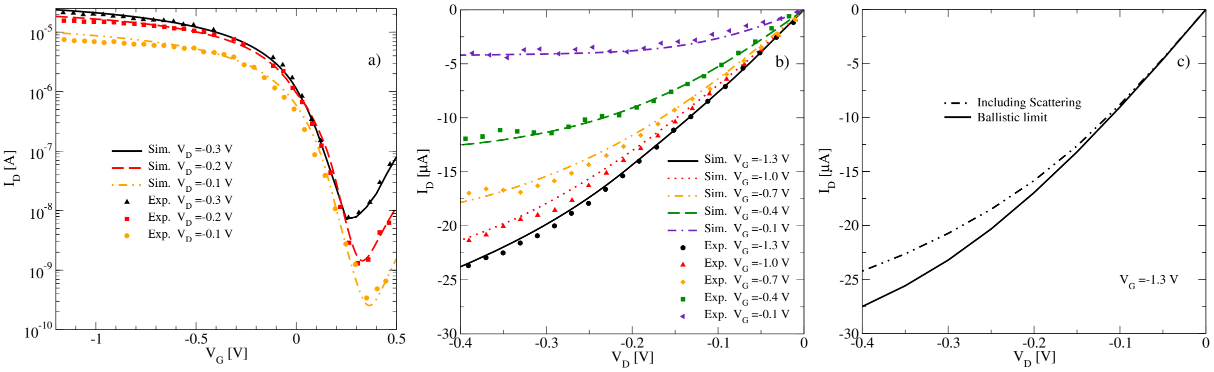

Figure 3. The comparison of the simulation results and experimental data for the transfer characteristics (a), and the output characteristic (b). Comparison of the output characteristic based on the ballistic transport and with scattering (c).

For comparison with experimental data, we used the same material composition and geometrical parameters as reported in [2]. These parameters give excellent agreement between simulation and experimental data (Fig. 3). As shown in Fig. 3-c even at high bias condition the drain current is close to its ballistic limit.

4. Conclusions

We theoretically investigated the effect of scattering on the performance of CNTFETs. Due to strong quantum effects like tunneling, the NEGF is a very well suited method to study transport phenomena in such devices. Because of back-scattering, elastic scattering has a detrimental effect on the device performance. Due to a long mean free path for this process, the performance of short devices (less than several hundred nano-meter) is only weakly affected. On the other hand, the mean free path for inelastic scattering in CNTs is quite short, but this process does not degrade device performance. Our analysis shows that even in the presence of inelastic scattering, short CNTFETs can operate close to their ballistic limit.

Acknowledgments

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

5. References

[1] Radosavljevic M. *et al.* 2004 *Appl.Phys.Lett.* **84**(18) 3693–3695
[2] Javey A. *et al.* 2004 *Nano Lett.* **4**(7) 1319–1322
[3] Appenzeller J. *et al.* 2004 *Phys.Rev.Lett.* **92** 048301
[4] Javey A. *et al.* 2003 *Letters to Nature* **424**(6949) 654–657
[5] Pourfath M. *et al.* 2005 *J.Appl.Phys.* **97** 106103
[6] Guo J. *et al.* 2004 *IEEE Trans. Electron Devices* **51**(2) 172–177
[7] Svizhenko A. *et al.* 2002 *J.Appl.Phys.* **91**(4) 2343–2354
[8] Venugopal R. *et al.* 2002 *J.Appl.Phys.* **92**(7) 3730–3739
[9] Svizhenko A. *et al.* 2005 *cond-mat/0503769*
[10] Xue Y. *et al.* 2002 *Chemical Physics* **281**(2-3) 151–170
[11] Guo G. *et al.* 2005 *Appl.Phys.Lett.* **86** 193103
[12] Datta S. 1995 *Electronic Transport in Mesoscopic Systems* (Cambridge University Press)
[13] Pourfath M. *et al.* *Microelectronic Engineering* **81**(2-4) 428–433
[14] Pourfath M. *et al.* 2006 *To appear in the Journal of Computational Electronics*
[15] Park J. *et al.* 2004 *Nano Lett.* **4**(3) 517–520