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Dissipative Transport in CNTFETs

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Introduction

Exceptional electronic and mechanical properties together with nanoscale diameter make carbon nanotubes (CNTs) candidates for nanoscale field effect transistors (FETs). High performance CNTFETs were achieved recently [1, 2]. In this work we focus on an n/i/n device [2, 3]. Using the non-equilibrium Green's function (NEGF) formalism quantum phenomena like tunneling and scattering processes can be rigorously modeled. Recently a semiclassical Monte Carlo analysis of the effect of scattering on CNTFET characteristics has been reported [4, 5]. 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. Based on this method the performance of CNTFETs 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. However, for short devices the performance is not affected because of the long mean free path for elastic scattering.

Approach

We have solved the coupled transport and Poisson equations. In this work we assume bias conditions in which the first sub-band contributes mostly to the total current. In the mode-space approach [6] the transport equations for each sub-band can be written as:

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

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

In (1) an effective mass Hamiltonian was assumed. All our calculations assume a CNT with $\mathrm{E_g} = 0.8$ eV, and $m^* = 0.05m_0$ for both electrons and holes. A recursive Green's function method is used for solving (1) and (2) [7]. 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 (3)-(6).

$$\Sigma^{<,>}_{\mathrm{el}}(E) = D_{\mathrm{el}} G^{<,>}(E) \quad (3)$$

$$\Sigma^{<}_{\mathrm{inel}}(E) = \sum_\nu D_{\mathrm{inel},\nu} [(n_B(\hbar\omega_\nu)+1)G^<(E+\hbar\omega_\nu) + n_B(\hbar\omega_\nu)G^<(E-\hbar\omega_\nu)] \quad (4)$$

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

$$\Im m[\Sigma^R_{\mathrm{e-ph}}(E)] = \frac{1}{2i}[\Sigma^>_{\mathrm{e-ph}} - \Sigma^<_{\mathrm{e-ph}}] \quad (6)$$

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 [8]. The transport equations are iterated to achieve convergence of the electron-phonon self-energies, resulting in a self-consistent Born approximation. 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 is calculated as (7) and (8).

$$n_j = -2i \int G^<_{j,j}(E) \frac{dE}{2\pi} \quad (7)$$

$$j_j = \frac{4q}{\hbar} \int 2Re\{G^<_{j,j+1}(E) H_{j+1,j}\} \frac{dE}{2\pi} \quad (8)$$

The coupled transport and Poisson system is solved iteratively.

SIMULATION RESULTS

The mean free paths of carriers in semiconducting CNTs at high energies approach those in metallic CNTs [4]. Reported values are $\lambda_{\mathrm{el}} \approx 1.6\ \mu\mathrm{m}$ and $\lambda_{\mathrm{inel}} \approx 10\ \mathrm{nm}$ for a metallic CNT with a diameter of $1.8\ \mathrm{nm}$, [9]. Elastic scattering is due to acoustic phonons, and inelastic scattering due to zone boundary and optical phonon modes with energies of $\hbar\omega_{\mathrm{op}} = 160\ \mathrm{meV}$ and $200\ \mathrm{meV}$, respectively [9]. 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 (Fig. 2), since scattered carriers lose their kinetic energy and the probability for back-scattering is low [4]. Due to a long mean free path for elastic scattering 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. Fig. 1 and Fig. 3 show the current spectrum in the absence and presence of scattering. In the presence of scattering the current decreases slightly and carriers at high energy states are scattered into lower energy states.

CONCLUSION

We theoretically investigated the effect of scattering on the performance of CNTFETs. Because of back-scattering, elastic scattering has a detrimental effect on the device performance. Our analysis shows that short CNTFETs can operate close to their ballistic limit.

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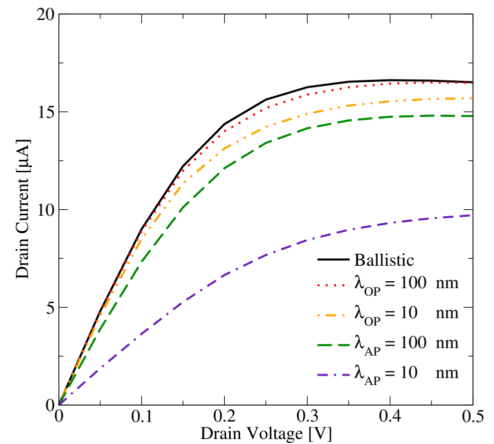

Fig. 2. The effect of scattering on the output characteristics.

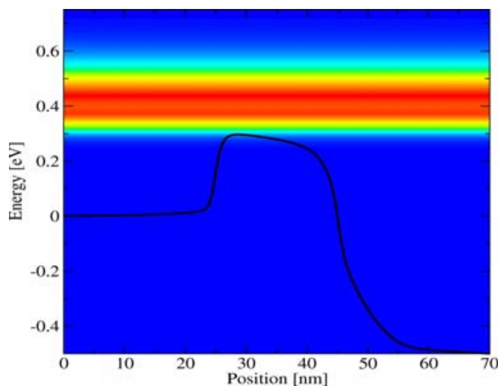

Fig. 1. The current spectrum for ballistic transport.

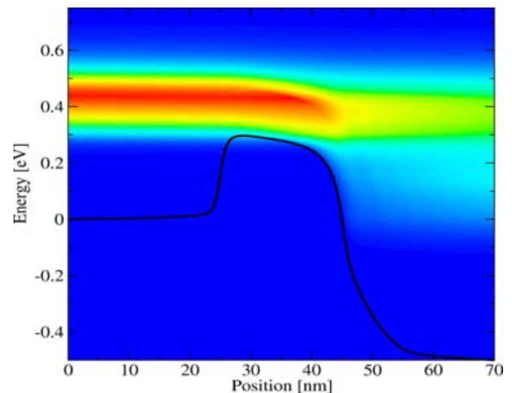

Fig. 3. Current spectrum in the presence of scattering.