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The Effect of Inelastic Phonon Scattering on Carbon Nanotube-Based Transistor Performance

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Abstract. Carbon nanotube (CNT) based transistors have been studied in recent years as potential alternatives to CMOS devices because of their capability of near ballistic transport. In this work the non-equilibrium Green's function (NEGF) formalism is used to perform a comprehensive study of CNT based transistors. The effect of inelastic phonon scattering on the gate-delay time of CNT based transistors is studied for a wide range of phonon energies. The results which confirm experimental data, show that depending on the phonon energy, inelastic scattering affects the steady-state on-current and switching response of CNT based transistors differently. The on-current can be close to the ballistic limit, whereas the gate delay time is above that limit.

1. Introduction

Novel structures and materials such as multiple gate MOSFETs, carbon nanotube field-effect transistors (CNT-FETs), and molecular based transistors, are expected to be introduced to meet the requirements for scaling. CNT-FETs have been considered in recent years as potential alternatives to CMOS devices due to excellent electronic properties of carbon nanotubes (CNTs). Some of the interesting electronic properties of CNTs are quasi-ballistic carrier transport [1], suppression of short-channel effects due to one-dimensional electron transport [2], and nearly symmetric structure of the conduction and valence bands, which is advantageous for complementary applications. Furthermore, the fact that there are no dangling bond states at the surface of CNTs allows for a wide choice of gate-insulators.

In this work the non-equilibrium Green's function (NEGF) formalism is used to perform a numerical study of the effect of inelastic phonon scattering on the performance of CNT-FETs. The gate-delay time is studied for a wide range of phonon energies.

2. Approach

Using the NEGF formalism quantum phenomena such as tunneling and scattering processes can be rigorously modeled [3, 4]. Based on the NEGF formalism we investigated the effect of the electron-phonon interaction on the performance of CNT-FETs.

The transport equations are solved on the surface of the CNT. We considered an azimuthal symmetric structure, in which the gate fully surrounds the CNT. Under the assumption that the potential profile does not vary sharply along the CNT, sub-bands are decoupled. As a result, transport equations need to be solved only along the CNT axis which is assumed to be the z direction in cylindrical coordinates. We assume bias conditions for which the first sub-band

contributes mostly to the total current. In the mode-space approach the transport equation for a sub-band can be written as [5]

$$G^{\mathrm{r,a}}_{z,z'}(E) = [EI - H_{z,z'}(E) - \Sigma^{\mathrm{r,a}}_{z,z'}(E)]^{-1} \tag{1}$$

$$G^{\gtrless}_{z,z'}(E) = G^{\mathrm{r}}_{z,z'}(E)\Sigma^{\gtrless}_{z,z'}(E)G^{\mathrm{a}}_{z,z'}(E) \tag{2}$$

In (1) an effective mass Hamiltonian was assumed. All our calculations assume a $(19, 0)$ zigzag CNT corresponding to a band gap of $\mathrm{E_g} = 0.6$ eV, a diameter of $\mathrm{d_{CNT}} = 1.5$ nm, and $m^* = 0.05m_0$. Here electrons are considered to be majority carriers. Since the dispersion relations for electrons and holes are symmetric, our discussions are valid for holes as well.

A recursive Green's function method is used for solving (1) and (2) [6]. The total self-energy in (1) consists of the self-energies due to the source contact, drain contact, and electron-phonon interaction, $\Sigma = \Sigma_{\mathrm{S}} + \Sigma_{\mathrm{D}} + \Sigma_{\mathrm{e-ph}}$. The calculation of the self-energies is presented in [5].

In this work the first-order self-energy for electron-phonon interaction within the self-consistent Born approximation is applied [7]. The interaction of electrons with optical phonons is inelastic. Assuming that the electron-phonon interaction occurs locally, $\Sigma_{z,z'}(E) = 0$ for $z \neq z'$ [8], the self-energy for inelastic electron-phonon interaction can be written as

$$\Sigma^{<}_{\mathrm{e-ph}}(E) = \sum_{\lambda} D_{\lambda}[(n_B(\hbar\omega_{\lambda}) + 1)G^{<}(E + \hbar\omega_{\lambda}) + n_B(\hbar\omega_{\lambda})G^{<}(E - \hbar\omega_{\lambda})] \tag{3}$$

where $\hbar\omega_{\lambda}$ denotes the phonon energy of branch λ, $n(\hbar\omega_{\lambda})$ the average phonon occupation number, and D_{λ} the electron-phonon coupling strength. Assuming that the bath of phonons is maintained in thermodynamic equilibrium, $n(\hbar\omega_{\lambda})$ is given by the Bose-Einstein distribution function. The electron-phonon interaction strength of a $(n, 0)$ zigzag CNT is given by

$$D_{\lambda} = \frac{\hbar|M_{\lambda}|^2}{2nm_{\mathrm{c}}\omega_{\lambda}} \tag{4}$$

where the matrix elements of the interaction Hamiltonian M_{λ} depend on the diameter and the chirality of the CNT. The calculation of these parameters is presented in [9, 10]. Phonons with $q \approx 0$ are referred to as Γ-point phonons, and can belong to the twisting acoustic (TW), the longitudinal acoustic (LA), the radial breathing mode (RBM), the out-of-phase out-of-plane optical (ZO), the transverse optical (TO), or the longitudinal optical (LO) phonon branch. Phonons inducing inter-valley transitions have a wave-vector of $|q| \approx q_{\mathrm{K}}$, where q_{K} corresponds to the wave-vector of the K-point of the Brillouin zone of graphene. K-point phonons, also referred to as zone boundary phonons, are a mixture of fundamental polarizations.

The transport equations (1) and (2) are iterated to achieve convergence of the electron-phonon self-energies, resulting in a self-consistent Born approximation. To solve the transport equations numerically, they need to be discretized in both the spatial and the energy domain. Uniform spatial grids have been employed. The energy grid, however, has to be non-uniform, since an adaptive integration method is generally required to resolve resonances at some energies with sufficient accuracy [11].

The coupled system of the transport and Poisson equations has to be solved self-consistently, where the convergence of the self-consistent iteration is a critical issue. To achieve convergence, fine resonances at some energies have to be resolved accurately [12]. For that purpose an adaptive method for selecting the energy grid is essential [13].

3. The Effect of the Electron-Phonon Interaction

In this section the effect of inelastic scattering on the steady-state on-current and gate delay time is studied. Depending on the phonon energy inelastic scattering affects the steady-state on-current and switching response quite differently.

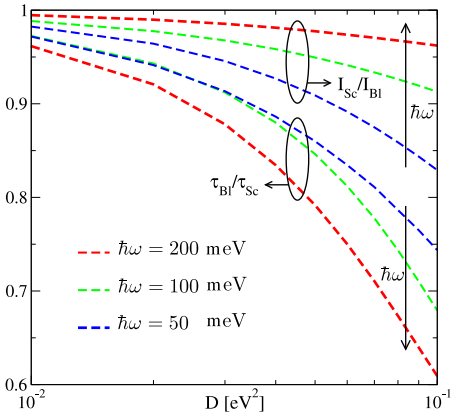

Figure 1. The ballisticity and the ratio of the gate delay time in the ballistic case to that in the presence of electron-phonon interactionas a function of the electron-phonon coupling strength.

3.1. Steady State On-Current

Fig. 1 shows the ballisticity as a function of the electron-phonon coupling strength for some phonon energies. The ballisticity is defined as $I_{\rm Sc}/I_{\rm Bl}$, the ratio of the steady-state on-current in the presence of electron-phonon interaction to the current in the ballistic case [14]. The left part of Fig. 2-a illustrates an electron losing its kinetic energy by emitting a phonon. The electron will be scattered either forward or backward. In the case of backward scattering the electron faces a thick barrier near the source contact and will be reflected with high probability, such that its momentum will again be directed towards the drain contact. Fig. 1 shows that with increasing phonon energy the effect of phonon scattering on the current is reduced, because scattered electrons lose more kinetic energy and the probability for traveling back to the source contact decreases.

The considerable decrease of ballisticity for low energy phonons is due to the phonon absorption process. The right part of Fig. 2-a shows an electron absorbing energy from a phonon and scattering into a higher energy state. In this case, the probability for arriving at the source contact increases. This process can severely reduce the total current. Fig. 2-b separately shows the effects of the phonon emission and absorption processes on the ballisticity. As the phonon energy decreases, the phonon occupation number increases exponentially, and the contribution of both phonon emission and absorption processes increases. However, due to the higher probability for back-scattering of electrons in the case of phonon absorption, this component reduces the total current more effectively than the phonon emission process does.

3.2. Gate Delay Time

To investigate the dynamic response of the device we consider the gate delay time defined as $\tau = C_{\rm G}V_{\rm D}/I_{\rm on}$, where $C_{\rm G}$ is the gate capacitance $C_{\rm G} = {C_{\rm Ins}}^{-1} + {C_{\rm Q}}^{-1}$, $C_{\rm Ins}$ is the gate-insulator capacitance. The quantum capacitance is given by $C_{\rm Q} = 8{\rm q}^2/{\rm h}\upsilon_{\rm F} \approx 400{\rm aF}/\mu{\rm m}$, including the twofold band and spin degeneracy. If thin and high-κ insulators are used, then $C_{\rm Ins} \gg C_{\rm Q}$ and $C_{\rm G} \approx C_{\rm Q}$, implying that the potential on the tube becomes equal to the gate potential (perfect coupling). This regime is called quantum capacitance limit in which the device is potential-controlled rather than charge-controlled [15]. It should be noticed that $C_{\rm Ins}$ of planar gate geometries is smaller than that of cylindrical gate geometries. Therefore, the condition $C_{\rm Ins} \gg C_{\rm Q}$ needs to be verified for such structures. However, by employing high-κ and thin dielectrics this condition can be satisfied even for planar structures. Assuming the quantum capacitance limit, one gets $C_{\rm G}V_{\rm D} \approx Q_{\rm Ch}$, where $Q_{\rm Ch}$ is the total charge in the CNT channel. The gate delay time can be written as $\tau \approx Q_{\rm Ch}/I_{\rm D}$.

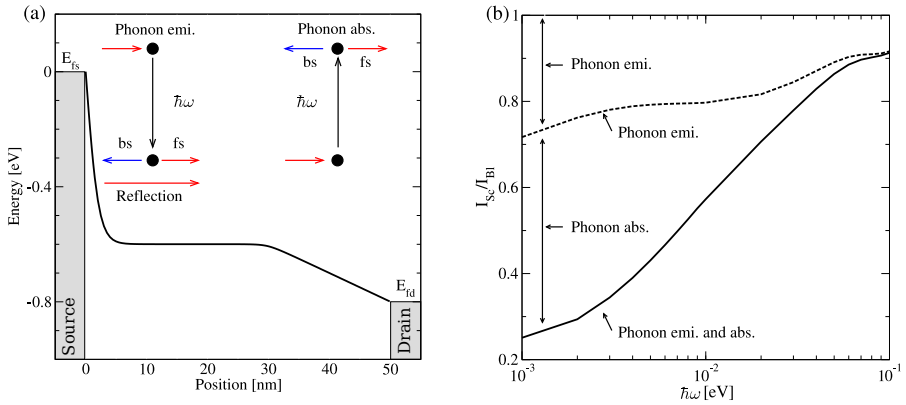

Figure 2. (a) Sketch of phonon emission and absorption processes in the channel. (b) Ballisticity versus phonon energy with $D = 10^{-1}$ eV^2 at the bias point $V_G = V_D = 1$ V. The contributions due to phonon absorption and emission are shown.

Fig. 1 shows the ratio of the gate delay time in the ballistic case to that in the presence of electron-phonon interaction, τ_{Bl}/τ_{Sc}, as a function of the electron-phonon coupling strength for some phonon energies. As the phonon energy increases the gate delay time increases. This behavior can be attributed to the electron group velocity in the channel, which is high for ballistic electrons and low for electrons scattered to lower energy states. Fig. 3 shows the spectra of the source and drain currents for different phonon energies. Electrons can emit a single phonon or a couple of phonons to reach lower energy states. The probability of n sequential electron-phonon interactions decreases as n increases. Fig. 3 shows a considerable increase of the electron population close to the conduction band-edge as the phonon energy increases. Therefore, the mean velocity of electrons decreases and the carrier concentration in the channel increases. The increased charge in the channel results in an increased gate delay time.

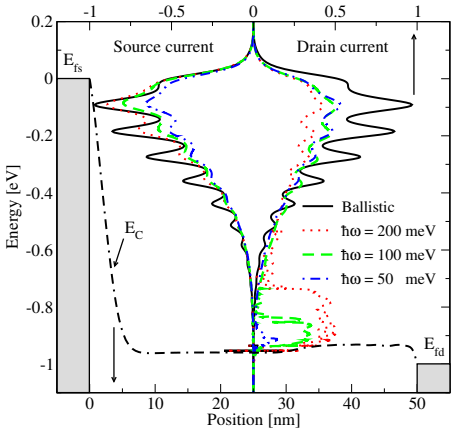

Figure 3. The normalized spectra of the source and drain currents. The effect of inelastic scattering with different phonon energies is shown. The electron-phonon coupling strength is $D = 2 \times 10^{-1}$ eV^2. The figure shows a considerable increase of the electron population close to the conduction band-edge as the phonon energy increases.

4. Discussion

For CNTs with diameters in the range $d_{\mathrm{CNT}} = 1 - 2$ nm the energies of important inelastic phonons are $\hbar\omega_{\mathrm{OP}} \approx 200$ meV, $\hbar\omega_{\mathrm{RBM}} \approx 30$ meV, $\hbar\omega_{\mathrm{K_1}} \approx 160$ meV, and $\hbar\omega_{\mathrm{K_2}} \approx 180$ meV [14, 16]. The corresponding coupling coefficients are $D_{\mathrm{OP}} \approx 40 \times 10^{-3}$ eV^2, $D_{\mathrm{RBM}} \approx 10^{-3}$ eV^2, $D_{\mathrm{K_1}} \approx 10^{-4}$ eV^2, and $D_{\mathrm{K_2}} \approx 50 \times 10^{-3}$ eV^2 [9, 14].

As discussed before high energy phonons such as OP and K-point phonons reduce the on-current only weakly, but can increase the gate-delay time considerably due to charge pileup in the channel. Low energy phonons such as the RBM phonon can reduce the on-current more effectively, but have a weaker effect on the gate-delay time. In a CNT at room temperature scattering processes are mostly due to electron-phonon interaction with high energy phonons. Therefore, the on-current of short CNT-FETs can be close to the ballistic limit [1], whereas the gate-delay time can be significantly above that limit [17]. The intrinsic (without parasitic capacitances) gate-delay time for the ballistic case can be approximated as $\tau \approx 1.7$ ps/μm, or equivalently $f_T \approx 100$ GHz/μm [18]. The highest reported intrinsic cutoff frequency for a device with a length of 300 nm is $f_T \approx 30$ GHz [19], which is far below the ballistic limit. Inelastic electron-phonon interaction with high energy phonon has to be considered to explain these results.

5. Conclusion

The effect of the electron-phonon interaction parameters on the performance of CNT based transistors was studied, using the NEGF formalism. Inelastic scattering with high energy phonons reduces the on-current only weakly, whereas it can increase the gate delay time considerably. The results explain the reason why the measured on-currents of short CNT-FETs can be close to the ballistic limit, whereas the highest achieved cutoff frequency is significantly below that limit.

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