Effects of contacts to electrodes and phonon scattering on transport of carbon-nanotube devices

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Abstract. We study the effects of longitudinal acoustic and optical phonon scatterings on the transport properties of carbon-nanotube devices with micron-order channel length, within the Kubo formula. We investigate the effects of the phonon scatterings with various wave numbers on the conductance. Furthermore, we evaluate the device properties of carbon nanotubes using the cut-off frequencies when the acoustic phonon is excited in the devices. The results presented here indicate the implication to high performance nanotube transistors.

1. Introduction

Applications of carbon nanotubes (CNTs) as electronic devices have long been expected, because the nanotubes are remarkable quasi-one-dimensional materials exhibiting ballistic transport. In practice, simple circuits based on semiconducting CNT field-effect transistors (FETs) have already been demonstrated [1]. The ballistic transport properties are disturbed by various scattering, such as impurities, vacancies and phonons. To realize the applications of CNT devices, it is important to understand the mechanism of the conductance reduction due to various scatterings by simulating the CNTs, whose sizes are the same as those observed in experiments.

In this paper, we have investigated the electron-phonon-coupling effects on the quantum transport properties of CNTs with micron-order channel lengths, within the Kubo formula [2, 3]. Furthermore, we have studied the effects of both electrode contacts and phonon scatterings on the cut-off frequencies of CNT-FETs.

2. Model and calculation method

We investigate the effects of the Schottky barrier and electron-phonon scattering on the electronic quantum transport in CNT-FETs using the time-dependent wave-packet approach within a tight-binding approximation. The vibrational atomic displacements by phonons in the CNTs are introduced through the time-dependent electron-transfer energies as following equation,
\[ \hat{H}(t) = -\sum_{i,j} \gamma_c(t) (\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i) + \sum \mathbf{V}(\mathbf{R}_j) \hat{c}_j^\dagger \hat{c}_j , \]  

where \( \hat{c}_i \) and \( \hat{c}_i^\dagger \) are the creation and annihilation operators of electrons at the \( i \)th orbital, and \( \gamma_c(t) \) is the time-dependent electron transfer energy between the \( i \)th and \( j \)th orbitals. The on-site energies, \( \mathbf{V}(\mathbf{R}_j) \), are deformed by the connection to metallic electrodes. We assume the time-dependent transfer energies as

\[ \gamma_c(t) = \gamma_0^c [\mathbf{R}_i - \mathbf{R}_j] \mathbf{R}_i^2 [\mathbf{R}_i(t) - \mathbf{R}_j(t)]^2 , \]

where \( \gamma_0^c \) is the transfer energy between two nearest-neighbor orbitals in the case of no phonons. The atomic displacement for the phonon mode with the wave vector \( \mathbf{q} \) and the frequency \( \omega_q \) is given by

\[ \mathbf{A}(t) = \mathbf{R}_i \mathbf{e}^{i \omega_q t} + \mathbf{e}^{i \omega_q t} \mathbf{R}_i^\dagger \mathbf{e}^{i \omega_q t} \mathbf{R}_i^\dagger , \]

where \( \mathbf{e}^{i \omega_q t} \mathbf{R}_i^\dagger \mathbf{e}^{i \omega_q t} \) is the phonon eigenvector. We assume that the amplitude is \( A_q = 0.5 \left( \frac{\hbar (2n_q + 1)}{2M \omega_q} \right)^{1/2} \). Here, \( M \) is the mass of carbon atom, and \( n_q \) is the phonon occupation number defined as \( (e^{\hbar \omega_q / k T} - 1)^{-1} \). The time-dependent diffusion coefficient is defined as

\[ D(E, \tau) = (2\tau)^{-1} \langle (\hat{x}(t) - \hat{x}(0))^2 \rangle_E , \]

where \( \hat{x}(t) \) is the electron-position operator along the tube axis in the Heisenberg representation. To compute the time-dependence of the diffusion coefficients for large systems, we develop the time-evolution operator using Chebyshev polynomials and Bessel functions. When an electron with energy \( E \) goes through a nanotube with length \( L \) for time \( \tau \), the conductance under a zero-bias limit is obtained within the Kubo-Greenwood formula using the diffusion coefficient [2, 3],

\[ G(L, E) = \frac{2e^2}{L} \text{Tr} \left[ \frac{\delta(E - \hat{H})}{L} D(E, \tau(L, E)) \right] . \]

Further, to evaluate the device properties, we calculate the cut-off frequency defined by

\[ f_c = 1/2 \pi \tau_f , \]

where \( \tau_f \) is the time in which the electron reaches the drain electrodes from the source electrode.

In this paper, we consider the longitudinal acoustic (LA) phonon and longitudinal optical (LO) phonon modes at room temperature. For the simplification, we assume that the frequency of LA phonon dispersion relation is proportional to the phonon wave number \( \mathbf{q} \), namely \( \omega_q = vq \). Here, \( v \) is the sound velocity and is set as 20 km/s. On the other hand, the LO phonon modes have the uniform energy 0.21 eV for every phonon wave number. We took the transfer energy \( \gamma_0^c \) as 2.5 eV. The time step was chosen as 0.41 fs.

3. Results and discussion

First, we calculated the conductance of (5, 5)-metallic CNTs with 1\( \mu \)m channel length in case of no phonon. We use the random-phase states as the initial wave packets [3]. Note that we do not consider the electrode-contact effects yet. The calculated conductance vs energy characteristic is shown in figure 1(b). The conductance takes quantized values corresponding to the number of one-dimensional electronic subbands. When the zone-center LA phonon modes with small phonon wave number are excited in the CNT, the intra-valley backscattering can be considered as shown by arrows (i) in figure 1(a). However, these scattering processes are prohibited reflecting the symmetry of the eigenstates of electrons and phonons. Thus, the conductance keeps the quantized values as shown in figure 1(b). It has good agreement with the result from the effective-mass theory [4]. When the wave number \( q \) becomes larger, the scattering processes change from the intra-valley scattering to the inter-valley scattering, as shown in arrows (ii) in figure 1(a). The conductance is reduced by such processes. For example, we show the effect of zone-boundary LA phonon on the conductance in figure 1(c). For the comparison, we also show the conductance in case of no phonon by the broken line. The conductance decreases around energy \( E=1 \) and 2 eV, corresponding to the scattering processes shown by arrows (ii) in figure 1(a). Then, we investigate the LO phonon effects on the conductances. It is found that the inter-valley scattering indicated by arrows (iii) in figure 1(d) is prohibited among the LO phonon
modes, although the scattering is permitted under the LA phonon modes. On the other hand, the intra-valley scattering due to LO phonons produces the conductance reduction. Figure 1(e) and 1(f) represent the calculated conductance in case that the LO phonon modes with $q=0$ and $q=0.3\pi/T$, which correspond to the processes shown by arrows (i) and (ii) in figure 1(d) respectively, are excited in the CNTs. Here, $T$ represents the length of a unit cell.

Then, we investigate the LA and LO phonon effects on the conductance of (10, 0)-semiconducting CNTs. For around zone-center LO phonon modes, the conductance keeps the quantized values, because there are no backscattering processes. However, it is found that the other phonon modes among LA and LO phonon modes decreases the conductance. We show the effects of LA phonons with $q=0.1\pi/T$ and $q=\pi/T$ on the conductances in figure 2(b) and 2(c), respectively. The conductance reduction around $E=0.6$ eV in figure 2(b) originates from the back-scattering process (i) in figure 2(a). The scattering processes (ii) decreases the conductance around $E=2$ eV. The zone-boundary LO phonon effect on the conductance is also shown in figure 2(e). The mechanism of conductance reduction is the similar to the case of zone-boundary LA phonon.

![Figure 1](image)

**Figure 1.** For the metallic (5, 5)-CNTs, possible backscattering processes by LA and LO phonons are shown by gray arrows in (a) and (d), respectively. The calculated conductances are shown in case that (b) zone-center LA phonon with a wave number $q=0.1\pi/T$, (c) zone-boundary LA phonon with $q=\pi/T$, (e) zone-center LO phonon with $q=0$ and (f) LO phonon with $q=0.3\pi/T$ are excited in the CNTs.

Finally, we investigate the contact effects on the transport properties of semiconducting (10, 0)-CNT-FETs. We evaluate the cut-off frequency, which is used by the estimation of switching speed of the devices. The on-site energies, $V(R_y)$, deformed by the contact and gate voltages are calculated self-consistently using Poisson’s equation [5]. We place a localized state at the middle position of the CNT as the initial wave packet. The Schottky barrier prevents a wave packet from diffusing. The time $\tau_\gamma$ is defined as the time in which the wave packet reaches the edge of the CNT. Table 1 shows the channel-length dependence of the cut-off frequencies when the gate voltage 0.8 V is applied to the FETs. The cut-off frequency is inverse proportional to the channel length according to the general rule. Furthermore, we investigate how the LA phonon scattering affects the cut-off frequencies. Table 2 shows the calculated cut-off frequencies with and without the LA phonon scattering under the gate voltage 1.0 V. The LA phonon decreases the cut-off frequency. However, the obtained frequency of the CNT-FET is still much higher than that of usual Si devices with same channel length.
Figure 2. For the (10, 0)-semiconducting CNTs, possible backscattering processes by LA and LO phonons are shown by gray arrows in (a) and (d), respectively. The calculated conductances are shown in case that the (b) zone-center LA, (c) zone-boundary LA, and (e) zone-boundary LO phonons are excited in the CNTs.

Table 1. Channel-length dependence of the cut-off frequency at gate voltage 0.8 V.

| Channel length [µm] | 0.5 | 1.0 | 2.0 |
|---------------------|-----|-----|-----|
| Cut-off frequency $f_T$ [GHz] | 117 | 54  | 26  |

Table 2. Effect of the LA phonon on the cut-off frequency of FET with 1µm channel length.

| τ | No phonon | LA phonon |
|---|-----------|-----------|
| $\tau_T$ [ps] | 1.768 | 2.156 |
| Cut-off frequency $f_T$ [GHz] | 90 | 74 |

4. Conclusion
We have investigated the effects of both the contact to electrodes and the phonon scattering on the transport properties of the CNT devices with micron-order channel length, using the time-dependent wave-packet approach based on the Kubo-Greenwood formula within a tight-binding approximation. For the metallic (5, 5)-CNTs, among LA phonons, zone-boundary modes decrease the conductance. On the other hand, the conductance becomes smaller by the zone-center modes among LO phonons. The reduction of conductance around the Fermi energy is dominated by LO phonon scattering. For semiconducting (10, 0)-CNTs, the conductance at the bottom of conduction band is mainly decreased by LA phonons. Under the LA phonon scattering, the obtained cut-off frequency of the CNT-FETs with 1 µm channel length is 74 GHz. This value is much higher than usual Si devices with same channel length. It indicates the possibility of application of CNTs to high-speed transistors.

References
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