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Influence of Hot Phonons on the Transport Properties of Single-Wall Carbon Nanotubes

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Single-wall carbon nanotubes (SWCNTs) are promising candidates for future electronic applications. The development of high performance nanotube devices requires a thorough investigation of their fundamental transport properties. At high applied fields, the interactions of electrons with optical phonons are the dominant scattering mechanisms in SWCNTs. Calculations of the optical mean free path ($l_{\rm op}$) in metallic SWCNTs according to the density functional theory (DFT) [1] lead to values which strongly disagree with those obtained by fitting the results of transport simulations to measured IV-characteristics [2]. Very recently, it was suggested that this disagreement is due to a nonequilibrium behavior of the optical phonons [3].

In order to quantify the hot-phonon effect in metallic SWCNTs, we perform simulations of the electron transport by taking into account the full dynamics of optical Γ- and K-phonons. The considered kinetic model is based on the coupled set of semiclassical Boltzmann transport equations (BTEs)

$$\left[\partial_t \pm v_f \partial_z \mp eEv_F \partial_\varepsilon\right] f_{R/L} = \mathcal{C}_{R/L}, \qquad (1)$$

$$\left[\partial_t + \frac{\partial \omega_{\Gamma/\rm K}}{\partial q}\partial_z\right] g_{\Gamma/\rm K} = \mathcal{D}_{\Gamma/\rm K} \qquad (2)$$

for electrons and phonons. Linearly dispersive electrons which move right (R) and left (L) with the Fermi velocity v_F are characterized by the distribution functions $f_{R/L}(z,\varepsilon,t)$ depending on position z, energy ε and time t. The distribution functions $g_{\Gamma/\rm K}(z,q,t)$ describe optical Γ-phonons and zone-boundary phonons with wave vector q and energy $\hbar\omega_{\Gamma/\rm K}$. The electron and phonon BTEs (1) and (2) are coupled by the collision terms $\mathcal{C}_{R/L}$ and $\mathcal{D}_{\Gamma/\rm K}$ which model backscattering processes of electrons via phonon absorptions and emissions.

A new deterministic numerical method is applied to solve the kinetic equations (1) and (2). This method is based on fixed uniform discretizations of the phase-space variables z, ε and q. The numerical grid is constructed so that the collision operators can be evaluated exactly at the grid points. A high-order conservative finite-difference scheme [4] is used to approximate the derivatives of the distribution functions with respect to the phase-space variables. The time integration of the discretized kinetic equations is performed with the help of total variation diminishing Runge-Kutta type schemes. The developed numerical method provides highly accurate results for the distribution functions without statistical noise (see Figs. 1-3). This is the main advantage over the usually applied Monte Carlo techniques.

The transport simulations performed for metallic SWCNTs with several lengths and diameters clearly show that the Γ- and K-phonons are driven far from equilibrium (see Figs. 1 and 3). We observe that these hot phonons have major influence on the electron transport. Comparisons of experimental data with results obtained by using DFT-values for the electron-phonon coupling strength exhibit very good agreement (see Fig. 4).

ACKNOWLEDGMENT

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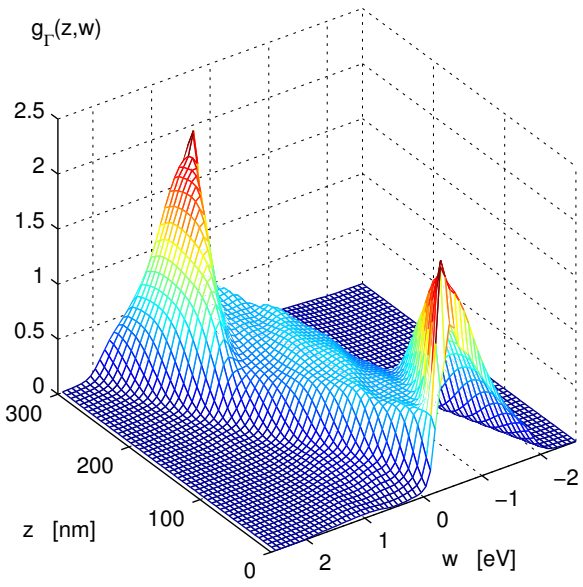

Fig. 1. Steady-state results for a 300 nm long SWCNT at 1 V bias: distribution of Γ-phonons as a function of position z and energy $w = \hbar v_F q$.

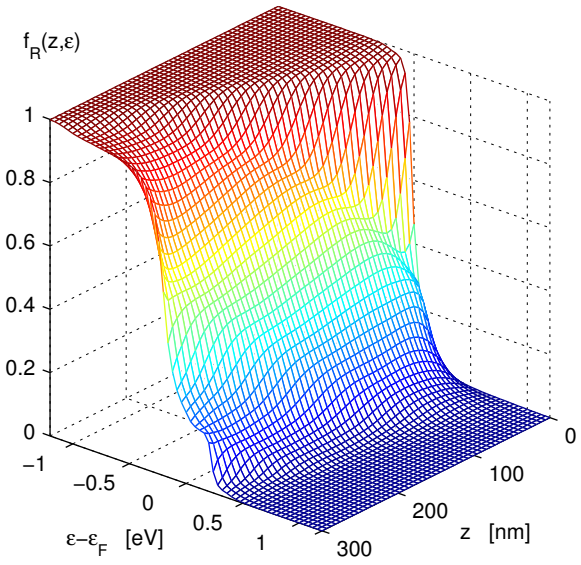

Fig. 3. Steady-state results for a 300 nm long SWCNT at 1 V bias: distribution of right moving electrons as a function of position z and energy ε.

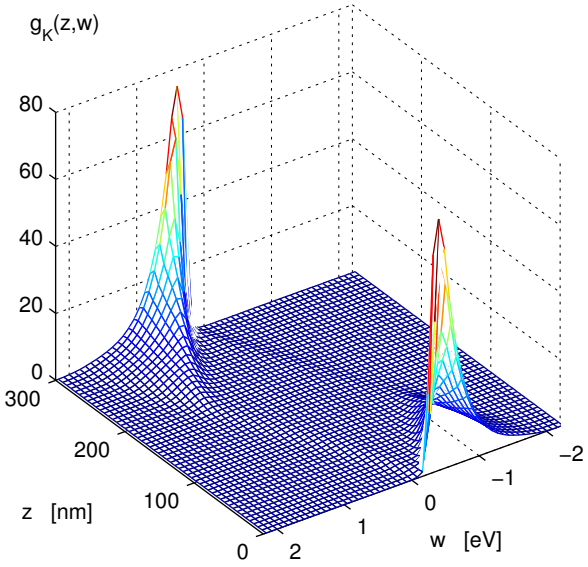

Fig. 2. Steady-state results for a 300 nm long SWCNT at 1 V bias: distribution of K-phonons as a function of position z and energy $w = \hbar v_F q$.

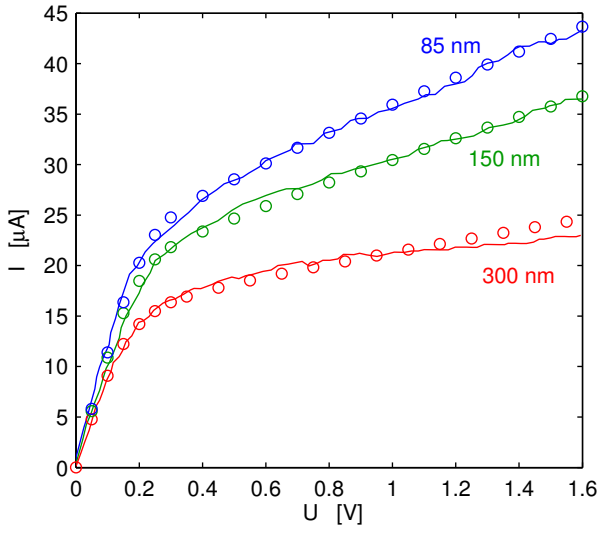

Fig. 4. Current-voltage (I-U) characteristics of SWCNTs with different lengths: solid lines refer to experimental data [2] and markers represent results of our transport simulations.