Carbon Nanotube Based Transistors: A Computational Study

M. Pourfath, H. Kosina, and S. Selberherr

Institute for Microelectronics, TU Wien, Gußhausstraße 27–29, 1040 Wien, Austria
{pourfath\|kosina\|selberherr}@iue.tuwien.ac.at

Abstract. In this work the non-equilibrium Green's function formalism is used to study the role of the electron-phonon interaction on carbon nanotube based transistors. Electron-phonon interaction parameters depend on the chirality and the diameter of the nanotube. The device response is studied for a wide range of electron-phonon interaction parameters. Results indicate the importance of the effect of phonon absorption on the device characteristics.

Keywords: Carbon nanotube transistors, Non equilibrium Green's function formalism, Electron-phonon interaction
PACS: 61.46.Fg, 85.35.Kt, 63.20.Kr

INTRODUCTION

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 [1]. In this work the non-equilibrium Green's function (NEGF) formalism is used to investigate the effect of the electron-phonon interaction parameters on the ballisticity of CNT based transistors. It is explained, why both ballistic and diffusive carrier transport in CNTs have been observed.

THEORY

The NEGF formalism applied to CNTs is discussed in [2]. The total self-energy is due to the coupling of the device to the source contact, drain contact, and electron-phonon interaction, $\Sigma = \Sigma_{\rm s} + \Sigma_{\rm d} + \Sigma_{\rm e-ph}$. The self-energy due to electron-phonon interaction comprises contributions of elastic and inelastic scattering mechanisms $\Sigma^{<,>}_{\rm e-ph} = \Sigma^{<,>}_{\rm el} + \Sigma^{<,>}_{\rm inel}$. Assuming local scattering ($\Sigma_{\mathbf{r},\mathbf{r}'} = 0$ for $\mathbf{r} \neq \mathbf{r}'$) the self-energies due to electron-phonon interaction for a single sub-band are given by:

$$\Sigma^{<,>}_{{\rm el},(\mathbf{r},\mathbf{r})}(E) = D_{\rm el} G^{<,>}_{\mathbf{r},\mathbf{r}}(E) \tag{1}$$

$$\begin{aligned}\Sigma^{<}_{{\rm inel},(\mathbf{r},\mathbf{r})}(E) = &\sum_{\nu} D^{\nu}_{\rm inel} \\ &\times[(n_B(\hbar\omega_\nu)+1)G^{<}_{\mathbf{r},\mathbf{r}}(E+\hbar\omega_\nu) \\ &+n_B(\hbar\omega_\nu)G^{<}_{\mathbf{r},\mathbf{r}}(E-\hbar\omega_\nu)]\end{aligned} \tag{2}$$

$$\Im m[\Sigma^{\rm R}_{{\rm e-ph},(\mathbf{r},\mathbf{r})}(E)] = \frac{1}{2i}[\Sigma^{>}_{{\rm e-ph},(\mathbf{r},\mathbf{r})} - \Sigma^{<}_{{\rm e-ph},(\mathbf{r},\mathbf{r})}] \tag{3}$$

where ν is the phonon mode. $\Sigma^{>}_{\rm inel}$ is calculated similar to (2) [2]. The first term in (3) is due to phonon emission and the second term due to phonon absorption. Assuming thermal equilibrium for phonons, their occupation number is given by the Bose-Einstein distribution function:

$$n_{\rm B}(\hbar\omega_\nu) = \frac{1}{\exp(\hbar\omega_\nu/k_{\rm B}T)-1} \tag{4}$$

THE EFFECT OF ELECTRON-PHONON INTERACTION PARAMETERS

To compare the effect of different scattering mechanisms, we define the ballisticity as the ratio of the current in the presence of electron-phonon interaction to the current in the ballistic case ($I_{\rm Sc}/I_{\rm Bl}$).

With increasing coupling coefficients (D_ν) the self-energies, (1) to (3), increase which adds dissipation to the Hamiltonian and decreases the total current. Fig. 1-a shows the ballisticity as a function of D_ν. Elastic scattering conserves the energy of carriers, but decreases the current due to elastic back-scattering. On the other hand, with inelastic scattering the energy of carriers is not conserved. Carriers acquiring enough kinetic energy can emit phonons and scatter into lower energy states.

With the increase of phonon energy (ω_ν) scattered carriers lose more kinetic energy and the probability for back-scattering decreases, such that the current is less reduced. As ω_ν decreases the phonon occupation number increases (4), as a result the contribution due to phonon absorption (the second term in (3)) increases. In this case carriers gain kinetic energy and the probability of back-scattering increases. As a consequence, the ballisticity decreases, see Fig. 1-b. For a better comparison, Fig. 1-c shows regions of ballistic and diffusive transport for inelastic scattering. These results are for a device of 50 nm length. Ballisticity is inversely proportional to the device length [3].

CP893, *Physics of Semiconductors, 28th International Conference*
edited by W. Jantsch and F. Schäffler

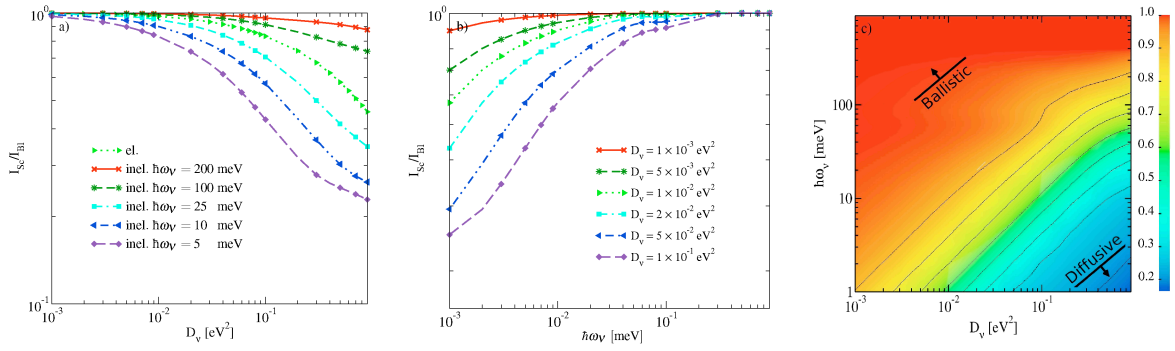

FIGURE 1. a) The ballisticity versus the strength of electron-phonon coupling for a CNT of 50 nm length. The ballisticity is defined as the ratio of the current in the presence of electron-phonon interaction to the current in the ballistic case $I_{\mathrm{Sc}}/I_{\mathrm{Bl}}$. b) The ballisticity versus the phonon energy. c) Ballisticity versus both the strength of electron-phonon coupling and phonon energy.

DISCUSSIONS

In general electron-phonon interaction parameters depend on the diameter and the chirality of the CNT. The calculation of these parameters is presented in [4]. We limit our study to semiconducting CNTs with diameters in the range of $d_{\mathrm{CNT}} = 1-2$ nm corresponding to a band gap in the range of $E_{\mathrm{g}} = 0.8-0.4$ eV, which is suitable for nanoelectronic applications.

In CNTs elastic scattering is caused by acoustic phonons (AP) and inelastic scattering by zone boundary (ZB), optical (OP), and radial breathing (RBM) phonon modes. Considering the parameter range discussed above, the energies of the these phonon modes are $\hbar\omega_{\mathrm{ZB}} \approx 160$ and 180 meV, $\hbar\omega_{\mathrm{OP}} \approx 200$ meV, and $\hbar\omega_{\mathrm{RBM}} \approx 30$ meV [5]. The corresponding coupling coefficients are $D_{\mathrm{inel}}^{\mathrm{ZB}} \approx 10^{-4}$ and 50×10^{-3} eV^2, $D_{\mathrm{inel}}^{\mathrm{OP}} \approx 40\times10^{-3}$ eV^2, and $D_{\mathrm{inel}}^{\mathrm{RBM}} \approx 10^{-3}$ eV^2 [6]. As discussed in the previous section high energy phonons, such as OP and ZB phonon modes, degrade the performance only weakly, whereas the RBM phonon mode can have a detrimental effect. However, due to weak electron-phonon coupling the RBM mode has a negligible effect at room temperature. The electron-phonon coupling is also weak for AP modes ($D_{\mathrm{el}}^{\mathrm{AP}} < 10^{-3}$ eV^2), which implies weak elastic backscattering of carriers. Therefore, CNT based transistors can operate close to the ballistic limit [1]. However, increasing the applied voltage increases phonon generation rate. If this rate becomes greater than the rate at which they can be thermalized, the assumption of equilibrium phonons (4) does not hold any longer [7]. For an accurate analysis coupled electron and phonon transport equations should be solved. Reference [8] has shown that, phonon occupation number can increase considerably, especially close to the contacts. The increase of phonon occupation number increases the phonon absorption rate (3). As a result, at high biases (> 0.2 V) ballisticity can reduce considerably.

CONCLUSIONS

Based on the NEGF formalism we investigated the effect of electron-phonon interaction parameters on the performance of CNT based transistors. For elastic scattering, the electron-phonon coupling strength plays an important role. For inelastic scattering not only the coupling strength, but also the phonon energy is an important factor. In CNTs either the electron-phonon coupling is weak or the phonon energies are high. Therefore, CNT based transistors have the potential to operate close to the ballistic limit. However, at high biases phonon occupation number increases above its equilibrium value. In this case, the phonon absorption rate increases, and ballisticity decreases. As a result, short CNT based transistors at low biases can operate close to the ballistic limit.

ACKNOWLEDGMENTS

This work has been partly supported by the Austrian Science Fund, contract I79-N16.

REFERENCES

1. A. Javey, J. Guo, D. Farmer, Q. Wang, E. Yenilmez, R. Gordon, M. Lundstrom, and H. Dai, *Nano Lett.* **4**, 1319–1322 (2004).
2. A. Svizhenko, and M. Anantram, *Phys.Rev.B* **72**, 085430–085440 (2005).
3. M. Lundstrom, *IEEE Electron Device Lett.* **18**, 361–363 (1997).
4. G. Mahan, *Phys.Rev.B* **68**, 125409 (2003).
5. J. Park, S. Rosenblatt, Y. Yaish, V. Sazonova, H. Ustunel, S. Braig, T. Arias, P. Brouwer, and P. McEuen, *Nano Lett.* **4**, 517–520 (2004).
6. S. Koswatta, S. Hasan, M. Lundstrom, M. Anantram, and D. Nikonov, *cond-mat/0511723* (2005).
7. M. Lazzeri, S. Piscanec, F. Mauri, A. Ferrari, and J. Robertson, *Phys.Rev.Lett.* **95**, 236802 (2005).
8. M. Lazzeri, and F. Mauri, *Phys.Rev.B* **74**, 165419 (2006).