Influence of Electron-Phonon Interactions on the Electronic Transport in Nanowire Transistors

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Abstract—Based on the nonequilibrium Green's function formalism, we study the influence of electron-phonon interactions on the electronic transport in silicon nanowire transistors as we change the channel length from 7 to 45 nm. Intravalley and intervalley phonon scattering mechanisms are taken into account in the simulation. The validity of the pure quantum ballistic transport model and the semi-classical drift-diffusion model for different channel lengths is also discussed.

Keywords-quantum transport; nonequilibrium Green's function formalism; electron-phonon interactions

I. INTRODUCTION

As the feature size of the MOSFETs enters into the nanoscale, the semi-classical approaches based on the Boltzmann transport equation to the modeling of the electronic transport are faced with difficulties arising from the quantum mechanical effects. Therefore, approaches based on more rigorous quantum transport theory such as the nonequilibrium Green's function (NEGF) formalism [1-2] become necessary. Up to now, there have been many works on the application of the NEGF formalism to the electronic transport in the semiconductor devices. Nevertheless, two-dimensional (2D) or three-dimensional (3D) NEGF simulation including the microscopic scattering mechanisms still remains a difficult problem.

Recently, we have developed a 3D simulation framework capable of handling electronic transport in nanoscale silicon devices based on the NEGF formalism within the effective mass and Hartree approximations, where we include the intravalley and intervalley phonon scattering mechanisms using the deformation potential theory and the self-consistent Born approximation [3]. After several assumptions on the electronphonon interactions that are also usually adopted in the Monte Carlo simulation, we can obtain the spatially local self-energy functions for both of the intravalley and intervalley phonon scattering mechanisms. Therefore, the quantum kinetic equations in the steady-state condition can be simplified to those reported in [4]. The obtained quantum kinetic equations are further simplified by the mode space approach suitable for the device whose cross section is relatively uniform along the transport direction. Finally, the self-consistent solution is obtained by solving the quantum kinetic equations and the

Poisson equation iteratively. Fig. 1 shows the procedure of the NEGF based quantum transport simulation.

Using this framework, we study the influence of electronphonon interactions on the electronic transport in nanowire transistors as we change the channel length from 7 to 45 nm. Using the proposed NEGF formalism that includes the phonon scattering mechanisms as a reference, we compare the drain current obtained from the pure quantum ballistic transport model and the semi-classical drift-diffusion (DD) transport model. In the DD model, the subband quantization is taken into account [5].



Figure 1. Flow chart illustrating the simulation procedure of the quantum transport.



Figure 2. Structure of the nanowire transistor ($t_{si}=5$ nm, $t_{ox}=0.8$ nm, $L_S=15$ nm, $L_D=15$ nm, and $L_G=7 \sim 45$ nm). Transport occurs along the z-direction and the spatial coordinate and the k-space coordinate are aligned. Ellipsoidal and parabolic energy band with three pairs of valley is considered.

II. SIMULATION RESULTS AND DISCUSSION

We simulate cylindrical nanowire transistors as shown in Fig. 2 with the channel lengths varying from 7 to 45 nm. In the simulation, we fix the lattice temperature to 300 K and consider five subbands per each valley, which gives fifteen subbands in total. In Fig. 3, we show the squared magnitudes and the corresponding energy levels of these fifteen wave functions at the source cross section.

The bulk scattering parameters reported in [6] are used for the six kinds of intervalley phonon scattering mechanisms, whereas the scalar deformation potential constant for the intravalley phonon scattering mechanism is calibrated to 14.6 eV to reproduce the phonon-limited low field mobility in the MOS inversion layer [7]. The calculated low field mobility in the channel of the nanowire from the NEGF formalism decreases from 670 to 614 cm²V⁻¹s⁻¹ as the gate voltage V_G is ramping up from -0.4 to 0.3 V, and we assume that the low field mobility and the saturation velocity in the DD model are equal to 614 cm²V⁻¹s⁻¹ and 1.07×10^7 cm/s, respectively.



Figure 3. Squared magnitude of the wave functions of three valleys and five modes at the source cross section.

In Fig. 4, we compare I_D -V_G characteristics of the nanowire transistor with $L_G=7$ nm obtained from the DD model and the NEGF formalism with and without the electron-phonon interactions. Regardless of the phonon scattering, the NEGF formalism predicts larger subthreshold leakage current compared with the DD model due to the tunneling current from the source to drain, which is excluded in the DD model. The subthreshold currents obtained from the three different methods become very similar when L_G>10 nm because the tunneling probability decreases exponentially as the thickness of the barrier (channel length) increases. To compare the drain current in the above threshold region, we compare on-currents (I_D when $V_G=0.3$ V and $V_D=0.5$ V) obtained from the three different models as well as their ratio as a function of the channel length in Fig. 5. When the channel length is 7 nm, the on-current obtained from NEGF method with the phonon scattering is about 75 % of its ballistic limit, whereas the DD model predicts about 57 % of the NEGF method with the phonon scattering. Therefore, the electronic transport in the nanowire transistor with $L_G=7$ nm can be thought to be close to its ballistic limit. As the channel length increases, however, the on-current obtained from the NEGF formalism in the presence

of the phonon scattering is getting close to that from the DD model, whereas the overestimation of the drain current from the NEGF method in the ballistic limit is getting larger.

In Fig. 6, we plot the average electron velocity and the electron density along the z-direction for $L_G=45$ nm. In the ballistic limit, the electron velocity and density do not change much from the entrance of the channel to the pinch-off region, whereas the electron velocity gradually increases and the electron density gradually decreases in the channel when the phonon scattering is present. In the DD model, the electron velocity is limited by the saturation velocity, and the electron density is largest in the channel. We also plot the energy spectrum of the electron density along the z-direction when $L_G=7$ and 45 nm in Fig. 7. When $L_G=7$ nm, the electrons injected from the source to channel do not have enough time to interact with phonons before they exit the channel. Therefore, the average energy loss of electrons in the channel is not significant and the electron transport can be regarded as quasiballistic. When $L_G=45$ nm, the electrons have more chance to interact with phonons, and the average energy loss of electrons in the channel is larger than in the shorter channel device. Also, we can observe that the electric field in the channel before the pinch off region is relatively small, which suggests that the electron transport in this region can be treated macroscopically.

III. CONCLUSION

In this paper, we present the 3D simulation results of the nanowire transistor obtained from the NEGF formalism with the electron-phonon interactions, and check the validity of the ballistic transport model and the semi-classical DD model. It is found that the ballistic transport model is valid only when the channel length is smaller than 10 nm, whereas the DD model may give reasonable terminal characteristics if the channel length is longer than 45 nm.

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Figure 4. Comparison of the I_D - V_G characteristics of the nanowire transistor with L_G =7 nm obtained from the NEGF formalism with and without the phonon scattering mechanisms and from the semi-classical DD model.



Figure 5. Comparison of (a) the on-currents (I_D when $V_G=0.3$ V and $V_D=0.5$ V) and (b) their ratio as a function of the gate length calculated from the NEGF formalism with and without the phonon scattering mechanisms ($I_{\text{scattering}}$ and $I_{\text{ballistie}}$) and from the DD model (I_{DD}).





Figure 6. Comparison of (a) the average electron velocity and (b) the electron density of the nanowire transistor with L_G =45 nm along the z-direction calculated from the NEGF formalism with and without the phonon scattering mechanisms and from the DD model.

Figure 7. Energy spectrum of the 1D electron density [in $(10^8 \text{ eV}^{-1}\text{m}^{-1})$] along the z-direction when the channel length is (a) 7 nm and (b) 45 nm obtained from the NEGF formalism with the phonon scattering mechanisms. The minimum subband energy level and the average energy of the electron flux are also plotted.