Development of Quantum Transport Simulation Model by Considering Phonon Scattering in Nanowire Device

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***Abstract*—In this paper, a simulation program using Non-Equilibrium Greens function formalism with electron-phonon (acoustic and optical phonon) is developed for studying carrier transport in a nanowire. The result shows that the carrier energy of the current density would be broadened and the current density would be lower after applying the scattering mechanism. The result suggests that a proper treatment for scattering mechanisms should be considered even in a small dimension nanostructure.**

Keywords: NEGF, phonon, scattering, nanowire

I. INTRODUCTION

As the progress of nanotechnology, it is important to consider the quantum transport behavior in the nanostructure. As we know, the advantage of scaling down the electronic device improves the device operation, increases transistors density on a single chip, and reduces the power consumption which results in lower average costs.

The development of the semi-classical transport model starts from Monte Carlo method with Poisson and drift-diffusion solver. However, when the dimension of the device has been pushed below 20 nm, the semiclassical Boltzman transport theory failed. The drift-diffusion equation model can not accurately describe the transport phenomenon in the device especially when the quantum tunneling process occurs. As a result, we are interested in developing a numerical simulation analysis including quantum mechanics to improve the prediction of the device behavior.

In this paper, we try to develop the non-equilibrium Green function theory including the phonon scattering effect. To examine the simulation model, we choose the surrounding gate since it is a more general device structure where the experimental results are much easier to be found and compared. We choose silicon nanowires as our simulation sample. We will examine device performance with the non-equilibrium Green's function (NEGF) [1] method by considering the electron-phonon scattering mechanism.

II. SIMULATION MODEL

At first, we use 3D Poisson and drift-duffusion solver to solve the potential and the Fermi level of the nanowire transistor. Then the 2D cross section is solved by Schrodinger solver to obtain the confined eigen states of the cross section of the nanowire. Secondly, the 1D Schrodinger equation is used to solve the wave function of different energy with the open boundary condition (OBC) along the electron transport direction of the nanowire. The optical phonon and acoustic phonon scattering are considered in the simulation. The scattering rate would be substituted back into the 1D Schrodinger equation using NEGF [1] formalism to yield a new set of wave function with phonon scattering. Then the Schrodinger equation are solved self-consistently until the scattering rate reaches the stable condition.

For the first step, Poisson and drift-diffusion equations are solved to obtain the potential profile and the Fermi energy in the device [2] Then, the 2D Schrodinger equation is used to solved the confined eigen states of the cross section of the nanowire as shown in Eqn. (1). The eigen energy along the transport direction of electron is the potential we use in the 1D NEGF solver as shown in Eqn. (2).

Secondly, we solve the 1D Schrodinger equation to find the propagating wave of different energy E_l as shown in Eqn. (2). In this paper, we use the finite difference (FD) method to solve the wavefunction and apply open bounday condition (OBC) on both ends. The propagation wave is injected from one boundary, and the boundary condition of the other end was considered as transparent for the outgoing wave.

$$\left[-\frac{\hbar^2}{2m^*}\nabla^2_{y,z} + E_c\left(x_i, y, z\right)\right]\psi_\perp\left(y,z\right) = E_{mn}\left(x_i\right)\psi_\perp\left(y,z\right) \tag{1}$$

$$\left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2} + E_{mn}\left(x\right) + \Sigma\right]\psi_l\left(x\right) = E_l\psi_l\left(x\right) \tag{2}$$

$$\Sigma = \frac{i\hbar}{2}\left(W_{in} - W_{out}\right) \tag{3}$$

The Σ term as shown in Eqn. (2). is to include the scattering rate in the Schrodinger equation. W_{in} and W_{out} as shown in Eqn. (3) represent how many electrons transit in or out to a certain state per unit volume per unit second. The Schrodinger equation with different energy E_l is calculated iteratively to get a stable solution.

In the simulation, the material of the nanowire device is Si. Therefore, we need to consider acoustic phonon scattering and

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optical phonon scattering rates. Followed by Fermi-Golden rule, the scattering rate can be shown below:

$$W_{ac}(E_l) = \sum_{n,m} \frac{n(E_l)}{A} \times \frac{2\pi k_B T D_{ac}^2}{\hbar \rho v_s^2} \times F_{nm} \times N_{1D}(E_l) \quad (4)$$

$$W_{op}(E_l) = \sum_{n,m} \frac{n(E_l)}{A} \times \frac{\pi D_{op}^2}{\rho \omega_0} \times \left[n_{\omega_0} + \frac{1}{2} \pm \frac{1}{2} \right] \times F_{nm} \times N_{1D}(E_l \mp \hbar\omega_0) \quad (5)$$

$$W_{out}(E) = W_{op}(E) + W_{ac}(E) \quad (6)$$

$\hbar\omega_0$ is the energy of the optical phonon in Si which is 0.062 eV. By the Bose Einstein distribution function, the occupation of the optical phonon n_{w_0} is 0.092 at room temperature. D is the deformation potential. The density of Si ρ = 5.36×10^3 kg/m^3. The sound velocity in Si υ_s = 5.22×10^5cm/s which is used in the calculation of the acoustic phonon scattering. A is the area of the cross section of the nanowire. $n(E) = N_{1D}(E) \times f(E) \times |\psi_l|^2 \times dE$. $f(E)$ is the Fermi Dirac distribution. D_{ac} and D_{op} are acoustic and optical deformation potential. $F_{nm} = \int\int \mid \psi_n(y,z) \mid^2 \mid \psi_m(y,z) \mid^2 dydz$ is the electron phonon wavefunction overlap integral of subbands n and m. The electron will transit from states to states according to the transition rate calculated.

III. RESULTS AND DISCUSSIONS

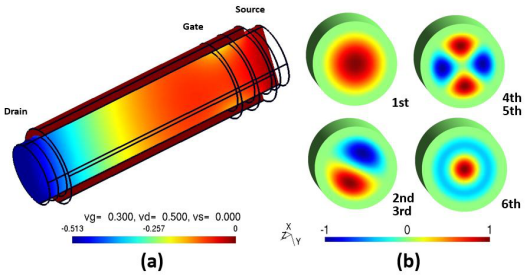


Fig. 1: (a)The potential profile of the Si nanowire along the transport direction of electrons. The radius of the channel is 16 nm and the radius including the oxide is 20 nm.(b)The eigen state wavefunction of the cross section of the nanowire which are the ground state to the sixth state

The Si nanowire is heavily n-type doped 10^{18}cm^{-3} on both sides, which is 5 nm respectively and the channel length is intrinsic which is surrounding by 120 nm oxide. We include eight subbands in our simulation. The electrons will be scattered from subband to subband by optical phonon and acoustic phonon.

Figure 2 shows that after considering optical and acoustic phonon scattering, the current density becomes lower because there are a few of electrons scattered backward by phonons.

Figure 3(a) shows that the energy distribution of the total current density that is the sum of the current density of eight

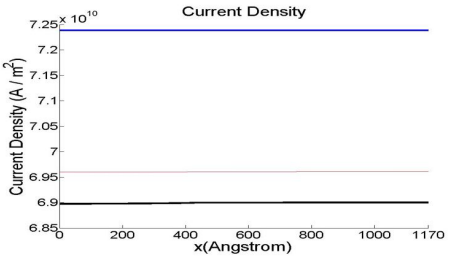
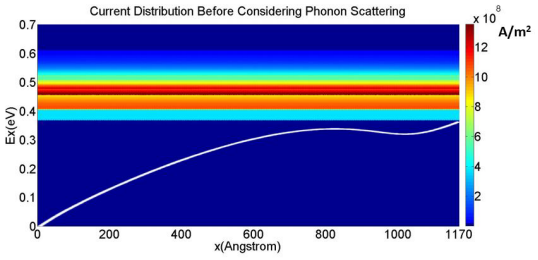
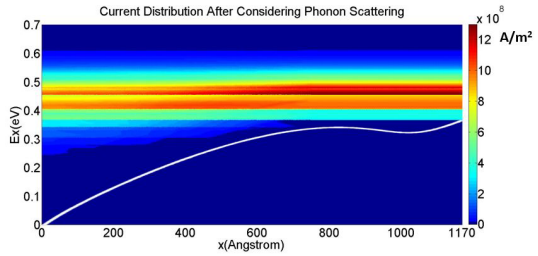


Fig. 2: The total current density of the device. The blue line is the current density without considering scattering and the black line is the current density with scatteing.



(a)



(b)

Fig. 3: The energy distribution of the current density (a) before considering the scattering rates (b) after considering the electron-phonon scattering. The white line represents the band of the ground state along the transport direction of the electron in the Si nanowire.

subbands without considering scattering effect. Compared with figure 3(b), we can observe that the energy distribution is broadened because the phonon would scatter electron to different subbands and lower energy states.

IV. ACKNOWLEDGEMENT

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