Journal of Computational Electronics 4: 35–38, 2005
© 2005 Springer Science + Business Media, Inc. *Manufactured in The Netherlands.*

Comparison of Non-Equilibrium Green's Function and Quantum-Corrected Monte Carlo Approaches in Nano MOS Simulation

HIDEAKI TSUCHIYA
Department of Electrical and Electronics Engineering, Kobe University, 1-1, Rokko-dai, Nada, Kobe 657-8501, Japan
tsuchiya@eedept.kobe-u.ac.jp

ALEXEI SVIZHENKO AND M.P. ANANTRAM
Mail Stop: 229-1, NASA Ames Research Center, Moffett Field, CA 94035-1000

MATSUTO OGAWA AND TANROKU MIYOSHI
Department of Electrical and Electronics Engineering, Kobe University, 1-1, Rokko-dai, Nada, Kobe 657-8501, Japan

Abstract. In this paper, we present a comparative study between non-equilibrium Green's function and quantum-corrected Monte Carlo approaches for an ultra-short channel MOSFET. As a result, we have found that the both models are equivalent in the simulation of quantum transport in a nano-scale MOSFET. We will also demonstrate that impurity scattering in the source region and plasmon scattering at the drain-end of the channel especially influence the drain current based on the quantum-corrected Monte Carlo approach.

Keywords: nano MOSFET, non-equilibrium Green's function, quantum-corrected Monte Carlo, scattering effects

1. Introduction

With the significant advances in lithography technology, nano-scale MOSFETs with channel length smaller than ten nanometers have been realized in several research laboratories [1]. Since the channel length becomes comparable to de Broglie wave length and scattering length, a quantum mechanical modeling of nano-scale MOSFETs involving carrier's quasi-ballistic behaviors will be indispensable. In the previous workshop (IWCE9), we have reported independently based on the non-equilibrium Green's function (NEGF) [2] and quantum-corrected Monte Carlo (QMC) [3] approaches that a detailed understanding of scattering effects is still important and crucial in determining the on-state current of ultra-short channel MOSFETs. In this paper, we present a joint study on comparison between the NEGF and QMC approaches for a nano-scale MOSFET. It is found that the both models are equivalent in the simulation of quantum transport in a nano-scale MOSFET. We will also discuss a role of impurity and plasmon scattering on drain current degradation.

2. Quantum Transport Models

The device model used in this study is a double-gate MOSFET shown in Fig. 1. The channel length, channel thickness and gate oxide thickness are 10 nm, 3 nm and 1.5 nm, respectively. The doping density in the source and drain regions are 10^{20} cm^{-3} and there is no doping inside the channel.

In the present NEGF approach, the one-dimensional non-equilibrium Green's function and the two-dimensional Poisson equations are solved self-consistently [2]. We retain only the lowest quantized



Figure 1. Schematic structure of a double-gate MOSFET used in the simulation. The channel is undoped.

subbands for the 2-fold and 4-fold valleys, to make a comparison with the QMC method. The subbands are coupled only via phonon scattering.

On the other hand, the QMC approach used in this study is based on a semi-classical MC technique with a quantum mechanical correction of potential derived by considering the lowest-order quantum correction in the Wigner transport equation [3]. The equations of motion for particles in free flight are given by

$$\frac{d\mathbf{r}}{dt} = \mathbf{v}, \quad \frac{d\mathbf{k}}{dt} = -\frac{1}{\hbar}\nabla_{\mathbf{r}}(U + U^{QC}) \tag{1}$$

where for two-dimensional problems, the quantum correction of potential is represented as [3]

$$U^{QC} = -\frac{\hbar^2}{12m_x}\frac{\partial^2 \ln(n)}{\partial x^2} - \frac{\hbar^2}{12m_y}\frac{\partial^2 \ln(n)}{\partial y^2}. \tag{2}$$

The n in Eq. (2) denotes the carrier density distribution, and m_x and m_y are the effective masses of the ellipsoidal multi-valleys of silicon conduction band. We define the quantum correction of potential for each valley by using the corresponding carrier density and effective masses, so the subband splitting due to the quantum confinement is automatically included in the present QMC approach [3,4].

So far, the NEGF and QMC approaches have been applied to simulate quantum transport of carriers in nano-scale MOSFETs, and provided a detailed understanding of scattering effects. We will demonstrate a comparison between the two quantum transport approaches in the next section.

3. Comparison Between NEGF and QMC Models

We consider only electron-phonon scattering. The parameters for the deformation potential and phonon energies in Si are taken from [5]. First, to elucidate the role of scattering, we calculate the drain current as a function of the right boundary of scattering, $Y_{\text{R-Scatt}}$, as shown in Fig. 2. Namely, scattering is included only from the edge of the source region (-20 nm) to the position of $Y_{\text{R-Scatt}}$, and otherwise electrons are ballistic. The solid line and the solid circles represent the results from the NEGF and QMC methods, respectively. The results from the classical Monte Carlo (CMC) method are also plotted in the open circles. The drain voltage is 0.6 V, while the gate voltage is adjusted so that the injection electron density at the source edge of the channel becomes identical in the three models.

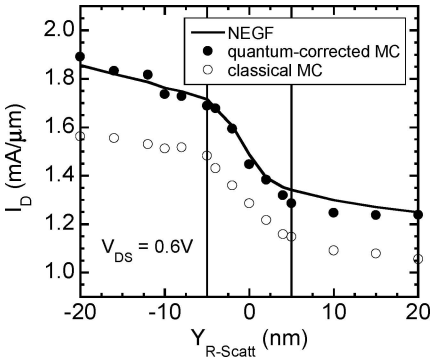


Figure 2. Drain current versus right boundary of scattering $Y_{\text{R-Scatt}}$. Channel extends from -5 nm to 5 nm. The solid line, solid circles and open circles represent the results from the NEGF, quantum-corrected MC and classical MC approaches, respectively. The drain voltage is 0.6 V. Note that only electron-phonon scattering is considered here.

As reported in ref. 2, the phonon scattering should be considered not only at the source-end of the channel but also throughout the device, because the drain-end scattering affects the electrostatic barrier height floating due to the reflected electrons [2]. Here, it should be noted that there is a good agreement between the NEGF and QMC results. The discrepancy in the drain region may be related to the accuracy in the description of hot electrons, which is presently under investigation. It is also found from Fig. 2 that the classical model underestimates the drain current. As shown in Fig. 3, the averaged electron velocity of the classical model is lower than that of the quantum-corrected model, because the classical model fails to capture the higher mobility resulting from the increase in occupancy of the 2-fold valleys, which has a smaller effective mass in the direction parallel to the oxide, as a result of energy quantization in the ultra-thin silicon channel [3,4]. Therefore, when the injection electron density is assumed to be the same, the drain current from the classical model is underestimated as found in Fig. 2. The above results

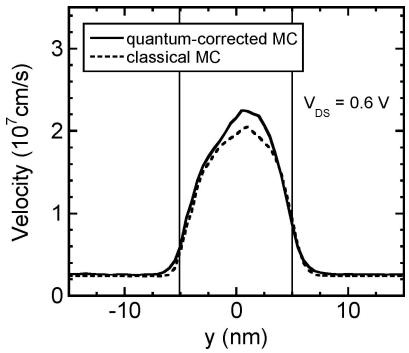


Figure 3. Comparison between quantum-corrected MC and classical MC approaches in averaged electron velocities. These results correspond to the case of $Y_{\text{R-Scatt}} = 20$ nm in Fig. 2.

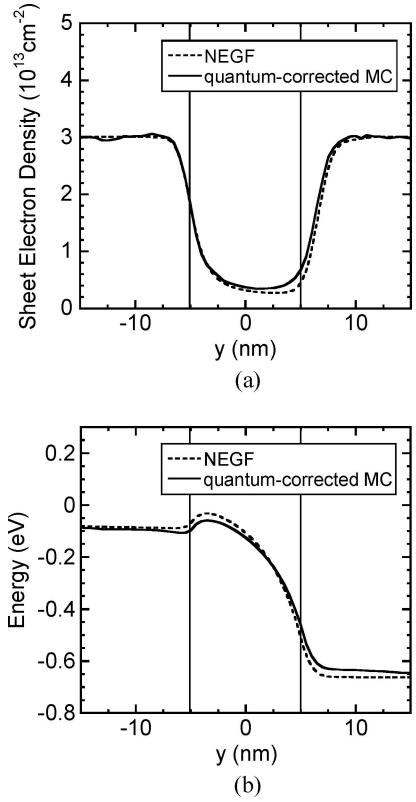


Figure 4. Comparisons of (a) sheet electron density and (b) potential profiles along the channel between NEGF and quantum-corrected MC approaches. These results correspond to the case of $Y_{\text{R-Scatt}} = 20$ nm in Fig. 2.

mean that an accurate modeling of quantized subbands in the inversion layer is important to estimate the drain current precisely, and that the quantum-corrected MC methodology will be applicable to nano MOS simulation.

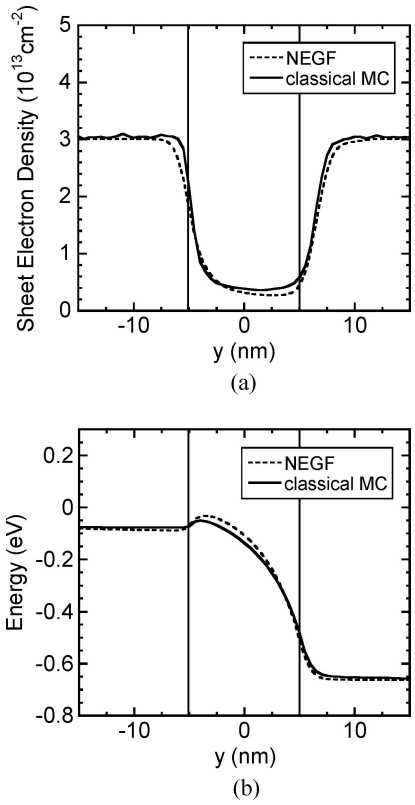


Figure 5. Comparisons of (a) sheet electron density and (b) potential profiles along the channel between NEGF and classical MC approaches. These results correspond to the case of $Y_{\text{R-Scatt}} = 20$ nm in Fig. 2.

Next, we have compared the sheet electron density and potential profiles along the channel as shown in Figs. 4 and 5, where the NEGF results are compared to QMC and CMC results in Figs. 4 and 5, respectively. The conduction band edges at the center of the channel ($x = 1.5$ nm) are plotted in Figs. 4(b) and 5(b). For the electron density profiles, a better agreement with the NEGF result is obtained with the QMC model as shown in Fig. 4(a), especially around the source edge of the channel. This is due to the fact that the potential barrier profile formed at the source-channel junction (potential bottleneck) is more accurately simulated with the QMC model as shown in Fig. 4(b). Although the barrier height in the QMC model looks smaller than that in the NEGF model, the effective barrier height from the local potential minimum at the junction is identical in both models. In the classical simulation, the electron density is the largest at the Si/SiO_2 interfaces, so the potential barrier at the channel center becomes

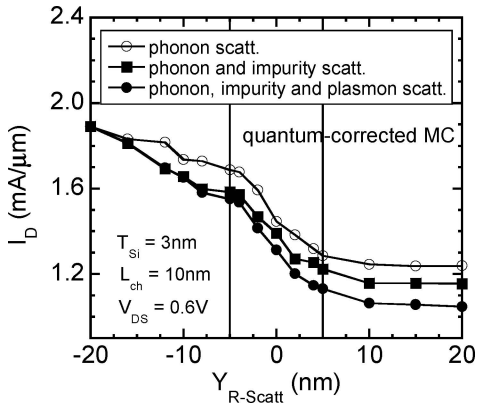


Figure 6. Role of impurity and plasmon scattering on drain current degaradation. These results are simulated by using the quantum-corrected MC method. The open circles denote the drain current with only phonon scattering, the solid squares the drain current with phonon and impurity scattering, and the solid circles the drain current with all of phonon, impurity and plasmon scattering. The drain voltage is 0.6 V.

smaller than that of the quantum simulation, as shown in Fig. 5(b). Since the carrier transport at the bottleneck point plays an important role in a ballistic MOSFET [6], the classical model will not be applicable for a ballistic transport simulation.

4. Role of Impurity and Plasmon Scattering

Finally, the role of impurity and plasmon scattering on drain current degradation is simulated based on the QMC model as shown in Fig. 6. The open circles denote the drain current with only the phonon scattering, the solid squares the drain current with the phonon and impurity scattering, and the solid circles the drain current with all of the phonon, impurity and plasmon scattering. Although the donors are doped both in the source and drain regions, a nontrivial current reduction is found to be caused by the impurity scattering in the source region. We consider that since the impurity scattering rate increases for electrons with smaller kinetic energies, the nearly thermal electrons in the source region are more likely to be scattered by the impurities. Moreover, the resultant series resistance of the source region can affect the drain current significantly, because a voltage drop in the source region corresponds to an effective change in the source-gate voltage.

On the other hand, the plasmon scattering is found to deteriorate the drain current mainly at the drain-end of the channel. This is because the plasmon scattering rate increases with electron kinetic energy, and hot electrons at the drain-end are more intensively thermalized by the plasmon emission.

5. Conclusion

We have presented a comparative study between the non-equilibrium Green's function and quantum-corrected Monte Carlo approaches for a MOSFET with ten nanometers channel length. As a result, we have found that the both approaches are equivalent in the quantum transport simulation of a nano-scale MOSFET. This result may be applicable to quantum correction models such as effective potential and Bohm potential, if the subband splitting is adequately incorporated. We have also demonstrated that the impurity scattering in the source region and the plasmon scattering at the drain-end of the channel are important to estimate the drain current.

Acknowledgment

This work is partially supported by the project of STARC and a grant-in-aid from the Ministry of Education, Culture, Sports, Science and Technology (No. 13750061).

References

1. H. Wakabayashi et al., "Sub-10-nm planar-bulk-CMOS devices using lateral junction control," *IEDM-03*, 989 (2003).
2. A. Svizhenko and M.P. Anantram, "Role of scattering in nanotransistors," *IEEE Trans. Electron Devices*, **50**(6), 1459 (2003).
3. H. Tsuchiya, M. Horino, M. Ogawa, and T. Miyoshi, "Quantum transport simulation of ultrathin and ultrashort silicon-on-insulator metal-oxide-semiconductor field-effect transistors," *Jpn. J. Appl. Phys.*, **42**(12), 7238 (2003).
4. H. Tsuchiya, M. Horino, and T. Miyoshi, "Quantum Monte Carlo device simulation of nano-scaled SOI-MOSFETs," *J. Comp. Electron.*, **2**, 91 (2003).
5. C. Jacoboni and L. Reggiani, "The Monte Carlo method for the solution of charge transport in semiconductors with applications to covalent materials," *Rev. Mod. Phys.*, **55**(3), 645 (1983).
6. K. Natori, "Scaling limit of the MOS transistor—A ballistic MOSFET-," *IEICE Trans. Electron.*, ***E*84-C**(8), 1029 (2001).