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Two-Dimensional Quantum Monte Carlo Device Simulation of Ultrasmall MOSFETs

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1. Introduction

Semiconductor device integration, typically in LSI circuits, has progressed rapidly in recent years. Device scaling is now pushing the gate length and gate oxide thickness of MOSFET's down below 0.1μm and 5nm, respectively. With the downsizing of the MOSFET's, the hot carrier and quantum mechanical effects have become more and more important. The Monte Carlo method, which is a general statistical numerical method for solving the Boltzmann equation directly, is a powerful tool for investigating electron transport in semiconductor devices. However, the Boltzmann equation as a basis for all Monte Carlo simulations is a fully classical equation though collisions are assumed as localized events in space and time and calculated quantum mechanically. So, the conventional Monte Carlo techniques have been unable to embody the carrier quantum transport effects such as tunneling and energy quantization.

In this paper, we present a newly developed quantum Monte Carlo device simulation applicable to ultrasmall semiconductor devices. In this model, the quantum effects are represented in terms of quantum mechanically corrected potential in the classical Boltzmann equation.

2. Quantum Monte Carlo Method

The quantum transport equation for the Wigner distribution function, which corresponds to a quantum mechanical distribution function, is given in the form of a modified Boltzmann equation with the infinite series of quantum corrections in potential [1]. The Wigner transport equation provides the general and powerful tool, but it is limited to one-dimensional problems in practical applications because of its computational expenses. So, we consider the lowest-order quantum correction in the Wigner transport equation, because the lowest-order term induces a major contribution in the quantum correction ingredients. Further, when the system is close to equilibrium, the following Boltzmann-like equation is finally obtained [2].

$$\frac{\partial f}{\partial t}+\frac{\hbar\mathbf{k}}{m^*}\cdot\nabla_{\mathbf{r}}f-\frac{1}{\hbar}\nabla_{\mathbf{r}}\left(U-\frac{\hbar^2}{12m^*}\nabla_{\mathbf{r}}^2\ln(n)\right)\cdot\nabla_{\mathbf{k}}f=\left(\frac{\partial f}{\partial t}\right)_C, \qquad (1)$$

where n is the carrier density and $U(\mathbf{r})$ the spatially varying potential energy. In the equation (1), the quantum effects are formulated in the form of the quantum corrected potential. Here, it is worth noting that the corrected term is identical to the quantum correction energy in the quantum moment theory [3]. Recently, we have demonstrated that the novel transport equation (1) is sufficiently applicable for nonequilibrium quantum transport analysis and multi-dimensional practical use [2]. In this paper, we will apply the ensemble Monte Carlo method to solve the quantum transport equation.

It is found from the equation (1) that the following equations of motion govern the particles in free flight.

$$\frac{d\mathbf{r}}{dt}=\frac{\hbar\mathbf{k}}{m^*} \qquad (2)$$

$$\frac{d\mathbf{k}}{dt}=-\frac{1}{\hbar}\nabla_{\mathbf{r}}\left(U-\frac{\hbar^2}{12m^*}\nabla_{\mathbf{r}}^2\ln(n)\right) \qquad (3)$$

The velocity equation (2) is the same as used in the standard Monte Carlo technique, but the force equation (3) is modified in the quantum transport so that the particles evolve under the enforcement by the classical built-in potential plus the quantum corrected potential. The quantum corrected potential serves to soften the potential variations that the particles feel at the quantum regions where the potential and the carrier density change abruptly. In the equations of motion (2) and (3), we can interpret that the $\mathbf{r}$ and $\mathbf{k}$ represent the centers of positions and momenta of traveling wave packets, respectively. This situation could be the same as the quantum mechanical treatment of scattering events in the semi-classical Monte Carlo approaches. To investigate the validity of our proposal, we first applied (2) and (3) to a single tunneling barrier. As a result, the quantum transport effects such as tunneling and quantum confinement have been successfully simulated in the standard Monte Carlo techniques.

3. Quantum Transport in Ultrasmall MOSFET's

Here, we study the two-dimensional quantum transport in ultrasmall MOSFET's by using the quantum Monte Carlo method at 300K. As a device model, the gate length is taken to be 0.1μm and the gate oxide thickness 3nm. The doping level of the source and drain regions is given as $3\times10^{18}\mathrm{cm}^{-3}$ and the p-Si substrate is assumed to be doped as $5\times10^{16}\mathrm{cm}^{-3}$. As a collisional process, the acoustic phonon scattering and the ionized impurity scattering are considered. For simplicity, hole transport is neglected in the calculation. Fig. 1 shows the computed electron distributions in the $x-y$ space at the gate voltage of 2.0V and the drain voltage of 1.0V, where (a)

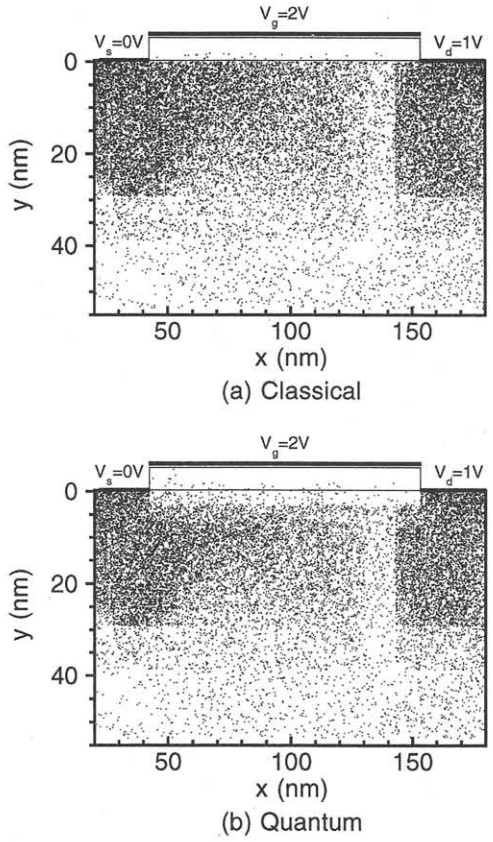

Figure 1: (a) Computed electron distributions in 0.1μm MOSFET at gate voltage of 2.0V and drain voltage of 1.0V. (a) and (b) correspond to the Monte Carlo simulations without and with the quantum corrected potential, respectively.

and (b) correspond to the Monte Carlo simulations without and with the quantum corrected potential, respectively. First of all, the classically simulated carriers are conducting from the source to drain regions just along the Si/SiO_2 interface as shown in Fig. 1 (a), while the quantum mechanically simulated ones are traveling away from the interface due to the wave nature of the inversion layer carriers as shown in Fig. 1 (b). Further, in the quantum model we can observe some tunneling particles through the oxide layer near the source side where the extremely high electric field exists. Here, we should emphasize that although the carrier transport changes from the two-dimensional (2D) behavior in the channel region to the three-dimensional (3D) one in the source and drain regions, we need not to distinguish them in the calculation if the quantum model is applied.

Finally, Fig. 2 shows (a) the drain current versus drain voltage characteristics at the gate voltage of 2.0V and (b) the gate leakage current versus gate voltage characteristics at the drain voltage of 1.0V, respectively. In Fig. 2 (a), the saturated drain current decreases for the quantum model. This is mainly because the induced charge in the channel region is smaller due to the quantum confinement effects at the same gate voltage. On the other

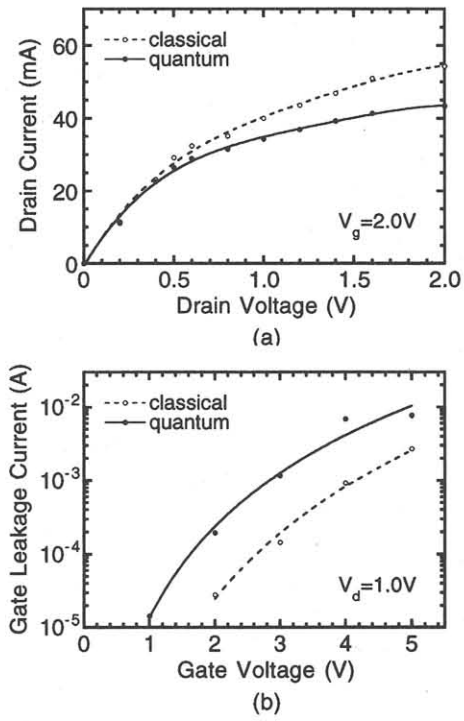

Figure 2: (a) Drain current versus drain voltage characteristics and (b) gate leakage current versus gate voltage characteristics.

hand, the gate leakage current increases in case of the quantum model because of the extra tunneling particles through the gate oxide as shown in Fig. 2 (b).

4. Conclusion

In this paper, we propose a quantum Monte Carlo device simulation applicable to ultrasmall semiconductor devices, where the quantum effects are represented in terms of quantum mechanically corrected potential in the Boltzmann equation. We have demonstrated that the quantum tunneling and quantum confinement effects of carriers can be simulated successfully in the standard Monte Carlo techniques. We believe that the proposed quantum Monte Carlo technique will provide a powerful tool in the device simulation of ultrasmall MOSFET's in ULSI circuits.

References

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