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Quantum Boltzmann equation solved by Monte Carlo method for nano-scale semiconductor devices simulation*

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A two-dimensional (2D) full band self-consistent ensemble Monte Carlo (MC) method for solving the quantum Boltzmann equation, including collision broadening and quantum potential corrections, is developed to extend the MC method to the study of nano-scale semiconductor devices with obvious quantum mechanical (QM) effects. The quantum effects both in real space and momentum space in nano-scale semiconductor devices can be simulated. The effective mobility in the inversion layer of n and p channel MOSFET is simulated and compared with experimental data to verify this method. With this method 50nm ultra thin body silicon on insulator MOSFET are simulated. Results indicate that this method can be used to simulate the 2D QM effects in semiconductor devices including tunnelling effect.

Keywords: quantum mechanical effect, Monte Carlo method, semiconductor device, carrier transport
PACC: 7115, 7280C, 6185, 7200

1. Introduction

The progress in CMOS technologies has resulted in scaling down devices to the nano-scale where quantum mechanical (QM) effects in the carrier transport become crucial for the device performance. The quantum Boltzmann equation (QBE) from the quantum kinetics equation and the Wigner distribution function can be used to describe the carriers transport including QM effects.[1,2] Compared to the semi-classical Boltzmann transport equation (BTE), quantum potential (QP) and collision broadening (CB) are two key QM effects in the QBE that describe the quantum effects in real space and K space respectively. Tsuchiya *et al* have introduced the QP correction for simulating ultra-small semiconductor devices.[3] This method has the least quantum correction to the BTE and only describes the spatially varying potential energy.[3] The CB effect in phonon–electron scattering[1,4,5] has also been investigated. However there is no work to solve the QBE with QP and CB effects at the same time for semiconductor device simulation up to now, to our knowledge.

Monte Carlo (MC) method is a powerful tool in semiconductor device research. In this paper a two-dimensional (2D) full band self-consistent ensemble MC method[6–8] for solving the QBE is developed to study the characteristics of nano-scale semiconductor devices with obviously QM effects.

Based on the QBE, CB and QP corrections are included at the same time by the MC method described in Section 2.1. The method is verified by comparing the simulation results of the effective mobility in the inversion layer of metal-oxide-semiconductor field effect transistor (MOSFET) with the experimental data. A 50nm ultrathin body (UTB) silicon on insulator (SOI) MOSFET is simulated by this method to investigate the QM effects on nano-scale MOSFET performance. The results indicate that the new developed MC method can simulate 2D quantum effect including tunnelling effect with full band structure and detailed scattering mechanism.

2. Simulation method

The MC method can solve the semi-classical

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BTE[6] without the assumption of distribution function, and has been proved a powerful tool for submicron device simulation. We developed a method to solve the QBE by the 2D full-band self-consistent ensemble MC device simulation. In this section the details of the 2D full-band self-consistent MC method for solving the QBE are described.

2.1. Quantum Boltzmann equation

From quantum kinetics equation, the QBE can be written as follows:[1−3]

$$\left[\frac{\partial}{\partial t}+\frac{\hbar k}{m^*}\nabla_r\right]G^<(k,\varepsilon;r,t) + \frac{1}{\hbar}\int\frac{\mathrm{d}^3k}{(2\pi)^3}V(r,k-k')G^<(k',\varepsilon;r,t) = \mathrm{i}\Big[\Sigma^<(k,\varepsilon;r,t)G^>(k,\varepsilon;r,t) - \Sigma^>(k,\varepsilon;r,t)G^<(k,\varepsilon;r,t)\Big]. \quad (1)$$

With the Wigner distribution function

$$f(k,r,t)=\int\frac{\mathrm{d}\varepsilon}{2\pi}[-\mathrm{i}G^<(k,\varepsilon,r,t)],$$

the QBE can be rewritten as

$$\left[\frac{\partial}{\partial t}+\frac{\hbar k}{m^*}\nabla_r\right]f(k,r,t) + \frac{1}{\hbar}\int\frac{\mathrm{d}^3k}{(2\pi)^3}V(r,k-k')f(k,r,t)=\left(\frac{\partial f}{\partial t}\right)_{\mathrm{c}}, \quad (2)$$

where

$$V(r,k-k')=\mathrm{i}\int\mathrm{d}^3u\mathrm{e}^{-\mathrm{i}(k-k')u} \times\left[U\left(r+\frac{u}{2}\right)-U\left(r-\frac{u}{2}\right)\right]$$

is the non-local potential function. In classical limit $\hbar\to 0$, it is reduced to the potential term in the BTE.

The collision term is on the right-hand side of Eq.(2):

$$\left(\frac{\partial f}{\partial t}\right)_{\mathrm{c}}=\int\mathrm{d}^3k'[W(k',k)f(k',r,t) - W(k,k')f(k,r,t)], \quad (3)$$

where

$$W(k,k')=\sum_{\eta=\pm1}|V(q)|^2\left(Nq+\frac{1}{2}+\frac{1}{2}\eta\right)K(k,k') \quad (4)$$

with

$$K(k,k')=\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}A(k,\omega+\eta\omega_q)A(k',\omega). \quad (5)$$

Equation (5) is the joint spectral function, and $A(k,\omega)$ describes the energy–momentum dispersion relation of electrons interacting with phonons. In the classical limit $\hbar\to 0$, the joint spectral function is reduced to $K(k,k')=\delta(\varepsilon-\varepsilon'\mp\hbar\omega_q)$, which is the well known Fermi golden rule.

Thus the QBE can be reduced to the BTE in the classical limit with the reduction of potential function and collision term.

2.2. 2D full band self-consistent ensemble Monte Carlo simulator

Just like the BTE, the QBE is also an integral-differential equation that is difficult to solve by the finite difference method without some kind of assumption, whereas the MC method is a statistical numerical approach to solve the BTE directly.

In order to include quantum effect in the conversional MC method, Tsuchiya *et al* introduced the QP correction and this is the lowest quantum effect of the potential term.[3−5] With the QP correction the QBE can be rewritten as[3]

$$\frac{\partial f}{\partial t}+\nu\cdot\nabla_r f-\frac{1}{\hbar}\nabla_r\left[U-\frac{\hbar^2}{12m^*}\nabla^2\ln(n)\right]\cdot\nabla_k f =\left(\frac{\partial f}{\partial t}\right)_{\mathrm{c}}, \quad (6)$$

where ν is the velocity of carrier, U is the potential solved self-consistently by the Poisson equation. Compared with the BTE, an additional potential $U_{\mathrm{q}}=-\dfrac{\hbar^2}{12m^*}\nabla^2\ln(n)$ is added to the driven term, which describes the spatially varying potential. In MC method, the QP correction gives the additional driven force during the process of carrier free flight. The QP is self-consistently calculated in every time step just like Poisson's potential.

In the QBE, the joint spectral function indicates that the CB affects both the initial state k and the final state k', and the CB is the main quantum effect due to collision. The joint spectral function can be calculated for the whole electron–phonon scattering process, just as Jauho and Reggiani[5] have done in the phonon–electron system.

For optical phonon emission scattering the joint spectral function in Eq.(4) can be written as[1,5]

$$K(x_{\rm i},x_{\rm f}) = \frac{2}{\pi\gamma^2}\left\{\int_{2x_0}^{\infty} {\rm d}x \frac{(x-x_0)^{1/2}(x-2x_0)^{\frac{1}{2}}\theta(x_{\rm i}-x_0)\theta(x_{\rm f}-x_0)}{\left[(x-x_{\rm i})^2+(x-x_0)\right]\left[(x-x_0-x_{\rm f})^2+(x-2x_0)\right]}\right.$$
$$\left. + \pi\frac{x_{\rm f}^{1/2}\theta(x_{\rm i}-x_0)\theta(x_0-x_{\rm f})\theta(x_{\rm f})}{(x_0+x_{\rm f}-x_{\rm i})^2+x_{\rm f}} + \pi^2\delta(x_0+x_{\rm f}-x_{\rm i})\theta(x_0-x_{\rm i})\theta(x_0-x_{\rm f})\right\}, \quad (7)$$

where the dimensionless energies are

$$x=\omega/\gamma^2; \quad x_{\rm i}=\varepsilon_{\rm i}/\gamma^2;$$
$$x_{\rm f}=\varepsilon_{\rm f}/\gamma^2; \quad x_0=\omega_0/\gamma^2, \quad (8)$$

where $\varepsilon_{\rm i}$ is the initial state energy, and $\varepsilon_{\rm f}$ is the final state energy, ω_0 is phonon energy, and γ^2 is the coupling strength.[1,5]

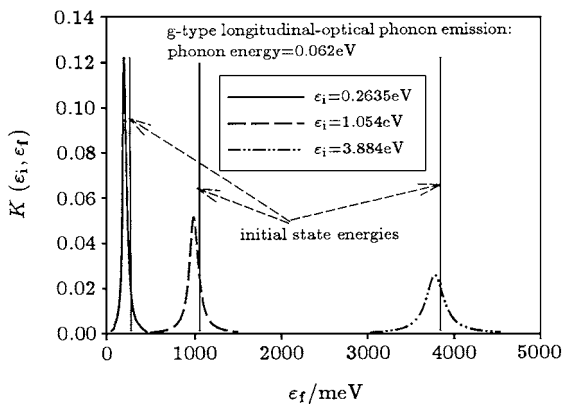


Fig.1. The joint spectral function of g-type longitudinal-optical phonon emission scattering in silicon.

Figure 1 shows the joint spectral function as a function of initial state energy for g-type longitudinal optical phonon emission scattering in silicon. Corresponding to lower initial state energy, the final state energy is distributed in a thinner region like a δ function (as Fermi's golden rule), but the final state energy distribution broadens at higher initial state energy. Thus the collision broadening effect mainly affects the transport of carriers with higher energy. In nanoscale semiconductor devices the electric field is rather strong and the carriers can obtain higher energy, thus the collision broadening effect will become obvious. The coupling strength γ^2 has scattering-type sensitivity, thus the collision broadening effect is different in different phonon scattering process. In the full band MC simulation for silicon devices, the collision broadening of f-type transversal optical phonon scattering, f-type longitudinal acoustic phonon scattering and g-type longitudinal optical phonon scattering are included. For simplicity, δ function (Fermi's golden rule) is used instead of the calculated joint spectral function when the broadening of joint spectral function is less than 1meV. Selection of the final energy after scattering occurs has to be changed according to the joint spectral function when the collision broadening effect is included. An additional random number will be used to select the final state energy according to the joint spectral function, and this function for each scattering process is calculated and stored in a table to save CPU time.

The 2D full-band self-consistent ensemble Monte Carlo method is used to solve the QBE. Both electron and hole are considered during the simulation. The band structure involves four conduction bands and three valence bands for silicon, but one conduction band for silicon oxide. Brooks–Herring model[6] is used for impurity scattering. For electron the intravalley acoustic scattering is assumed to be elastic, four intervalley acoustic scatterings and two optical scatterings are also included. The parameter of phonon scattering can be found in Ref.[6]. Impact ionization scattering, surface roughness scattering (the Si/SiO_2 interface scattering) are also included.

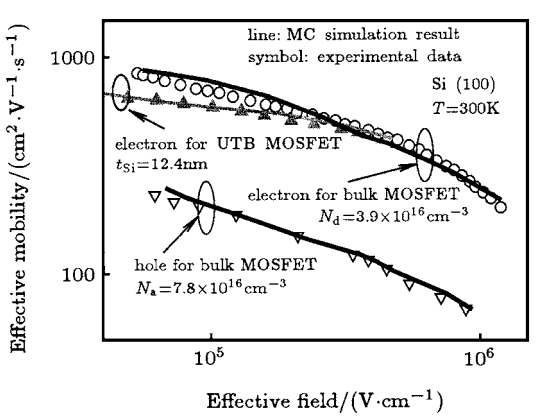


Fig.2. The effective mobility in the inversion layer of n and p channel MOSFET simulated by the new MC simulator.

The effective mobility in the inversion layer of n and p channel MOSFETs are simulated by the new

MC simulator and plotted in Fig.2. The electron effective mobility in the inversion layer of an UTB MOSFET with 12.4nm Si layer is also plotted. For comparison, the experimental data of n and p channel MOSFETs as well as the UTB MOSFET are also shown in the figure.[9,10] From the figure it can be seen that our MC simulation results match the experimental data excellently without adjusting any fitting parameters.

3. Simulated results of a 50 nm UTB MOSFET

A 50nm UTB MOSFET is simulated using the QBE based MC method introduced above. The device structure is shown in Fig.3: the gate length (L_g) is 50nm, the silicon layer thickness (t_{Si}) is 10nm, the equivalent oxide thickness (EOT) of gate oxide is 1nm, the channel doping is 10^{18}cm^{-3} of p-type Si, and the source/drain doping is 10^{20}cm^{-3} of n-type Si.

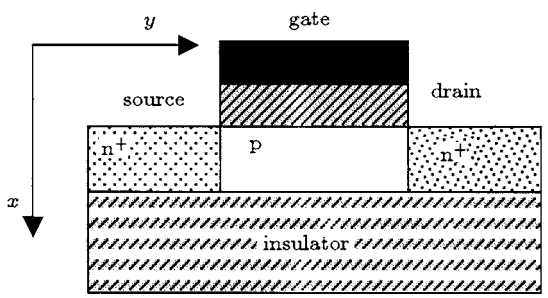


Fig.3. The structure of 50nm UTB MOSFET.

As the channel length of MOSFET devices scaling down to nano-scale region, the quantum effect along the channel direction has to be included. Figure 4 shows the inversion electron density distribution in different regions of the channel vertical to the Si/SiO_2 interface. The left figure shows the distribution in the channel 1nm from source junction, the middle of the plot displays the distribution in the middle of the channel, and the right figure exhibits the distribution in the channel 1nm from the drain junction. White symbols are the classical results solved by the BTE, and black symbols are the quantum results solved by the QBE. The results show that the peak of the electron distribution is pushed away from the interface with quantum confinement and this confinement is sensitive to the V_{ds} and the position due to the change of electric field in the channel. In order to investigate the influence of quantum effects along the channel direction, the inversion layer charge distributions along the channel with different V_{ds} are simulated.

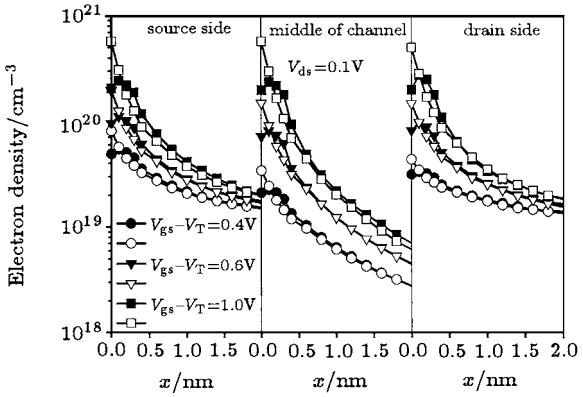


Fig.4. The quantum effect on the electron density distribution at vertical channel direction in channel area. The figures from left to right show the results for the channel 1nm from source junction, the middle of channel and that 1nm from the drain junction respectively. White symbols represent classical results, and black symbols represent quantum results.

Figure 5 plots the inversion layer charge distribution along the channel direction at $V_{gs} - V_T$=0.1V. The results indicates that the inversion charge in the channel is also pushed away from the source and drain junctions due to the QM confinement. Thus the distribution of inversion charge in the channel away from the junction increases, as compare with the classical case. The increase is more obvious in the drain side due to the stronger electric field. Our MC method based on the QBE simulates the 2D carriers transport in real space. Thus it can describe the 2D QM effects naturally.

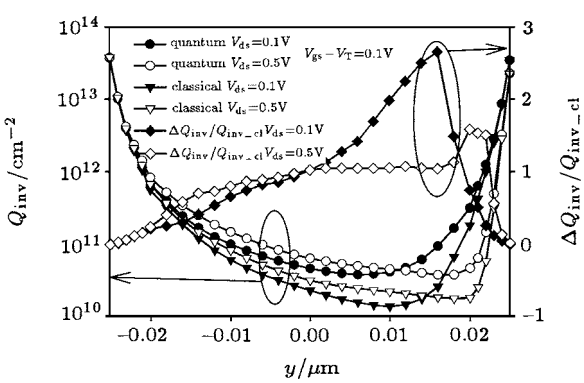


Fig.5. Quantum effect on the inversion layer charge distribution along the channel direction at $V_{gs} - V_T$=0.1V. Circles represent the quantum results, triangles the classical results, diamonds the charge increasing rate; black symbols represent results at V_{ds}=0.1V, and white symbols at V_{ds}=0.5V.

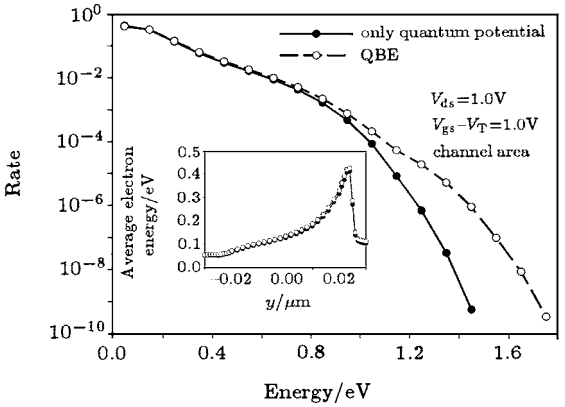


Fig.6. The electron energy distributions in the channel, at V_{gs}-V_T=1.0V and V_{ds}=1.0V. The average electron energy along the channel is plotted in the inset.

Figure 6 plots the electron energy distribution in the channel, at $V_{gs} - V_T$=1.0V and V_{ds}=1.0V, simulated with and without the CB effect. From the figure it can be seen that there are more electrons populating in the higher energy region when the CB effect is included. The inset plots the average electron energy along the channel direction. It shows that the electron average energy increases with the CB effect. Higher energy carriers can move across the potential barrier easily and have lower drift velocity due to the higher scattering probability, especially the inter-valley scattering. The particles injected into oxide in 2ps are statistical and the results are listed in Table 1. The number of particles injected into the oxide increases with the CB effect due to more high-energy particles in the channel. The phenomenon that in the case of the QP correction the number of particles injected into oxide is less than the classical case can be explained by the fact that the peak of the electron distribution is pushed away from the interface, then the amount of particles is reduced. From this result we can find that the QP correction can only involves the quantum effects in real space, yet it is not enough to simulate the nano-scale semiconductor devices in which high-energy carriers effect is important.[11] The CB effect describes the quantum effects in K-space and is important to describe the transport mechanism in devices, especially in nano region where the electric field is strong and the carriers have high energies.

Table 1. Number of particles injected into the oxide in 2ps.

$V_{gs} - V_T$=1.0V	Classical	Only Quantum potential	QBE
V_{ds}=0.6V	3	1	30
V_{ds}=0.8V	52	41	454
V_{ds}=1.0V	4098	3842	6675

4. Conclusion

A 2D full band self-consistent ensemble Monte Carlo method for solving the BE including CB and QP corrections has been developed. The CB effect describes the quantum effects in momentum space and is important for describing the transport mechanism in small devices, especially in sub-100nm region where the electric field is strong and the carriers have high energies. The simulated results of 50 nm UTB SOI MOSFET show that the QBE-based MC method can describe the 2D quantum effects in nano-scale MOSFET device.

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