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Quantum mechanical effects on heat generation in nano-scale MOSFETs*

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The Monte Carlo simulation is performed to investigate the quantum mechanical (QM) effects on heat generation in nano-scale metal oxide semiconductor field effect transistors (MOSFETs) by solving the quantum Boltzmann equation. The influence of QM effects both in real space and K space on the heat generation is investigated.

Keywords: heat generation, quantum potential, collision broadening
PACC: 7115, 7280C, 6500, 6780G

1. Introduction

Thermal effects have become one of the most important concerns of VLSI designers with the growing packing density and power consumption.[1] Heat generation in silicon devices is becoming increasingly important for its relevance to self-heating and reliability in nanoscale metal oxide semiconductor field effect transistors (MOSFETs).[2] In semiconductor devices, the carriers accelerated by electric field, gain energy and then are heated up. The carriers can be scattered to exchange energy and momentum with phonons (lattice vibrations), other carriers, impurity atoms or imperfections, and material interface. Among these scatterings, the carriers only lose net energy by scattering from phonons, and consequently heating up the lattice through the mechanism known as Joule heating.[3,4] Other scattering mechanisms mainly affect the carrier's momentum. The lattice absorbs the carrier energy and is heated to a higher temperature and in turn has impacts on the carriers transport property.

The Monte Carlo (MC) method has been used to investigate the microscopic details of Joule heating instead of the macroscopic method $J \cdot E$.[4] On the other hand, quantum mechanical effects become crucial for the device performance of the semiconductor devices scaling down to the nano-scale ones.[5,6] However, there has been no work of investigating the influence of quantum mechanical effects on heat generation, so far as we know.

The ultra thin body (UTB) silicon-on-insulator (SOI) MOSFETs device has been considered as one of the most promising candidates for nano-scale ULSI applications due to its suppressed short-channel effects,[7] nearly ideal sub-threshold swing and low junction capacitance. However, the UTB structure will suffer more severe self-heating, for the devices are separated from the substrate by poor thermal conducting layers. For example, the thermal conductivity of the oxide insulator is two orders of magnitude less than that of bulk silicon.[8] On the other hand, the quantum confinement becomes more serious in UTB MOSFETs due to the ultra thin body. In this work, the full band ensemble MC method based on solving quantum Boltzmann equation (QBE) is used to investigate the influence of quantum mechanical (QM) effects on the heat generation in 45 nm UTB MOSFET.

This paper is organized as follows. The simulation method is described in Section 2. The simulated heat generation based on QBE is compared with that by using the semi-classical Boltzmann transport equation, and the QM effects on heat generation in 45 nm UTB MOSFETs are investigated in Section 3. Section 4 is a summary.

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2. Simulation method and device structure

In this paper a 2D full band self-consistent ensemble Monte Carlo method[2,5,6] to solve QBE is used. The QBE from quantum kinetic equation and Wigner distribution function can be used to describe the carriers transport including QM effects.[9,10]

Compared to semi-classical Boltzmann transport equation (BTE), quantum potential and collision broadening are two key QM effects in QBE, which describe the quantum effects in real space and K space respectively, Eq.(2) in Ref.[5] or Eq.(1) in Ref.[11].

The quantum potential term is a non-local potential function, in classical limit $\hbar \to 0$; it reduces to the potential term in BTE. Here we use the quantum potential correction as the lowest quantum effect of the potential term introduced by Hideaki *et al.*[12] Collision broadening is the main quantum effect that affects both the initial and the final states. The joint spectral function is used to describe the energy–momentum dispersion relation of electrons interacting with phonons. In MC method, an additional random number is used to select the final states according to the joint spectral function. Then, the joint spectral function for each scattering process is calculated and stored in a table to save CPU time.[5,11] The acoustic and optical phonon scatterings, the ionized impurity scattering, intervalley scattering and the surface roughness scattering are taken into account; While the impact ionization is included as a kind of scattering. The heat generation rate is influenced by static phonon–electron scattering. Once one type of phonon–electron scattering occurs, the energy emission or absorption of that type is added to the total energy. So, the heat generation rate is equal to the total energy divided by the silicon area. Net generation rate (emission minus absorption) of different types of phonons in the UTB along the channel is plotted in Fig.1. However, the macroscopic method cannot describe any spectral information regarding the types of phonons emitted, which is important in heat transfer.[13] It can be observed that the g-type optical phonon emission is the dominant contribution to the total Joule heating.

The schematic structure of the 45 nm UTB MOSFET simulated in this paper is shown in Fig.2, the gate length (L_g) is 45 nm, the silicon layer thickness (t_{si}) is 15 nm, the equivalent oxide thickness (EOT) of the gate oxide is 1nm, the dopant in the channel is $N_A = 1.0 \times 10^{16}\,\mathrm{cm}^{-3}$, and in the source/drain region is $N_D = 1.0 \times 10^{20}\,\mathrm{cm}^{-3}$.

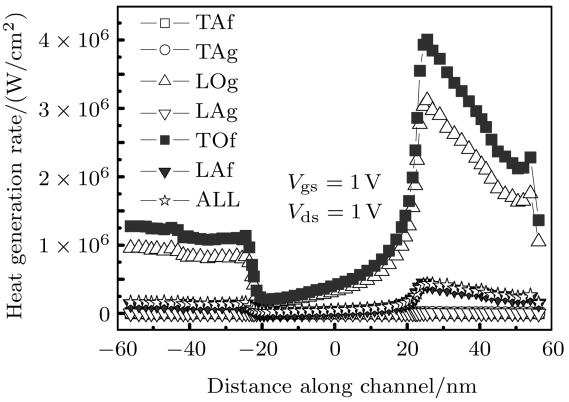


Fig.1. Net generation rate (emission minus absorption) of different types phonons in the UTB along the channel. L stands for longitudinal and T for transverse, O for optical and A for acoustic, g for g-type scattering and f for f-type scattering.

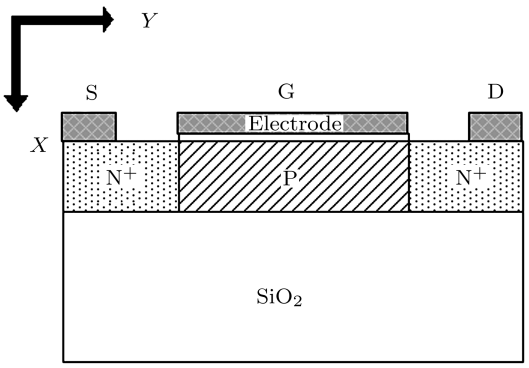


Fig.2. Schematic diagram of the 45nm UTB structure used in the simulation. The interface between the silicon and the gate dielectric is at $X = 0$, the pn junction for source and drain is at $Y = -22.5$ and $Y = 22.5$ respectively.

3. Results and discussion

The influence of the two key factors of the quantum mechanical effects on the heat generation in nanoscale UTB MOSFETs has been investigated.

Figure 3 shows the heat generation profile in the 45 nm UTB MOSFETs simulated by using the classical BTE. The difference between the classical BTE and the macroscopic method mainly appears near the drain side where the electric field is high. The hot spot region near the drain side is larger than for the

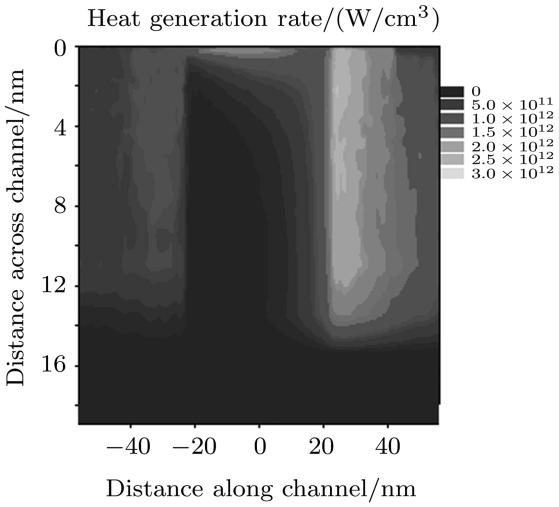


Fig.3. Heat generation profiles in the UTB obtained by semi-classical BTE solved by Monte Carlo method.

classical BTE, and even extending inside the drain region due to the electron non-local transport effect. This can be explained as follows: although electrons gain most of their energy at the location of the electric field peak, they typically travel several mean free paths.[3,4]

Figure 4 shows the heat generation profiles with QM effects. To investigate the influence of the collision broadening and quantum potential effects respectively, Fig.4(a) plots the results only including the quantum potential, and Fig.4(b) shows the results just including the collision broadening effect. As can be seen, compared to the semi-classical BTE, the quantum potential effects mainly have influence on the interface between the gate oxide and the silicon region. The hot spot region near the interface which may cause serious mobility degradation disappears when quantum potential effects are included. This can be explained by the fact that the peak of the electron distribution is pushed away from the interface due to quantum confinement, and the electron-phonon scattering decreases with the decrease of the electron density. The collision broadening effect causes more heat generation at the drain side as shown in Fig.4(b). To summarize, QM effects lead to the disappearance of hot region near the interface but increase the heat generation at the drain side, and the quantum effects

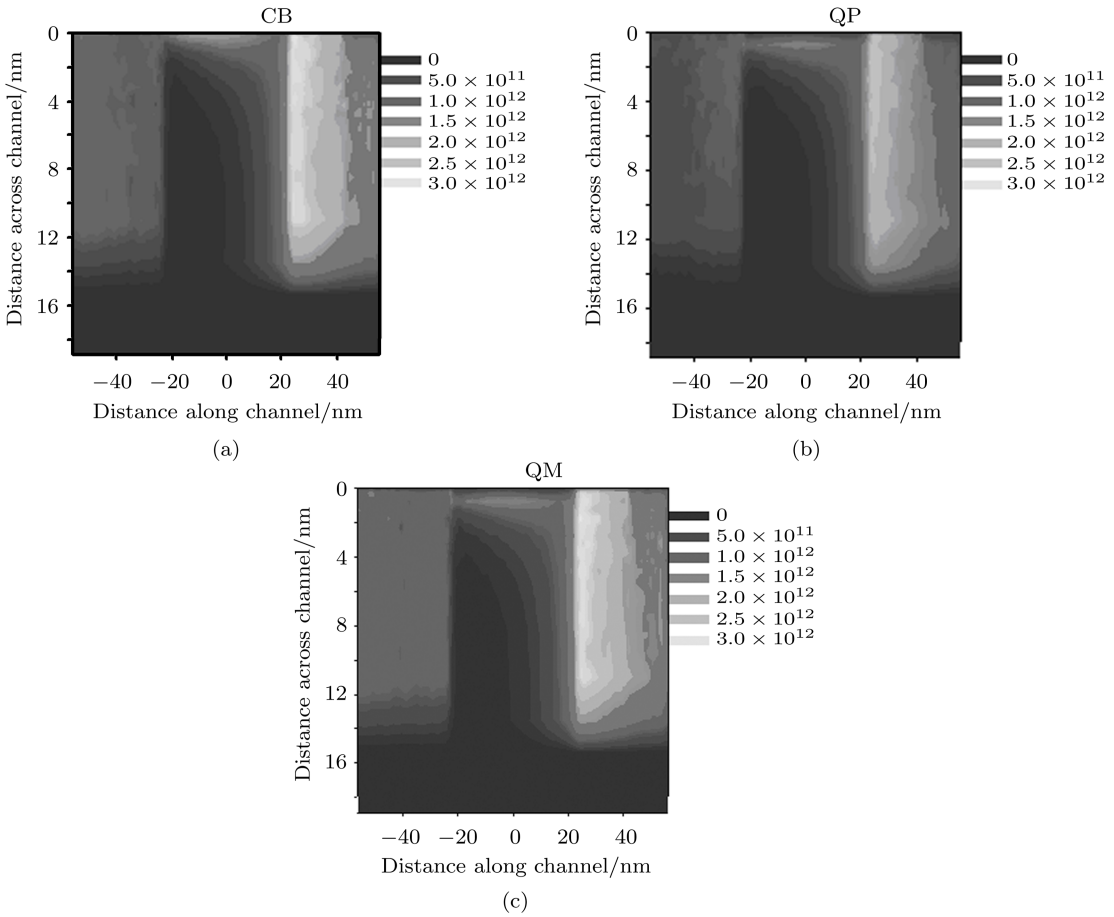


Fig.4. Heat generation profiles obtained by taking into account quantum mechanical effects (a). Collision broadening only, (b) quantum potential only (c) quantum mechanical including both collision broadening and quantum potential.

both in real space and K space should be considered at the same time during the investigation of the thermal effects in semiconductor devices. The heat generation profile vertical to the channel in the middle of the channel is plotted in Fig.5. It is obviously that the quantum potential confinement pushes the peak heat generation near the interface away from the interface and decreases the peak heat generation, while the collision broadening increases the heat generation.

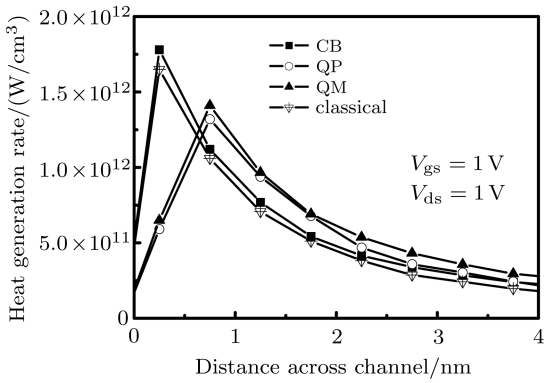


Fig.5. Heat generation in the direction vertical to the channel in the middle of it.

Figure 6 shows the heat generation along the channel integrated over the silicon body in the direction vertical to the channel. It can be observed that most of the heat is generated in the drain region by using the MC method.

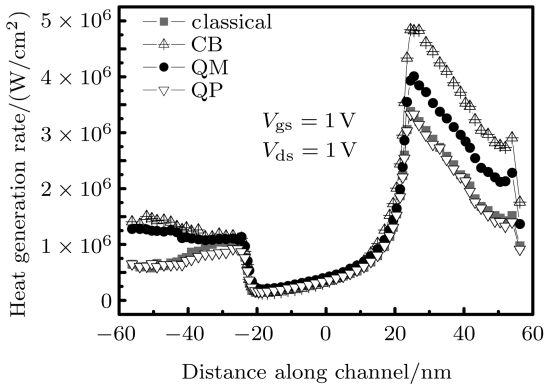


Fig.6. Heat generation profile integrated along the direction vertical to the channel.

The total heat generation obtained by integrating heat generation rate over the whole silicon region under various biases is given in Fig.7. The total heat generation increases with both gate voltage and drain voltage. The QM effects increase the total heat generation by approximately 25%.

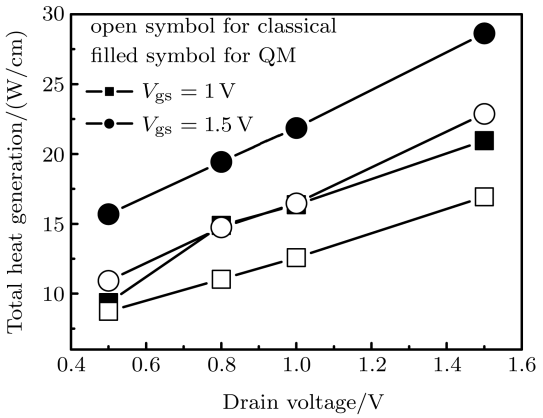


Fig.7. Total heat generation obtained under various biases, with and without QM effects.

4. Summary

The influence of the two key factors of the quantum mechanical effects on the heat generation in nanoscale UTB MOSFETs has been investigated.

The total heat generation obtained by QBE is larger than that by semi-classical Boltzmann transport equation. Quantum effects have obviously influence on the thermal effects in MOSFETs. It can lead to the incorrect distribution of the heat generation if the quantum potential is not included, while only considering the collision broadening will overestimate the total heat generation. It can be concluded that it is very important to take the QM effects into account in the accurate analysis of the nanoscale self-heating effects.

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