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Effects of quantum coupling on the performance of metal-oxide-semiconductor field transistors

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Abstract. Based on the analysis of the three-dimensional Schrödinger equation, the effects of quantum coupling between the transverse and the longitudinal components of channel electron motion on the performance of ballistic MOSFETs have been theoretically investigated by self-consistently solving the coupled Schrödinger–Poisson equations with the finite-difference method. The results show that the quantum coupling between the transverse and the longitudinal components of the electron motion can largely affect device performance. It suggests that the quantum coupling effect should be considered for the performance of a ballistic MOSFET due to the high injection velocity of the channel electron.

Keywords. Quantum coupling; metal-oxide-semiconductor field transistors.

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1. Introduction

Continuous success in downscaling MOSFETs (metal-oxide-semiconductor field transistor) has brought the gate length scaled down into sub-50 nm regime. Thus two non-classical physical mechanisms are generally recognized as playing a critical role in the determination of device characteristics: ballistic transport and quantum effects. As we know that the traditional approach to the performance of semiconductor devices is to assume the carrier scattering frequently so that the average distance between scattering is much shorter than the channel length of the device. The channel electron velocity is a critical device parameter. It can reach a value as high as 4.5×10^7 cm/s [1]. At the same time, the experimental value higher than 1×10^7 cm/s at 85 K has also been observed [2]. The drift-diffusion equations can be used to describe carrier transport when such conditions hold. According to the drift-diffusion, energy balance, and energy transport models, the calculated channel electron velocity varies from 1×10^7 cm/s to 9×10^7 cm/s [3]. However, when the channel length is much shorter than the mean-free-path of the channel electron, the scattering can be completely ignored. In such a case, the operation of a MOSFET is more like a vacuum tube than like a conventional device and the ballistic transport can be used to describe carrier transport when such conditions hold. As we know, the ballistic transport in a MOSFET can lead to a high channel electron velocity.

On the other hand, quantum mechanical effects become more and more important due to the continued success in downscaling MOSFETs. Among all methods considering the quantization in the inversion layer of a MOSFET, the most accurate one is to solve a set of coupled Schrödinger–Poisson equations subjected to an appropriate boundary condition at the interface of SiO_2 with the silicon substrate [4–6]. With the decreasing oxide thickness and the increasing substrate doping level, a very large electric field at the Si/SiO_2 interface is produced. It can give rise to a significant quantization in the inversion layer of a MOSFET, which results in the redistribution of carriers. Thus, the channel surface potential significantly increases with respect to the gate voltage even in the strong inversion regime [7]. The effects of the barrier height reduction caused by the channel electron velocity due to the effective electron mass difference between the silicon substrate and oxide on the gate leakage current in a MOSFET have been discussed in the previous work [8]. One can note that the quantization in such a potential well at the Si/SiO_2 interface with the silicon substrate will be affected by the barrier height. Thus quantum coupling effects can also affect the other performance of a ballistic MOSFET (for example, the inversion electron density).

The effective mass theory is one very powerful theoretical method for investigating the quantum feature of electrons in semiconductor heterostructures. The parabolic band effective mass approximation is successful in dealing with the quantum tunneling problems in semiconductor devices. For many studies, the components of electron motion in semiconductor devices have been assumed to be decoupled in the parabolic band effective mass approximation. The assumption is incorrect because the effective mass mismatch in the semiconductor devices will lead to a breakdown of the conservation of electron transverse kinetic energy. As we know, the ballistic transport in a MOSFET can lead to a high channel electron velocity. Thus the quantum coupling between the longitudinal and transverse components of electron motion could have a larger effect on the performance of ballistic MOSFETs due to high channel electron velocity.

2. Methods

Applying the parabolic band in the effective-mass theory, the one-dimensional Schrödinger equation for a MOSFET can be written as

$$\left(\frac{1}{2m_\perp(z)}\hat{p}_\perp^2 + \frac{1}{2m_z(z)}\hat{p}_z^2 + \phi(z)\right)\psi = E\psi, \tag{1}$$

where $\phi(z)$ represents the potential energy along z direction, $m_\perp$ and m_z denote the mass in and perpendicular to the plane of the Si/SiO_2 interface plane respectively, z is the tunneling direction which is perpendicular to the Si/SiO_2 interface, and E is the total energy of the tunneling electron, $p_\perp$ and p_z represent the electron momentum operators parallel and perpendicular to the Si/SiO$_2$ interface, respectively. Thus, the Schrödinger equation can be written as

$$\left[\frac{-\hbar^2}{2m_\perp(z)}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)-\frac{\hbar^2}{2m_z(z)}\frac{\partial^2}{\partial z^2}+\phi(z)\right]\psi=E\psi, \tag{2}$$

where $\hbar$ is the reduced Planck's constant. $\lfloor\widehat{p}_\perp,\widehat{H}\rfloor=0$ can be obtained by analysing eq. (2), which denotes that the transverse momentum of a channel electron preserves conservation in the direction perpendicular to the Si/SiO$_2$ interface.

$$\psi=\varphi(x,y)\Phi(z). \tag{3}$$

Then $\Phi(z)$ satisfies the following equation:

$$\left[-\frac{\hbar^2}{2m_z(z)}\frac{\mathrm{d}^2}{\mathrm{d}z^2}+\phi(z)\right]\Phi(z)=E_z(z)\Phi(z). \tag{4}$$

The transverse momentum of a channel electron keeps conservation in the direction perpendicular to the Si/SiO$_2$ interface. Therefore, for a MOSFET, in the substrate and the oxide regions, the Schrödinger equation along the direction perpendicular to the Si/SiO$_2$ interface can be written as

$$\left[-\frac{\hbar^2}{2m^*_{z-\mathrm{Si}}}\frac{\mathrm{d}^2}{\mathrm{d}z^2}+\phi(z)\right]\Phi(z)=E_z^{\mathrm{Si}}\Phi(z), \tag{5}$$

$$\left[-\frac{\hbar^2}{2m^*_{\mathrm{ox}}}\frac{\mathrm{d}^2}{\mathrm{d}z^2}+\left(\phi(z)-\frac{\hbar^2k_r^2}{2m^*_{\perp-\mathrm{Si}}}\left(1-\frac{m^*_{\perp-\mathrm{Si}}}{m^*_{\mathrm{ox}}}\right)\right)\right]\phi(z)=E_z^{\mathrm{Si}}\Phi(z), \tag{6}$$

where V is the applied voltage across the oxide, $m^*_{\perp-\mathrm{Si}}$ and $m^*_{z-\mathrm{Si}}$ are the effective electron masses in the substrate and gate regions. m^*_{ox} is the effective electron mass in the oxide (it is assumed to be independent of direction because the oxide is amorphous), E_z^{Si} is the longitudinal energy of channel electron. Because total energy and the transverse momentum of an electron in such a system preserve conservation, the longitudinal energy of an electron in the oxide can be obtained as

$$E_z^{\mathrm{ox}}=E-\frac{\hbar^2k_r^2}{2m^*_{\mathrm{ox}}}=\left(E_z^{\mathrm{Si}}+\frac{\hbar^2k_r^2}{2m^*_{\perp-\mathrm{Si}}}\right)-\frac{\hbar^2k_r^2}{2m^*_{\mathrm{ox}}}.$$

Thus a barrier height reduction can be found in the oxide region

$$\Delta\phi=0.5m^*_{\perp-\mathrm{Si}}v_e^2\left(1-\frac{m^*_{\perp-\mathrm{Si}}}{m^*_{\mathrm{ox}}}\right), \tag{7}$$

where v_e is the average electron velocity along the channel of a ballistic MOSFET. It is well-known that the ballistic transport in a MOSFET can result in a high channel electron velocity. It implies that the potential energy along the direction perpendicular to the Si/SiO$_2$ interface of a ballistic MOSFET will be largely affected due to the effective electron mass difference between the substrate and the oxide.

Thus the performance of a ballistic MOSFET will be affected by the quantum coupling of the longitudinal and transverse components of channel electron motion. More detail can be found in [8].

An accurate description of the electron in the inversion layer of a MOSFET required a self-consistent solution of the coupled Poisson and Schrödinger equation. In general, the one-dimensional Poisson equation along the z direction can be written as

$$\frac{\partial}{\partial z}\left[\varepsilon(z)\frac{\partial\varphi}{\partial z}\right] = -e\left[N_{\mathrm{D}}^{+}(z) - N_{\mathrm{A}}^{-}(z) + p(z) - n(z)\right], \tag{8}$$

where $\varphi(z)$ is the electrostatic potential, $\varepsilon(z)$ is the spatially dependent dielectric constant, $N_{\mathrm{D}}^{+}(z)$ and $N_{\mathrm{A}}^{-}(z)$ are the ionized donor and acceptor concentrations, respectively, and $n(z)$ and $p(z)$ are the electron and hole densities, respectively. In this work, the one dimension Poisson (eq. (8)) and the one dimension Schrödinger equation (eqs (5) and (6)) have been self-consistently solved with the finite-difference method. Starting with a trial potential, the wave functions and its corresponding eigenenergies can be calculated. Thus, the eigenenergies can be used to calculate the electron density distribution in the silicon substrate. The calculated electron density distribution and the given acceptor–donor concentration can be used to calculate the potential via eq. (8). The subsequent iteration can result in the final self-consistent solution.

The capacitance of a MOSFET generally consists of three components in series connection: the per unit area gate oxide capacitance ($C_{\mathrm{ox}} = \varepsilon_{\mathrm{ox}}/t_{\mathrm{ox}}$), depleted poly-gate capacitance (C_{GD}), and surface capacitance (C_{SB}). The total capacitance C is thus given by

$$C = \left(\frac{1}{C_{\mathrm{ox}}} + \frac{1}{C_{\mathrm{GD}}} + \frac{1}{C_{\mathrm{SB}}}\right)^{-1}. \tag{9}$$

Quantum mechanical effects and polydepletion delay the information of the inversion layer with respect to the applied gate bias. Obviously, quantum coupling will lead to a reduction in the barrier height, then the quantization in the inversion layer will be affected and lead to a redistribution of inversion channel electrons. These mean that the device characteristics such as threshold voltage and gate capacitance will also be affected by the quantum coupling between the transverse and the longitudinal components of channel electron motion.

3. Results and discussion

In this work, the coupled Schrödinger–Poisson equations from the gate/SiO_2 interface with the silicon substrate in a ballistic poly-Si gate MOSFET with the acceptor density in Si substrate of 3.0×10^{17} cm^{-3} have been numerically solved using the finite-difference method after the quantum coupling between the longitudinal and transverse components of channel electron motion is considered or not. The self-consistent solutions have been performed on the prolonged cylinders along z direction (from the gate/SiO_2 interface to the Si substrate with the thickness of

200 nm) The conduction band offset between Si and SiO_2 and the barrier height at the gate/SiO_2 interface have been chosen as 2.9 and 3.1 eV, respectively. The transverse mass $0.19m_0$, the longitudinal mass $0.98m_0$ of electron in silicon, and effective electron mass $0.5m_0$ in SiO_2 have been used in the calculations. The convergence criterion for the potential is 1×10^{-5} eV, and z-grid is 0.5 Å in the calculations. The oxide thickness has been assumed to be 2.5 nm in this work.

Figure 1 depicts the potential well in the silicon substrate, the eigenvalues together with the wave functions obtained by self-consistently solving the coupled Schrödinger–Poisson equations using the finite-difference method by neglecting the quantum coupling (a), when the channel electron velocity of a ballistic MOSFET is 5.0×10^7 cm/s (b) and 1.0×10^8 cm/s (c). The gate voltage used in the calculations is 1.0 V. One can easily find that the minimum of the potential well will increase after considering the quantum coupling between the longitudinal and transverse components of channel electron motion. Such a phenomenon implies that the surface potential will decrease with the increase in channel electron velocity when the quantum coupling between the longitudinal and transverse components of channel electron motion has been considered. The details of the effects of quantum coupling on the surface potential and the gate leakage current have been reported in [9,10].

Table 1 shows the three initial energy eigenvalues after neglecting quantum coupling and after considering quantum coupling with different channel electron velocities for a ballistic MOSFET obtained by self-consistently solving the coupled Schrödinger–Poisson equations using the finite-difference method. The gate voltage used in the calculations is 1.0 V. The energy is referenced to the Fermi energy in the silicon substrate that is set to zero. From table 1, one can find that a high channel electron velocity will have a large effect on the quantization in the inversion layer of a MOSFET. The energy level will shift to higher energy when the channel electron velocity increases. As we know, the electron concentration can be obtained via the following equation:

$$n(z) = \sum_i \frac{m^* kT}{\pi \hbar^2} \ln\left\{1 + \exp\left(\frac{E_\mathrm{f} - E_i}{kT}\right)\right\} |\psi_i(z)|^2, \tag{10}$$

where k is the Boltzmann's constant, T is the absolute temperature, E_f is the energy of Fermi level, E_i and ψ_i are the energy and the wave function of the i subbands. The sum is in i over all subband. According to eq. (10), one can easily draw a conclusion that the electron concentration will decrease when the energy level of the subband shift to high energy. The above discussion implies that the concentration of channel electrons will decrease after the quantum coupling between the longitudinal and transverse components of the channel electron motion has been considered.

Figure 2 depicts the capacitance–voltage curves of a ballistic MOSFET under inversion bias when the coupling between the longitudinal and transverse components of channel electron motion is considered or when not considered. The injection velocity of the channel electron used in the calculations is 5.0×10^7 cm/s, 8.0×10^7 cm/s, and 1.0×10^7 cm/s, respectively. It can be clearly seen in figure 2 that the quantum coupling will have a large effect on the capacitance–voltage curve of a ballistic MOSFET, and the capacitance–voltage curve shifts to higher voltage with increased injection velocity.

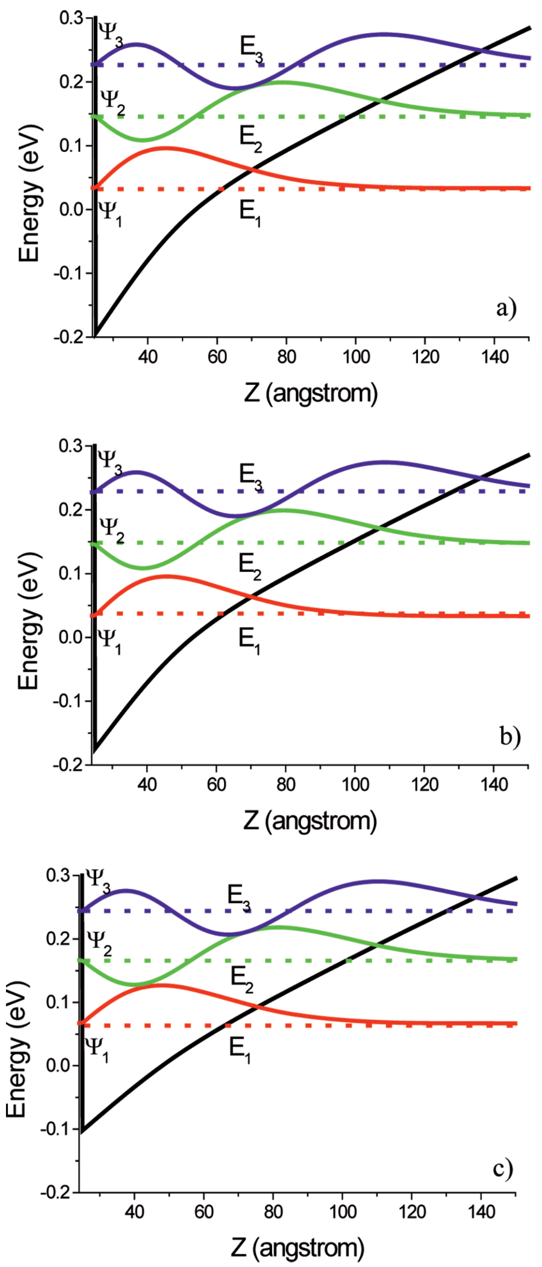

Figure 1. Calculated potential energy, wave function, and energy eigenvalues of a ballistic MOSFET with the acceptor density in Si substrate of 3.0×10^{17} cm^{-3} and the gate voltage of 1.0 V for neglecting quantum coupling (**a**) and considering quantum coupling for the channel electron velocity of 5.0×10^7 cm/s (**b**) and 1.0×10^8 cm/s (**c**).

Table 1. Energy eigenvalues in the inversion layer of a ballistic MOSFET with the acceptor density in Si substrate of 3.0×10^{17} cm^{-3} and the gate voltage of 1.0 V for different injection velocities of the channel electron.

Injection velocity (cm/s)	E_1 (eV)	E_2 (eV)	E_3 (eV)
1.0×10^6	3.2131E-2	1.4545E-1	2.2652E-1
1.0×10^7	3.2335E-2	1.4556E-1	2.2660E-1
2.0×10^7	3.2958E-2	1.4588E-1	2.2686E-1
3.0×10^7	3.4022E-2	1.4643E-1	2.2731E-1
4.0×10^7	3.5564E-2	1.4726E-1	2.2798E-1
5.0×10^7	3.7386E-2	1.4826E-1	2.2881E-1
6.0×10^7	4.0369E-2	1.4998E-1	2.3024E-1
7.0×10^7	4.3879E-2	1.5210E-1	2.3205E-1
8.0×10^7	4.8981E-2	1.5539E-1	2.3489E-1
9.0×10^7	5.4403E-2	1.5912E-1	2.3818E-1
1.0×10^8	6.3388E-2	1.6578E-1	2.4417E-1
Neglecting coupling	3.2129E-2	1.4545E-1	2.2652E-1

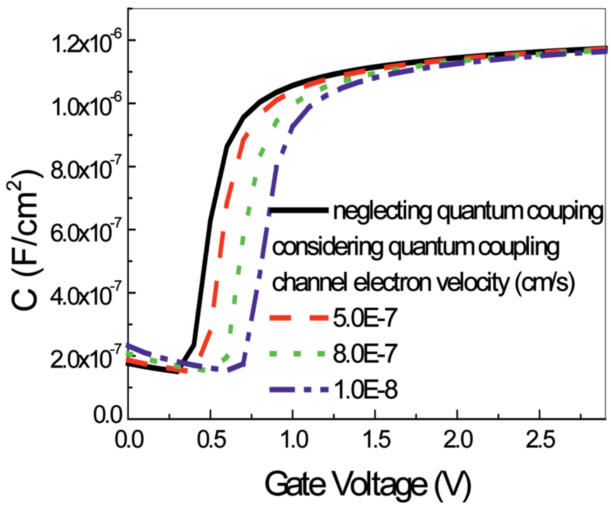

Figure 2. Calculated capacitance of a ballistic MOSFET with the acceptor density in Si substrate of 3.0×10^{17} cm^{-3} under inversion bias by considering the coupling and by not considering the coupling when the injection velocity of the channel electron is 5.0×10^7 cm/s, 8.0×10^8 cm/s and 1.0×10^6 m/s, respectively, as a function of voltage.

All these results imply that the coupling effect can be neglected for a conventional MOSFET but needs to be considered for a ballistic MOSFET where the ballistic transport ensures the electron velocity higher than the thermal injection velocity that varies from 1.2×10^7 cm/s to 2×10^7 cm/s.

4. Conclusion

The effects of the quantum coupling between the longitudinal and transverse components of channel electron motion on the performance of ballistic MOSFET have been theoretically investigated via the self-consistent solution to the coupled Schrödinger–Poisson equations. One can find that the quantum coupling effect is obvious when the ballistic transport ensures the velocity higher than 1×10^7 cm/s. With increasing channel electron velocity, the energy levels of all subbands shift to high energy and the capacitance–voltage shifts to higher voltage. This suggests that the concentration of channel electrons will decrease with the increase in channel electron velocity. The results also demonstrate that the capacitance–voltage will be affected by the quantum coupling for a ballistic MOSFET, which also means the threshold voltage will be affected by the quantum coupling. In all, the quantum coupling between the longitudinal and transverse components of channel electron motion can apparently affect the performance of a ballistic MOSFET that ensures a high channel electron injection velocity.

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