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Quantitative Evaluation of Quantum Mechanical Influence on Flat-Band Capacitance of Poly-Si/SiO₂/Si Substrate System and the Impact of Oxide Charge Density

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1. Introduction

The electron density near the Si/SiO₂ interface significantly decreases due to quantum mechanical effects [1,2]. This dark space near the SiO₂/Si substrate interface influences the characteristics of modern MOSFETs that use ultra thin SiO₂ films [3,4]. The dark space also influences the surface properties even in or close to the flat-band (FB) condition [2]. Therefore, it is anticipated that the semi-classically defined FB capacitance significantly differs from that derived using the quantum mechanical (QM) consideration [5,6].

In this paper, in the vicinity of the FB bias condition, an analytical probability density function of electrons near the Si/SiO₂ interface is derived theoretically on the basis of a tunneling probability formulation. The analytical expression of electron density is used to calculate the FB capacitances at both the poly-Si/SiO₂ and SiO₂/Si substrate interfaces. Finally, it is shown how the inherent error in the oxide charge evaluation becomes significant for actual devices.

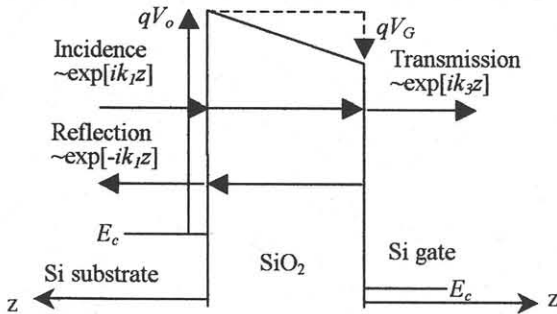


Fig. 1. A band diagram and wave function model for the theoretical formulation of electron probability density function.

2. Calculation of the electron density profile with QM effects

In calculating the electron density in the presence of QM effects, we assume a MOSFET with a band structure across the gate oxide (barrier height = qV_o), as shown in Fig. 1. The energy is measured from the conduction band bottom of the Si substrate. Fundamental definitions of incident, reflecting and transmitting electron waves are also described in the figure [7]. The applied surface potential is smaller than the thermal voltage ($k_B T/q$), where k_B is Boltzmann's constant. The bent barrier, bent due to V_G , is replaced with a flat barrier having a height of $qV_o - qV_G/2$ in order to simplify the theoretical formulation [8]. The probability density of electrons near the Si/SiO₂ interface can be expressed approximately as

$$f_{qm}(E_z, |z|, m^*) = 1 - \cos\left\{\frac{4\pi}{h}(2m^*E_z)^{1/2}|z|\right\} + 2\left(\frac{m_{ox}^*E_z}{m^*qV_o}\right)^{1/2} \sin\left\{\frac{4\pi}{h}(2m^*E_z)^{1/2}|z|\right\} \quad (1)$$

where E_z is the electron energy in the z -direction, m_{ox}^* is the electron effective mass inside the SiO₂ film. The probability density function of electrons is, for (001) Si, given by

$$f_{(001)} = \frac{1}{3} f_{qm}(E_z, |z|, m_l^*) + \frac{2}{3} f_{qm}(E_z, |z|, m_t^*) \quad (2)$$

where m_l^* and m_t^* are the longitudinal and transverse effective masses, respectively. Integration of the product of the density of states ($D(E)$), the Fermi-Dirac function ($f_{FD}(E)$) and $f_{(001)}$ over the possible energy range yields the electron density function ($n_{(001)}(z)$). Since $f_{FD}(E)$ can be replaced approximately with the Boltzmann distribution function at room temperature for the non-degenerate silicon, $n_{(001)}(z)$ is given by

$$n_{(001)}(z) = N_c e^{E_F/k_B T} \left[1 - \frac{1}{3} \left\{ 1 - 2 \left(\frac{m_{ox}^* k_B T}{m_l^* q V_o} \right)^{1/2} \frac{|z|}{\lambda_l} \right\} \exp\left\{-\left(\frac{|z|}{\lambda_l}\right)^2\right\} - \frac{2}{3} \left\{ 1 - 2 \left(\frac{m_{ox}^* k_B T}{m_t^* q V_o} \right)^{1/2} \frac{|z|}{\lambda_t} \right\} \exp\left\{-\left(\frac{|z|}{\lambda_t}\right)^2\right\} \right] \quad (3)$$

where E is the total electron energy, N_c is the effective density of states in the conduction band, E_F is the Fermi energy. λ_l and λ_t are the de Broglie wavelengths of electrons with longitudinal and transverse effective mass, respectively. It is known that the poly-Si bottom surface often has the (111) orientation in the present system. Since poly-Si is degenerate because of high doping levels, we employ the 0K approximation to simplify the calculation. The electron density function is given by

$$n_o(z) = n_o E_F^{3/2} \left[\frac{1}{3} + \frac{\cos(z')}{z'^2} - \frac{\sin(z')}{z'^3} - 2 \left(\frac{m_{ox}^* E_F}{m_t^* q V_o} \right)^{1/2} \left\{ \frac{\sin(z')}{z'^2} + \frac{3 \cos(z')}{z'^3} - \frac{3 \sin(z')}{z'^4} \right\} \right] \quad (4)$$

where $n_o = 48 \pi (2m_e^*)^{3/2}/h^3$ and $z' = 2|z|/\lambda_F$. λ_F is the Fermi wavelength.

3. Results and discussion

Figure 2a shows the electron density profile near the Si/SiO₂ interface for the surface potential of $k_B T/q$ at 300K. It is found that the dark space in (111) Si is slightly wider than that in (001) Si because of anisotropy in the effective mass of electrons. In both cases, the dark space is about 3 nm thick. Figure 2b shows the electron density profile near the poly-Si/SiO₂ interface at the surface potential of $k_B T/q$. In this case, the dark space is about 2 nm thick.

In Fig. 3, we show the FB capacitance (C_{fb}) as a function of the substrate doping concentration (N_d) [9]. For the low doping case, there is little difference between C_{fb} values in (111) and (001) Si surfaces. The difference of C_{fb} increases with N_d because the number of depleted electrons in the dark space increases with N_d . In the similar manner, we can simulate the surface capacitance of the poly-Si (C_p) at the FB condition. The total gate capacitance (C_G) at the FB condition is given as

$$C_G = (C_p^{-1} + C_i^{-1} + C_b^{-1})^{-1} \quad (5)$$

where C_i is the SiO₂ film capacitance per unit area. According to simulation results, the value of C_p is larger than C_{fb} by a factor of

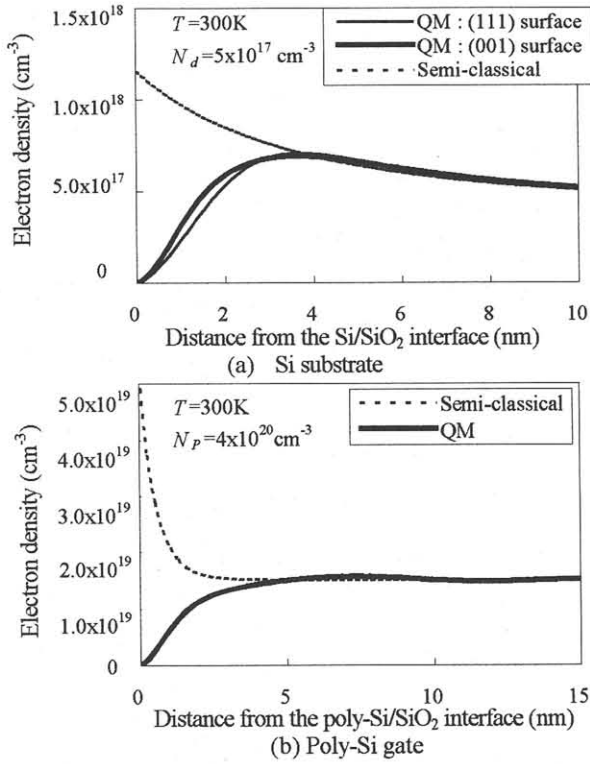


Fig. 2. Comparison of the semi-classically or quantum-mechanically simulated electron density profiles. The surface potential is equated to $k_B T/q$.

7 for N_d of $5 \times 10^{17} \text{ cm}^{-3}$. In other words, for N_d values higher than $1 \times 10^{17} \text{ cm}^{-3}$, C_P cannot be neglected in eq. (5) any longer. Figure 4a shows the normalized C_G dependences on gate SiO_2 film thickness (t_{ox}) for (111) and (001) Si surfaces. The normalized C_G decreases with t_{ox} . However, it is obvious that the difference between the values of C_G/C_i in (111) Si and (001) Si is virtually independent of t_{ox} . A similar behavior is seen in the difference between the quantum and the classical C_G/C_i values; the difference in C_G/C_i depends mainly on N_d . Figure 4b shows the normalized C_G dependence on t_{ox} for cases with and without C_P using eq. (5). Since N_d increases as the MOSFET is further miniaturized, it is anticipated that C_P will form a larger part of C_G in the future.

Finally, we show how the C_G/C_i determination affects the estimation of total oxide charge. Simulated C-V curves are partly shown in Fig. 5 for three cases: the semi-classical case, the QM case without C_P and the QM case with C_P [9]. When it is assumed that the QM case with C_P represents the real C-V curve, the semi-classical determination of C_G/C_i at the FB condition yields the error of the order of 10^{12} cm^{-2} in the oxide charge evaluation for t_{ox} of 2 nm. Therefore, the correct determination of FB capacitance is needed for accurately designing contemporary and future devices.

4. Summary

In this paper, the electron density function on the basis of tunneling wave mechanics is analytically formulated for both the non-degenerate and degenerate Si/SiO₂ systems. The FB surface capacitance in (111) Si is smaller than that in (001) Si because of anisotropy in the effective mass of electrons. It is also demonstrated that the FB surface capacitance of poly-Si will form a larger part of the total gate capacitance at the FB condition as the substrate doping concentration becomes higher.

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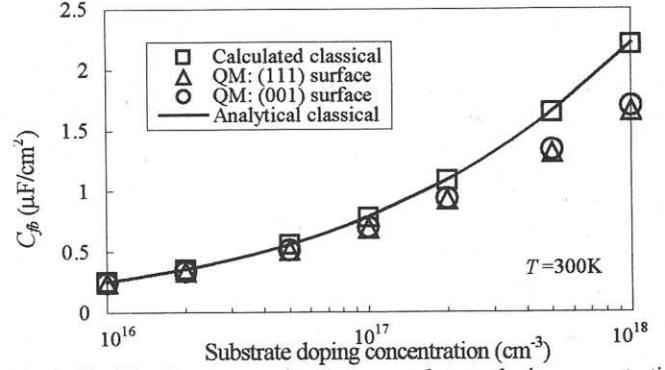


Fig. 3. The FB substrate capacitance versus substrate doping concentration.

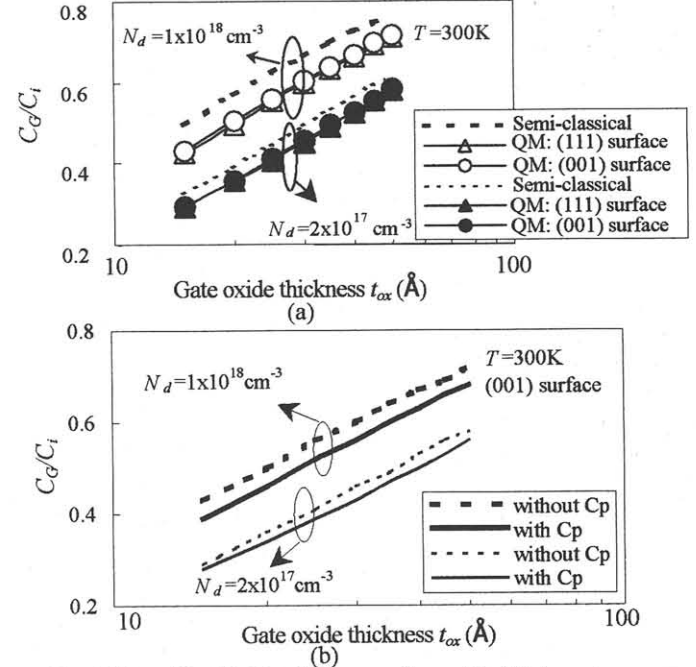


Fig. 4. Normalized flat-band gate capacitance (C_G/C_i) dependence on t_{ox} (b) with and (a) without C_P in eq. (5).

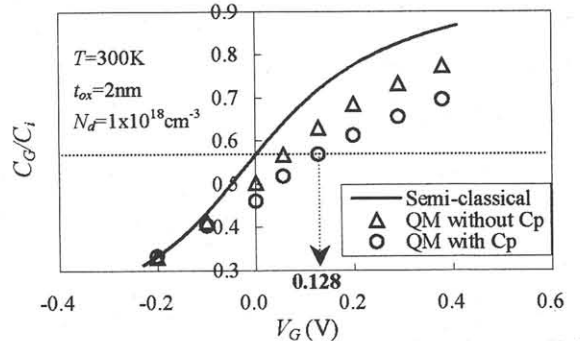


Fig. 5. Normalized gate capacitance (C_G/C_i) dependence on V_G for three cases; the semi-classical case, the QM case without C_P and the QM case with C_P .