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Threshold Voltage Modeling in (100), (110) and (111) Oriented Nanoscale MOSFET Substrates

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Abstract: An analytical model for the inversion layer quantization for nanoscale – Metal Oxide Semiconductor Field Effect Transistor (MOSFET) with different crystallographic substrate orientations, such as (100), (110) and (111) has been developed. The threshold voltage analysis has been studied using the quantum inversion charge model under three substrate orientations. The results indicate a significant impact of crystal orientation on the threshold voltage and the inversion charge density. The results have also been compared with the numerically reported results and show good agreement.

Keywords: Orientation, model, Inversion quantization, MOS device, Threshold voltage.

1 Introduction

MOSFET modeling is facing difficulties to achieve accurate description of extremely scaled down devices. The reason is that many complicated new phenomena are arising which are not easy to describe. One such phenomenon arising out of down scaling the MOSFET is the failure of classical physics at nanometer scale. As Complementary Metal Oxide Semiconductor (CMOS) technology scales down aggressively, it approaches a point, where classical physics is not sufficient to explain the behavior of a MOSFET. At this classical physics limit, quantum mechanics has to be taken into account to accurately assess the overall performance of a MOSFET. One of the major effects in the nanoscale MOSFETs is the inversion layer quantization. Accurate modeling of inversion layer quantization in the (100) substrate has received considerable attention [1]. However, very less research has taken place to study inversion layer quantization in other crystal oriented substrates. Whatever models developed so far for other orientations, are mainly numerical. The paper is organized as follows: The paper starts with an overview of the basic MOSFET models. Secondly, modeling of inversion layer quantization effect has been done by considering various crystal

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orientations. Thirdly, threshold voltage has been formulated by considering various crystal orientations and the inversion quantization effect in the substrate.

2 Mosfet Models

The charge based models include the basic Simulation Program with Integrated Circuit Emphasis (SPICE) Level 1, Level 2, Level 3, Berkeley Short Channel Insulated gate Field effect transistor model (BSIM) models and the other advanced models such as BSIM 4 and 5 [2-5]. Secondly, the potential based models include the Surface Potential (SP) model, MOS Model 11, Hiroshima Starc Insulated gate Field effect transistor model (HiSIM) model etc. [6-9] and thirdly, the conductance based models like the Enz, Krummenacher,Vittoz (EKV) model [10]. The other models which include the energy quantization effects though empirical in nature are Hansch model [11], Van Dort Model [11], Inversion charge model [12] etc. It can be concluded that attempts are being made to include inversion layer quantization in nanoscale MOSFET models in (100) crystal orientations, yet a MOSFET model largely analytical including inversion layer quantization in all the crystal orientations of the nanoscale MOSFET substrate is still to be developed.

3 Inversion Layer Quantization

As the MOSFET dimensions approach deep sub-micron and nanometer regions, the classical movement of the charge carriers is greatly affected by the non-classical behavior of electrons in the MOSFET. Due to aggressive scaling of the MOSFETs, the gate oxides are also scaled to nanometer regions. Also, the substrate doping is increased tremendously to negate the short channel effects at the deep sub-micrometer or nanometer scales. This results in very high electric fields in the silicon/silicon oxide interface and hence the potential at the interface becomes steep. This results in a potential well between the oxide field and the silicon potentials. During the inversion condition, the electrons are confined in this potential well. Due to confinement, the electron energies are quantized and hence the electrons occupy only the discrete energy levels. This results in the electrons residing in some discrete energy levels which are above the classical energy level by some fixed value of energy as shown in Fig. 1.

The inversion layer results in the lifting of the energy sub bands in different energies because the electron quantization masses are different in three orientations as shown in Fig. 1. Solving the Poisson equation in the inverted MOSFET substrate channel, we get the total charge density "Q_s" [13]:

$$Q_s = -(2qN_a e_{si} e_0)^{1/2}\left[\varphi_s + V_t\, \mathrm{e}^{-2\varphi_f/V_t}\left(\mathrm{e}^{\varphi_s/V_t} - 1\right)\right]^{1/2}, \tag{1}$$

q is electron charge, e_{si} is silicon relative permittivity, e_0 is permittivity of free space, φ_s is surface potential, φ_f is fermi potential, N_a is substrate concentration, and $V_t = kT/q$ is thermal potential. Similarly, the depletion charge Q_b is approximated as

$$Q_b = -(2e_{si} e_o q N_a \varphi_s)^{1/2}\,. \tag{2}$$

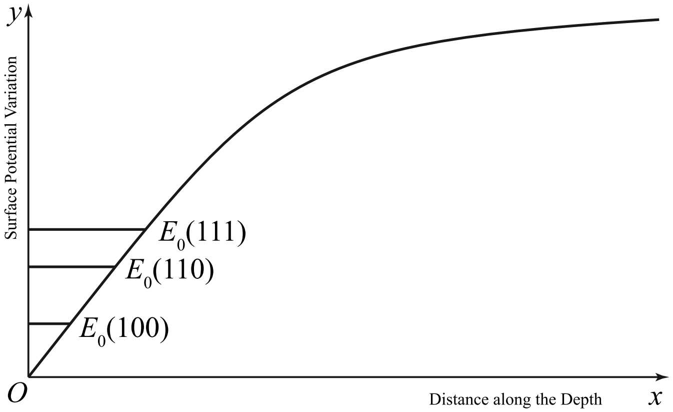

Fig. 1 – *Inversion layer quantization in the substrate for different crystal orientations.*

Therefore, the inversion charge density Q_{inv} is given by (1) and (2):

$$Q_{inv} = -\gamma C_{ox}\left\{\left[\varphi_s + \frac{kT}{q}\exp\left(\frac{q\left(\varphi_s - 2\varphi_f\right)}{kT}\right)\right]^{1/2} - (\varphi_s)^{1/2}\right\}, \tag{3}$$

$\gamma = (2qN_a e_{si} e_o)^{1/2} / C_{ox}$ is body effect parameter and C_{ox} is the unit area oxide capacitance (Fcm^{-2}). The main problem with (3) is that the surface-potential has to be evaluated explicitly in all the regions of electron inversion and then only, the (3) can be solved. An explicit solution has been evaluated in the [14].

The wave function solution of the Schrödinger's equation is given by using variation approach [1]:

$$\psi(x) = \frac{b^{3/2} x}{\sqrt{2}}\exp\left(\frac{-bx}{2}\right), \tag{4}$$

where

$$b = \left[\frac{48\pi^2 m^* q^2}{e_{si} e_0 h^2} \left(0.33 Q_{inv} + Q_{dep} \right) \right]^{1/3},$$

and m^* is effective quantization mass. After solving the Schrödinger's equation using variation approach, the corresponding shift in the sub band electron energy [1] is

$$E_o = \frac{3h^2 b^2}{8m^*}, \tag{5}$$

and shift in the surface potential

$$\text{“}\delta\varphi\text{”} = E_o / q. \tag{6}$$

The (6) is then included in the explicit surface potential expression given by [13]:

$$\varphi_s = f + a, \tag{7}$$

$$f = \varphi_f + 0.5\varphi_{swi} - 0.5\left[(\varphi_{swi} - 2\varphi_f)^2 + 0.0016 \right]^{1/2},$$

$$a = 0.025 \ln\left\{ \left[x - y \left(1 + 100 y^2 \right)^{-1/2} \right]^2 \left(0.16\,\gamma \right)^{-2} - 40 f + 1 \right\},$$

$$\varphi_{swi} = \left[\left(V_{gs} - V_{fb} + 0.25\gamma^2 \right)^{1/2} - 0.5\gamma \right]^2,$$

and φ_{swi} is the weak inversion surface potential, $x = V_{gs} - V_{fb} - f$, and $y = \varphi_{swi} - f$.

The quantum surface potential is hence given by adding the classical surface potential with the shift in the surface potential due to inversion layer quantization from (5).

$$\varphi_{sqm} = \varphi_s + \delta\varphi = 2\varphi_f + \delta\varphi. \tag{8}$$

Using the surface potential model (8) in (2) and (3), we can calculate explicitly inversion charge density and depletion charge density. The shift in the surface potential due to inversion layer quantization in the substrate can hence be calculated from (6). Using (6-8), the quantum depletion charge density (2) and inversion charge density (3) can be evaluated for quantum mechanical case.

The results in Fig. 2 match quite closely with the reference 1 (BSIM 5 results) [15] and reference 2 results [16]. The results show that the inversion layer quantization leads to reduced inversion charge densities in the substrate. The situation further worsens as the substrate orientation changes from (100) to (110) and (111). The inversion layer charge density further reduce in these orientations.

Table 1
Variation of effective electron quantization mass with crystal orientation in silicon substrate [1].

Substrate crystal orientation	Effective quantization transverse mass (m^*) and m_o= electron free mass
<100>	$0.916m_o$
<110>	$0.315m_o$
<111>	$0.258m_o$

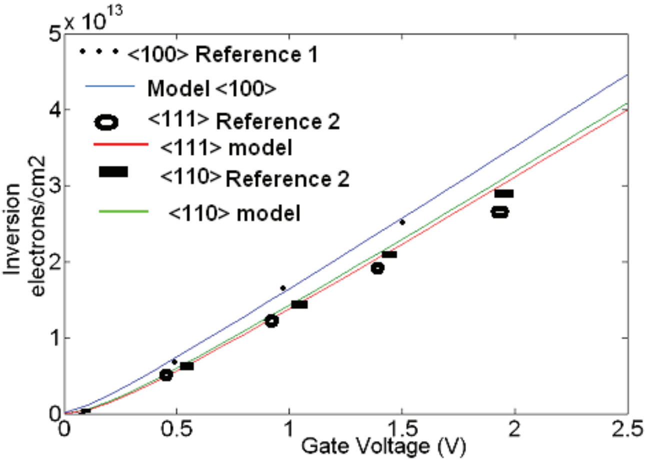

Fig. 2 – *Simulated Results of quantized inversion charge density in three crystal orientations* (*lines on the graph from top*: *Model* <100>, <110> *model,* <111> *model*).

4 Threshold Voltage

The voltage required to turn on the MOSFET is called the threshold voltage. As the gate voltage is increased above the threshold voltage, electrons from the substrate, source and drain start accumulating at the surface of the substrate thus creating a sheet of charge called as inversion layer which is enough for the conduction from the source to the drain. In the case of inversion layer quantization in the substrate, the energy band-gap widens due to the electrons staying at higher energy levels. So less electron contribution is available at the same gate voltage. This results in increased threshold voltage. So, in order to invert the channel, more band bending is required and voltage greater than classical voltage has to be applied at the gate terminal. This is called threshold voltage shift. So, this shift in the threshold voltage is added to the classical threshold voltage to obtain the net threshold voltage. An analytical model of this effect has been developed in this section. Various crystal orientations have been taken to study the impact of inversion layer quantization. The gate to source voltage is given by:

$$V_{gs} = V_{fb} + \varphi_s + Q_s / C_{ox}, \tag{9}$$

total substrate charge = $= Q_s = -Q_b$ (before inversion).

The threshold voltage is defined for the depletion potential at the onset of inversion i.e. before $\varphi_s = 2\varphi_f$. Here the inversion charge density is negligible and hence can be ignored. Therefore (9) becomes,

$$V_{gs} = V_{fb} + \varphi_s - Q_b / C_{ox}. \tag{10}$$

Using (2) in (10), we get,

$$V_{gs} = V_{fb} + \varphi_s + (2\varepsilon_0\varepsilon_{si} q N_b \varphi_s)^{1/2} / C_{ox}. \tag{11}$$

Hence at $\varphi_s = 2\varphi_f$, $F_{gs} = V_T$, V_T is the classical threshold voltage, Therefore,

$$V_T = V_{fb} + 2\varphi_f + 2(\varepsilon_0\varepsilon_{si} q N_b \varphi_f)^{1/2} / C_{ox}. \tag{12}$$

Differentiating (10) with respect to surface potential (φ_s), we get,

$$\frac{\mathrm{d}V_{gs}}{\mathrm{d}\varphi_s} = 1 + 0.5(2\varepsilon_0\varepsilon_{si} q N_b)^{1/2} / (\varphi_s)^{1/2} C_{ox}. \tag{13}$$

Putting the condition $\varphi_s = 2\varphi_f$, we get

$$\frac{\mathrm{d}V_{gs}}{\mathrm{d}\varphi_s} = 1 + 0.5(\varepsilon_0\varepsilon_{si} q N_b)^{1/2} / (\varphi_f)^{1/2} C_{ox}. \tag{14}$$

The shift in the surface potential due to inversion layer quantization is given by (6) which is multiplied with (14) to get the shift in the threshold voltage. Therefore, the shift in the threshold voltage is

$$\frac{\mathrm{d}V_{gs}}{\mathrm{d}\varphi}\delta\varphi_s = \frac{\mathrm{d}V_T}{\mathrm{d}\varphi}\delta\varphi_s. \tag{15}$$

As shown in Fig. 3, threshold voltage shift in the crystal orientations (110) and (111) is larger as compared to (100) crystal orientations. This shows the extent of impact of inversion layer quantization on the (110) and (111) crystal orientations making them less useful for the nanoscale MOSFETs. At higher substrate concentrations, the shift in the threshold voltage increases and is of the order of 50 mV and more. The parameters taken are oxide thickness 2.5 nm, substrate doping variation from 1×10^{15} cm^{-3} to 1×10^{18}cm^{-3}. The results have been compared for the (100) crystal orientation with the numerical results as predicted in reference 3 [17].

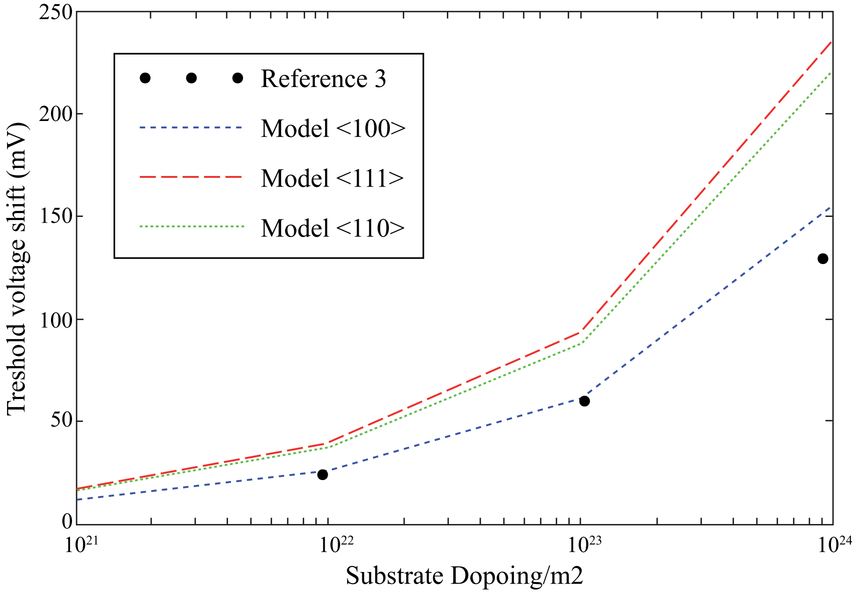

Fig. 3 – *Threshold voltage shift with substrate doping in the presence of inversion layer quantization in the substrate at oxide thickness of* 2.5nm. *The case of three crystal orientations viz*; (100), (110) *and* (111) *has been taken.*

5 Conclusion

Quantization effects on carrier distribution in substrate are studied based on the variation approach. The threshold voltage with inversion layer quantization analytically derived shows that crystal orientations also have a significant effect on the threshold voltage and inversion charge density of MOSFET at nanoscale levels.

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