

# A Comparative Study of Hole and Electron Inversion Layer Quantization in MOS Structures

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**Abstract:** In this paper, an analytical model has been developed to study inversion layer quantization in nanoscale Metal Oxide Semiconductor Field Effect Oxide p-(MOSFET). n-MOSFETs have been studied using the variation approach and the p-MOSFETs have been studied using the triangular well approach. The inversion charge density and gate capacitance analysis for both types of transistors has been done. There is a marked decrease in the inversion charge density and the capacitance of the p-MOSFET as compared to n-MOSFETs. The results are compared with the numerical results showing good agreement.

**Keywords:** Inversion quantization, hole, Modeling, Inversion layers, MOS devices.

## 1 Introduction

N type MOSFETs have been studied intensively since their evolution in early 1950s. Since then scaling down of both p-MOSFETs and n-MOSFETs has been taking place for their use in Complementary Metal Oxide Semiconductor (CMOS) technology. Very less attention has been given to the modeling process of p-MOSFET mainly because of the complex nature of valence band structure. 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 nanoscale. Due to extremely thin oxide and high doping concentration very high electrical fields at the oxide/substrate interface occur. This results in the charge carriers occupying quantized two-dimensional sub-bands which behave differently from the classical three-dimensional case. An appreciable amount of work has been performed to account for these effects in electron inversion layers [Stern, 1972; Fang et al, 1966; Stern et al, 1967; F. Stern, 1972; and Ando et al, 1982], while the hole inversion layers has not been studied

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analytically but mainly experimental work has been done and whatever, theoretical work done already has yielded complex solutions not suitable for device simulation [Takagi et al, 1999; S. Jlallepalli et al, 1996; G. Chindalore et al, 1997; S. Hareland et al,1998; T. Hou et al, 2001; T. Hou et al, 2001; T. Hou et al, 2001; C. Hu et al, 1996]. One of the reasons for this is that the valence energy levels under very high electrical fields at the oxide/silicon interface tend to mix up or intermingle and hence simple approach to study hole inversion layers has not been dealt with. More so, mixing of valence band becomes fiercer at high electrical field at the oxide/silicon interface. This makes simple formulations of hole quantization much more difficult to calculate accurately. Moreover, step wise step analytical formulation is missing in most of the literature yielding very less information about the hole quantization modeling process. An attempt has been made in this paper to give a simple and yet accurate description of the energy quantization process in the p-MOSFETs.

## **2 Inversion Layer Quantization**

Various models [Takagi et al, 1999; S. Jlallepalli et al, 1996; G. Chindalore et al, 1997; S. Hareland et al,1998; T. Hou et al, 2001; T. Hou et al, 2001; T. Hou et al, 2001; C. Hu et al, 1996] have been reported in literature to understand the energy quantization effect in a pMOSFET. The problem with these existing models is that either they are empirical in nature, or involve lengthy and complex numerical calculations. These types of approaches seriously affect the processing speed and the accuracy of the model is sometimes sacrificed.

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. To accurately model the quantization effect, Schrödinger and Poisson equations need to be solved.

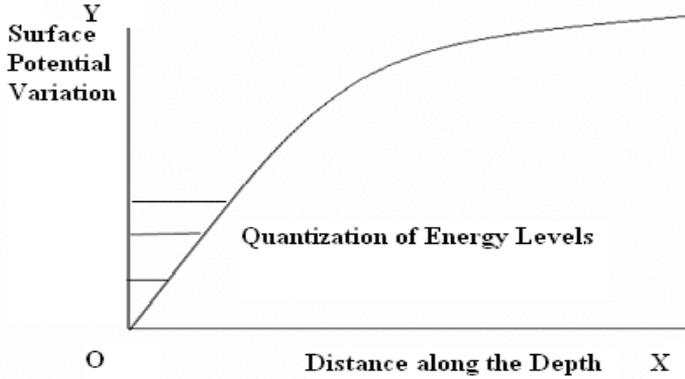


Fig. 1 – Energy quantization in the substrate.

## 2.1 Modeling of channel electrostatics

To solve the Schrödinger's equation, some approximations are required. These are triangular well approximation and variation approximation. Using these approximations, the Schrödinger's equation generates the electron energies and hence the electron potentials. The shift in electron potentials is then used to find the total surface potential in the presence of energy quantization by including it in the existing classical surface potential in the channel. For this purpose, depletion charge density and inversion charge density calculation is required.

The inversion charge density including weak and strong inversion can be found using the Poisson's equation in the MOSFET substrate channel:

$$\frac{d^2}{dx^2}\phi = \frac{qN_t}{\epsilon_o\epsilon_{si}}, \text{ for } 0 < x < X_d. \quad (1)$$

Total charge  $N_t$  is the sum of bulk depletion charge and electron inversion charge in the channel,  $\epsilon_o$  is the permittivity of air and  $\epsilon_{si}$  is the relative permittivity of silicon,  $q$  is the electron charge and  $X_d$  is the depletion depth in the substrate. Upon solving the (1) and applying necessary boundary conditions, the total surface charge density is:

$$Q_s = -(2qN_b\epsilon_o\epsilon_{si})^{1/2} \left[ \phi_s + V_t e^{-2\phi/V_t} (e^{\phi_s/V_t} - 1) \right]^{1/2}. \quad (2)$$

The depletion charge is obtained using (1) in the substrate using the depletion approximation:

$$Q_b = -(2\epsilon_o\epsilon_{si}qN_a\phi_s)^{1/2}, \quad (2a)$$

where  $N_a$  is substrate concentration ( $\text{cm}^{-3}$ ) and  $\phi_s$  is surface potential (V).

Subtracting (2a) from (2), we get the surface inversion charge density as

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

where  $C_{ox}$  is oxide capacitance ( $\text{Fm}^{-2}$ ),  $V_t = 0.025 \text{ V}$  at room temperature, and Fermi potential in the substrate  $\varphi_f = V_t \ln(N_a / n_i)$ .

The potential-based models are more physics-based, and are therefore, more accurate. However, a major disadvantage of the potential based models is that potential is related to the MOSFET terminal voltages such as gate voltage or drain voltage by an implicit relation that needs to be solved iteratively, incurring expensive computation time. Several solutions have been proposed for finding surface potential explicitly, and a very brief review of several of these approaches can be found in [Van Langevelde et al, 2000]. By solving the Poisson's equation in the substrate, the surface potential is obtained as:

$$\varphi_s = \left( \frac{2qN_b}{\epsilon_o \epsilon_{si}} \right)^{1/2} \left[ \varphi_s + V_t \exp \left( -\frac{2\varphi_f}{V_t} \right) \left( \exp \left( \frac{\varphi_s}{V_t} \right) - 1 \right) \right]^{1/2}. \quad (4)$$

Solving (4) requires numerical techniques and can be solved only in separate regions of inversion. However, some efforts have been made to determine it analytically also. The analytical explicit surface potential model has been reported in [Van Langevelde et al, 2000].

$$\varphi_s = f + a \quad (5)$$

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

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

where  $\varphi_{swi} = \left\{ (V_{gs} - V_{fb} + 0.25\gamma^2)^{1/2} - 0.5\gamma \right\}^2$  is the weak inversion surface potential, and  $x = V_{gs} - V_{fb} - f$ ,  $y = \varphi_{swi} - f$ .

Using the surface potential model (5) in (1) and (3), we can calculate explicitly inversion charge density, depletion charge density and the shift in the surface potential due to energy quantization effect.

## 2.2 Variation approximation for electron quantization

Using the variation approximation to the problem, we get the energies of the electrons at the bottom of the potential well, which ultimately decide the

shift in the potential. The main assumption is that all the carriers are present at the bottom of the conduction band. The solution of the Schrödinger's equation is given by the wave function [Stern, 1972]:

$$\psi(x) = \frac{b^{3/2}x}{\sqrt{2}} \exp\left(-\frac{bx}{2}\right), \quad (6)$$

$b$  is a constant [Stern, 1972] given by

$$b = \left[ \frac{48\pi^2 m_{ee} q}{\epsilon_o \epsilon_{si} h^2} (0.33Q_{inv} + Q_b) \right]^{1/3}, \quad (7)$$

and  $m_{ee} = 0.98m_o$  is effective mass in longitudinal direction for (100) crystal orientation of substrate [Stern, 1972]. The value of  $b$  has been chosen so as to minimize the energy of the electrons, i.e., finding the energy of the electrons in the lowest energy band. The corresponding minimum energy shift [Stern, 1972] is given by

$$E_{oe} = 3\hbar^2 b^2 / (8m_{ee}). \quad (8)$$

The shift in the surface potential is given as

$$\delta\phi_{se} = 3\hbar^2 b / (8m_{ee} q), \quad (9)$$

where (9) can be written as by putting the value of ' $b$ ' from (7)

$$\delta\phi_{se} = \frac{3\hbar^2}{8m_{ee} q} \left[ \frac{48\pi^2 m_{ee} q}{\epsilon_o \epsilon_{si} h^2} (0.33Q_{inv} + Q_b) \right]^{2/3}. \quad (10)$$

The quantum surface potential is hence

$$\phi_{sqm} = 2\phi_f + \delta\phi_{se}. \quad (10a)$$

Using the surface potential model (10a) in (1) and (3), we can calculate explicitly depletion charge density and inversion charge density. The quantum inversion charge density from (3) can be evaluated for quantum mechanical case.

$$Q_{invqm} = -\gamma C_{ox} \left[ \left\{ \phi_{sqm} + \frac{kT}{q} \exp\left(\frac{q(\phi_{sqm} - 2\phi_f)}{kT}\right) \right\}^{1/2} - (\phi_{sqm})^{1/2} \right]. \quad (10b)$$

The results in Fig. 2 match quite closely with the BSIM 5 results [J. He et al, 2007]. The results show that the energy quantization leads to reduced inversion charge densities and increased surface potentials in the substrate. It has been analytically proved that the classical theory overestimates the value of inversion layer charge density as compared to the quantum mechanical charge

density. The inversion charge density has been obtained with the applied gate voltage ranging from  $-0.5\text{V}$  to  $2.5\text{V}$  at zero drain voltage p-type substrate, Doping  $N_a = 1 \times 10^{18} \text{cm}^{-3}$ ,  $t_{ox} = 1.5 \text{nm}$ . At  $1.5 \text{V}$  gate voltage, the classical charge density is  $2.5 \mu\text{Ccm}^{-2}$  and quantum mechanical Charge density is  $2.138 \mu\text{Ccm}^{-2}$ . The BSIM 5 inversion charge density [J. He et al, 2007] in similar conditions including the energy quantization is approximately  $2.0 \mu\text{Ccm}^{-2}$ . The value is quite close.

### 2.3 Triangular well approach for hole quantization

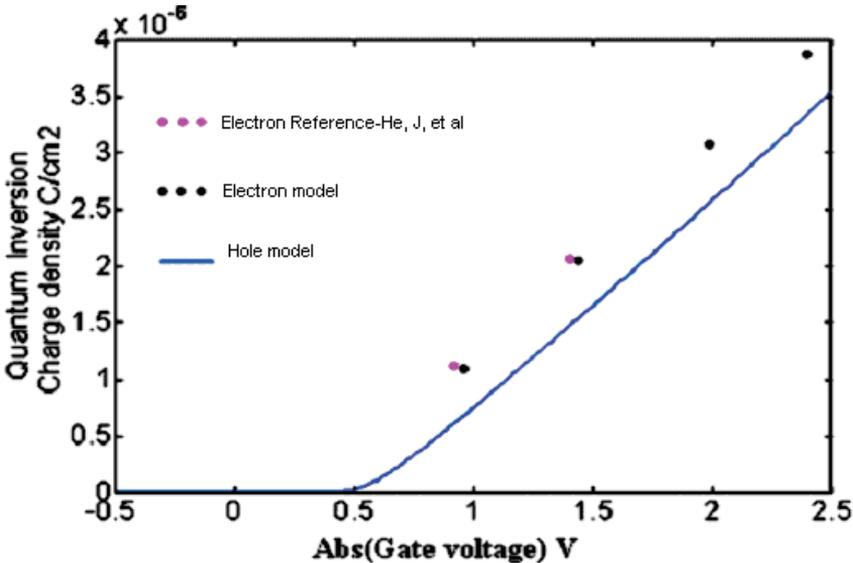
The hole inversion layers are studied using the triangular well approximation for solving the Schrödinger's equation [Y. Ma et al, 2000]

$$E_{oh} = (\hbar^2 / 8\pi^2 m_{hh})^{1/3} (1.1\pi q E_s)^{2/3}, \quad (11)$$

$m_{hh} = 0.16m_0$  [S. Takagi et al, 1999]. The shift in the surface potential is obtained using (11) as:

$$\delta\phi_{sh} = E_{oh} / q, \quad (12)$$

where  $E_s = (\eta Q_{inv} + Q_b) / \epsilon_{si} \epsilon_0$ ,  $\eta = 0.8$  for holes [Y. Ma et al, 2000].



**Fig. 2** – Simulated results of quantum mechanical electron inversion charge density using variation approach and hole inversion charge density using triangular well approach.

(12) is then included in the explicit surface potential expression given by (5) and the total quantum surface potential is obtained. The individual potentials

can be calculated and hence the inversion quantum charge densities can be found from (10b). The results in Fig. 2 show that the hole density is much lower than the electron density showing that the energy quantization effect is more severe in p-MOSFETs than the n-MOSFETs.

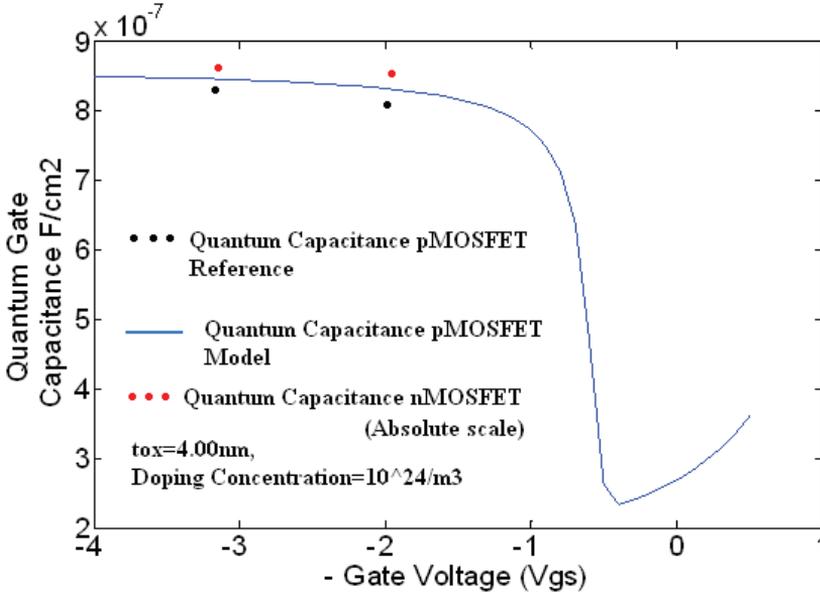
### 3 C-V Modeling

Approximating the inversion charge density for the weak inversion region and strong inversion regions separately, we get after differentiating (3) with respect to surface potential, the weak inversion and strong inversion capacitances. The inversion capacitance in the presence of energy quantization is

$$C_{invqm} = C_{wi} C_{si} / (C_{si} + C_{wi}), \quad (13)$$

where  $C_{wi} = (q / kT) Q_{invqm}$  is the weak inversion capacitance,  $C_{si} = (q / 2kT) Q_{invqm}$  is the strong inversion capacitance, and  $Q_{invqm}$  is Quantum inversion charge density.

Total gate capacitance is  $C_{ox} (C_d + C_{invqm}) / (C_{ox} + C_d + C_{invqm})$ , where  $C_{ox}$  is Oxide capacitance, and  $C_d$  is Depletion capacitance obtained by differentiating (2a) with respect to surface potential.



**Fig. 3** – Simulated results of the gate capacitance ( $F/cm^2$ ) including energy quantization in the substrate. The results are compared with the reference reported in [S. Takagi et al].

## 4 Conclusion

In this paper, an analytical model has been developed to study inversion layer quantization in nanoscale p-MOSFET. The inversion charge density and capacitance analysis for both types of transistors has been done. The results are compared for the similar cases in n-MOSFETs and the numerical results also and show good agreement. A detailed study has been done to evaluate the electrical parameters like C-V in the p-MOSFETs. Based on the variation approach and triangular well approach, all these parameters have been derived. In the presence of energy quantization, the inversion charge capacitance has been obtained. The total gate capacitance with quantum mechanical effects in p-MOSFETs reduces as compared to the n-MOSFETs. This is due to reduced charge density at interface of the substrate and the oxide.

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