# Quantum Surface Potential Model Suitable for Advanced MOSFETs Simulation

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*Abstract*— An analytical solution physically accounting for the quantum mechanical effects within the context of an explicit surface-potential-based MOSFET model is presented. The quantum model does not need any additional parameter, and is fully dependent on all terminal voltages. It gives an accurate and continuous description of the surface potential and its derivatives in all regions of operation. The validity of our new modeling approach is confirmed by both comparisons with simulation data (obtained using self-consistent Schrödinger-Poisson numerical calculations) and experimental data from an advanced deep-submicron CMOS technology.

#### I. INTRODUCTION

The trend toward smaller MOSFET devices with thinner gate oxide and greater doping level is resulting in the increased importance of the quantum mechanical effects (QME) [1], [2]. Quantum effects drastically reduce performances of state-of-the-art MOSFETs, in a rather similar way to the polysilicon gate depletion effect (PDE) [3]–[5]. From a physical point of view, both phenomena result in a decreased inversion charge layer density at a given gate voltage compared to predictions of the classical theory. Hence, numerous characteristics and measurable parameters of the device change, such as the surface potential, the drain current, the transconductance and the transcapacitances, etc. [6]–[9]. To ensure the accuracy of simulations, compact MOSFET models for circuit simulation need to account for the observed changes in device characteristics.

Predicting all the new important effects apparent in modern CMOS technologies has led to the current trend of increasing the model complexity and the number of parameters (e.g. BSIM3, BSIM4). In an attempt to increase the physical content, especially in the moderate inversion region, over the years the focus has gradually shifted from threshold-voltagebased models to charge sheet models based on the surface potential formulation ( $\phi_s$ -models) [6]–[13]. However a major drawback of the  $\phi_s$ -models is that the surface potential is given by an implicit relation and thus, can only be solved iteratively. For this reason, the original  $\phi_s$ -models required an expensive computation time. To overcome this difficulty, several solutions have been proposed [13]-[15]. The model presented in [13] is accurate and close to the physics but does not include the QM effects. In [14], a solution suitable for circuit simulation is reported, but the lack of physics of this purely empirical approach results in a questionable predictivity of the model. In [15], a new closed-form analytical approximation for the surface potential is proposed. This modeling

approach is able to provide accurate results. Nevertheless from the engineering and circuit design point of view, it would be desirable to have a model that further simplifies the analytical expressions, while keeping the physical basis inherent to the surface potential approach.

In this paper, we present an explicit description of the surface potential physically accounting for the QM effects. The inclusion of QM effects is achieved in a physical way, using a new approximation — the concept of moderate inversion approximation— of the variational approach to the solution of the Schrödinger and Poisson equations. We show how the new surface potential formulation allows us to simply compute the various charges of the MOSFET, thus enabling accurate and fast simulations of the transcapacitances. The quantum  $\phi_s$ -model is finally implemented in a charge sheet model and verified on aggressively scaled MOSFET devices.

# II. MODELING THE QUANTUM EFFECTS

# A. Variational theory

In the quantum theory the conduction band can no longer be regarded as a continuum of states, but rather splits into discrete subbands. Nonetheless it is largely recognized that in the inversion regime the contribution of the carriers in the lowest subband is dominant [2], [16], [17]. Therefore a variational approach to the exact solution of the Schrödinger and Poisson equations instead of the usual triangular potential approximation will be used in our model. The triangular potential approximation is a good method when there is little or no charge in the inversion layer, but fails when the charge density in the inversion layer is comparable to or exceeds that in the depletion layer [1]. On the contrary, within this condition i.e. when a quasi-only single subband is occupied, the variational approach gives an accurate estimation for the energy of the lowest subband. The inversion layer quantization is then calculated using a variational wave function  $\zeta_h(x)$ , associated to the lowest energy level and depending on the so-called b parameter [1], [2].

The value of b is chosen to minimize the first energy level:

$$b(n_{inv},\phi_s) = \left[\frac{12 \cdot m^* \cdot q^2}{\epsilon_{si} \cdot \hbar^2} \cdot \left(\frac{n_{inv}}{3} + n_{dep}(\phi_s)\right)\right]^{1/3}$$
(1)

where  $m^*$  is the electron longitudinal effective mass,  $\epsilon_{si}$  the silicon dielectric constant,  $n_{inv}$  the electron density in the inversion layer, and  $n_{dep}$  the fixed charge density in the depletion layer.

## B. The moderate inversion approximation

For an explicit calculation of the surface potential, ideally, the increase of the surface potential  $\delta \phi_s$  due to QM effects should be included within a single relationship of the following form:  $\delta \phi_s \propto V_g, V_{ch}$ , where  $V_g$  is the gate voltage and  $V_{ch}$ the drain or source voltage (all these voltages are defined with respect to substrate, e.g.  $V_q \equiv V_{qb}$ ). In this respect, we have defined the concept of an equivalent carrier density  $n_{all}$ , accounting for both free carrier density in the inversion layer, and fixed charge density in the depletion layer. The equivalent carrier density is considered to be zero when the gate voltage is smaller than  $V_{to} + V_{ch}$  (with  $V_{to}$  the classical long-channel threshold voltage). Using (4), we ensure a continuous transition from zero for  $V_g \leq V_{to} + V_{ch}$  to  $n_{all}$  for  $V_g \ge V_{to} + V_{ch}$ . This approach results in a new formulation of the *b* parameter, valid in all operation regions and particularly accurate in the moderate inversion region, which is defined as follows

$$b(V_g, V_{ch}) \simeq \left[\frac{12 \cdot m^* \cdot q^2}{\epsilon_{si} \cdot \hbar^2} \cdot \frac{n_{all}(V_g', V_{ch})}{3}\right]^{1/3}$$
(2)

with

$$n_{all}(V_{g}', V_{ch}) = \frac{2 \cdot C_{ox}}{q} \cdot (V_{g}' - V_{to} - V_{ch})$$
(3)

and

$$V_{g}' = \frac{1}{2} \cdot \left[ V_{g} + \sqrt{(V_{g} - V_{to} - V_{ch})^{2} + 4\varepsilon^{2}} + \sqrt{(V_{to} + V_{ch})^{2} + 4\varepsilon^{2}} \right]$$
(4)

where  $C_{ox}$  is the gate oxide capacitance per unit area, and  $\varepsilon$  is a fixed constant.

Due to this new formulation of b, we can accurately describe the quantum shift of the first energy level of the silicon conduction band as follows

$$E_w(V_g, V_{ch}) = \frac{3}{8} \frac{\hbar^2}{m^*} \cdot b(V_g, V_{ch})^2$$
(5)

The shift of the first energy level is then expressed in terms of surface potential increment by the function  $\delta \phi_s$ , fully dependent on terminal voltages, and given by

$$\delta\phi_s(V_g, V_{ch}) = E_w(V_g, V_{ch})/q \tag{6}$$

This provides an explicit relationship between the quantum increment of the surface potential and the gate and source/drain voltages. Thus with this method, taking into account the QM effects is not at all time consuming. Moreover it should be noticed that the above modeling does not introduce any additional parameter with respect to a classic  $\phi_s$ -model.

## III. SURFACE POTENTIAL MODEL DESCRIPTION

Incorporating the moderate inversion approximation in an explicit surface potential model is the final goal of this work. Towards this end, we have modified the model recently introduced in [13] in a rigorous way. In order to preserve

all the physics of both the basic model and the moderate inversion approximation, no additional smoothing function has been used. At first sight a natural way to incorporate the moderate inversion approximation to the basic model is to add the two expressions  $\delta \phi_s$  and  $\phi_s$  together. In reality this method is really too simplistic and would not provide the best possible model. In addition it is well known that adding two functions without helping from smoothing functions leads sometimes to discontinuity problems when the derivatives of the resulting function are addressed. Owing to previous observations, we have transformed the basic model from the inside. These changes result in a new expression for the so-called f function [13]. This leads to the following relationships

$$f_{[qm]}(V_g, V_{ch}) \equiv f(V_g, V_{ch}) \Big|_{\phi_s \leftarrow \phi_s + \delta \phi_s} \tag{7}$$

and hence,

$$\phi_{s[qm]}(V_g, V_{ch}) = \phi_s(V_g, V_{ch}, f_{[qm]}(V_g, V_{ch}))$$
(8)

In Fig. 1, the surface potential as obtained from (8) is shown for n-channel MOSFETs with no source/drain bias applied. An excellent agreement between the analytical model and the self-consistent calculations is found, even for very high doped substrates and ultra-thin gate oxides. Self-consistent solutions have been obtained by coupling the Schrödinger equation to the traditional Poisson equation. We have performed this with the Berkeley quantum-mechanical C-V simulator [18].

Fig. 2 shows the surface potential for various drain bias conditions. It can readily be seen that significant errors will be made in the prediction of the surface potential if QM effects are neglected. Since numerous basic MOSFET characteristics directly depend on the surface potential (within the context of a charge sheet model), some errors in the calculation of  $\phi_s$  may lead to huge errors in the estimation of the drain current, transconductance and transcapacitances [19]. For ultra-thin oxides, errors in estimation of the drain current can be almost



Fig. 1. Surface potential  $\phi_s$  as a function of gate voltage  $V_{gb}$  computed with the new explicit relation (8) (*solid lines*). The quasi-Fermi potential  $V_{ch}$  is set to zero. Symbols represent numerical results obtained by self-consistent quantum calculations.



Fig. 2. Surface potential  $\phi_s$  as a function of gate voltage  $V_{gb}$  for different drain voltage values as obtained from the new explicit expression (8) (*solid lines*), and according to the classical one [13] (*dashed lines*).

80% which will definitely lead to unwanted results, e.g. when designing devices to have maximum drive currents or transconductance. More in-depth validation will be considered in the next section by comparing results of our model with experimental data.

## IV. RESULTS

Simulating a MOSFET with a surface potential model has two major advantages, on the one hand such a model offers insight into the physical phenomena, and on the other it gives a straightforward and accurate description of all crucial electrical characteristics thanks to the use of a charge sheet model. In fact, within the context of a charge sheet model, a single continuous equation yields the drain current for the whole operation range (from depletion to inversion), and the computation of charges is straightforward [13].

Fig. 3 displays the simulated drain current of an advanced n-MOS transistor with a high doped substrate of  $N_a = 8 \times 10^{17}$  cm<sup>-3</sup> and a very thin gate oxide of  $t_{ox} = 2.5$  nm. This graph illustrates the relative importance of both QM and PD effects



Fig. 3. Simulated drain current using the classical model [13], the quantum model without the polydepletion effect and the full quantum model. The model parameters are  $W/L = 10/10 \ \mu m$  and  $t_{ox} = 2.5 \ nm$ .



Fig. 4. Comparison of the measured and modeled drain current at low drain bias, for n-channel MOSFETs with various gate oxide thicknesses  $t_{ox}$  and  $W/L = 10/10 \ \mu$ m. Symbols represent experimental results.

on the drain current, and clearly shows that the QM effects dominate. In fact, the polydepletion effect is by far more important for the charges and transcapacitances calculation. Let us notice that the complete procedure of implementing the polydepletion effect into the quantum surface potential model can be found in [20].

Further evidence for the accuracy of the present  $\phi_s$ -model is achieved by comparing the results with Philips' experimental data. Two measurement sets of n-channel MOSFETs are considered. The first one corresponds to specifically processed devices with uniform substrate doping of  $N_a = 5 \times 10^{17}$  $cm^{-3}$  and various oxide thickness values, while the second one corresponds to a typical 0.18  $\mu$ m CMOS technology. Fig. 4 illustrates the good agreement between the experimental results and the  $\phi_s$ -model for predicting the drain current in devices with very thin gate oxides ( $t_{ox} = 2$  and 5 nm) that are considered to have many applications in deep-submicron design. The drain current is also plotted on a logarithmic scale to demonstrate the characteristics in the subthreshold region. It appears that the slope in the weak inversion region is correctly predicted for both devices. Another important point is that our model is not only valid for the surface potential  $\phi_s$ , but also for its derivative  $\partial \phi_s / \partial V_q$ . As shown in Fig. 5, this leads to an accurate description of the transconductance  $g_m$ , whereas the classical model incorrectly predicts the peak of  $g_m$ .

Finally, Fig. 6 gives the normalized gate transcapacitance  $C_{gg}/C_{ox}$  of an actual MOSFET device from a 0.18  $\mu$ m CMOS technology. As depicted in the latter, both the quantum and polydepletion effects, which strongly affect the total gate capacitance  $C_{gg}$  are correctly described by the present model. Note that the device simulated in Fig. 6 has an oxide thickness equal to 3.2 nm, a polysilicon doping of about  $1.2 \times 10^{20}$  cm<sup>-3</sup>, and a non-uniform substrate doping, but in the order of magnitude of  $6 \times 10^{17}$  cm<sup>-3</sup>. Regarding the oxide thickness, all the simulations were performed without making it an adjustable parameter; only the technological oxide thickness was used in the model.

To conclude this section, let us emphasize that in order to



Fig. 5. Simulated transconductance  $g_m$  and drain current  $I_d$  as a function of gate voltage  $V_{gb}$  for both the quantum and classical  $\phi_s$ -models. Failing to account for QME can lead to errors both in the design of MOSFETs and in the interpretation of experimental data.



Fig. 6. Comparison between simulated and measured normalized gate transcapacitances  $C_{gg}/C_{ox}$  for a device from a 0.18  $\mu$ m CMOS technology.

demonstrate that our quantum  $\phi_s$ -model is ready for integrated circuit simulators, we introduced in [19] two operating implementations of the model in both VHDL-AMS and Verilog-AMS Hardware Description Languages (HDLs).

# V. CONCLUSION

An analytical MOSFET model, physically accounting for the QM effects has been proposed. A new concept is used to include the QM effects within an effective closed-form analytical expression for the surface potential  $\phi_s$ . No additional parameter with respect to the basic  $\phi_s$ -model is necessary. We show that the model leads to excellent results in comparison with numerical QM calculations and actual devices, for any substrate doping and oxide thickness. In a forthcoming study, we will focus on the development of a fully analytical model that independently accounts for the QM effects in accumulation and inversion modes. Thus, it will be possible to have a comprehensive quantum surface-potentialbased model suitable for both simulation and characterization of state-of-the-art MOSFET devices.

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