Compact Modeling of Quantum Effects in Undoped Long-Channel Cylindrical Surrounding-Gate MOSFETs

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Abstract. Quantum effects have been incorporated in the analytic potential model for cylindrical surrounding-gate or gate-all-around metal oxide semiconductor field effect transistors (MOSFETs). By extracting some constants parameter from the self-consistent Schrödinger and Poisson equations, two physical parameters, threshold voltage shift and inversion layer centroid, are expressed as closed form function of device radius and charge density. The quantum version of inversion charge density is obtained by incorporating of those parameters into the classical procedure as modifications for gate work function and inversion layer capacitance. The model represented here has been able to reproduce simulation data obtained from self-consistent calculation. The calculated results show that the model fits well with the self-consistent calculation.

1. Introduction
Since the bulk CMOS scaling is approaching the limit [1], multi-gate field-effect transistors in particular cylindrical surrounding-gate (SG) MOSFETs have been becoming intense subject of research due to their abilities to better control short channel effects (SCEs) [2-8]. For better understanding of device physics and in order to implement the device characteristics into further applications, for example in the context of circuit simulator, development of compact modeling could play an important role. A good compact model is not only designed for its accuracy but also for the ability to catch hidden underlying physics for example quantum quantization effects. In the case of cylindrical SG MOSFETs, carriers are confined in a thin cylindrical potential well of the oxide barrier hence the quantum quantization effects on the cylindrical SG MOSFETs are assumed to be greater than in bulk device in which the carriers are only confined by electric field from the gate.

In this paper, we propose a simple analytical model for obtaining inversion charge that includes quantum confinement effects of the cylindrical SG MOSFET. Roldan et al. [2] have developed a good semiempirical model for cylindrical SG MOSFETs that include quantum confinement effects by performing modification on classical charge control based approach [3]. We will demonstrate in this letter that an analogous formulation of quantum correction for potential based approach [4] as proposed by Wang et al. for the double-gate (DG) MOSFET [5] can be carried out for the cylindrical SG MOSFET [6, 7]. For this purpose, we organize this letter as follows: In section 2, solutions to the coupled Schrödinger and Poisson equations in cylindrical coordinate system are developed using a one
dimensional Poisson-Schrödinger solver. Influences of quantum confinement on device characteristics, namely, threshold voltage shift and inversion layer centroid are expressed as closed form functions of device radius and inversion charge density (section 3). In section 4, quantum effects are implemented in an analytic potential compact model for the final result. Conclusions are finally drawn.

2. Self-consistent solution of Schrödinger-Poisson Equation

Figure 1 shows the geometrical dimensions of a cylindrical SG MOSFET. A silicon nanowire with radius \( R \) is surrounded by thin gate oxide with thickness \( t_{\text{ox}} \). For a long-channel SG-MOSFET with channel length \( L \), quantum confinement effects arise not only due to 1-D confinement of electron motion by surface or field potential like in bulk device but also caused by the 2-D structural confinement from the surrounding oxide barrier. To obtain the quantum electrical characteristics of the MOSFET, one needs to solve the coupled Poisson and Schrödinger equations self-consistently.

The Poisson equation connecting the electrostatic potential \( \psi(r) \) to the electron density \( n(r) \) is [2, 6, 7]

\[
\frac{d^2 \psi(r)}{dr^2} + \frac{1}{r} \frac{d \psi(r)}{dr} = \frac{q}{\varepsilon_{\text{si}}} n(r). \tag{1}
\]

Instead of using classical Boltzmann’s statistics \( n = n_i \exp q\psi/kT \) like in the classical model, \( n \) is modeled quantum mechanically as [2]

\[
n(r) = \sum_{v,n_r,n_{\phi}} g_v \left( \frac{2m^*_{d,v} kT}{\pi^2 \hbar^2} \right)^{1/2} \left| \Psi_{v,n_r,n_{\phi}}(r) \right|^2 F \left( \frac{E_f - E_{v,n_r,n_{\phi}}}{kT} \right), \tag{2}
\]

due to the application of Fermi-Dirac statistics. Here \( q \) is the electronic charge, \( \varepsilon_{\text{si}} \) is the silicon permittivity, \( k \) is Boltzmann’s constant, \( T \) is temperature, \( E_f \) is the Fermi level, \( g_v \) and \( m^*_{d,v} \) are the degeneracy and density-of-state effective mass in the \( v^{\text{th}} \) valley, respectively, \( \hbar \) is Planck’s constant, \( \Psi_{v,n_r,n_{\phi}}(r) \) is the normalized wave functions and \( E_{v,n_r,n_{\phi}} \) is the energy of the \( n_r^{\text{th}} \) and \( n_{\phi}^{\text{th}} \) subband in the \( v^{\text{th}} \) valley satisfying the Schrödinger equation

\[
-\frac{\hbar^2}{2m^*_{r,v}} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} \right) \Psi(r, \phi) + E_c(r) \Psi(r, \phi) = E_{v,n_r,n_{\phi}} \Psi(r, \phi). \tag{3}
\]

Here \( m^*_{r,v} \) is the electron effective mass in the \( v^{\text{th}} \) valley in the radial direction and the conduction band \( E_c(r) \) is coupled to the electrostatic potential \( \psi(r) \) through \( E_c = E_g/2 - q\psi(r) \).

The boundary condition relates the potential and electric field at the silicon-oxide interfaces to the applied gate voltage [4, 6]
where $C_{ox} = \varepsilon_{ox}/R \ln(1 + t_{ox}/R)$ is the oxide capacitance per unit area, $\Delta \phi$ is the work function difference between the gate electrode and the intrinsic silicon, $V_g$ is gate voltage, and $Q$ is the electron charge sheet density. The wave function is forced to be zero at the silicon-oxide interface mimicking impenetrable barrier but continues at the center ($r = 0$).

A 1-D coupled Poisson-Schrödinger solver was developed to solve numerically these two radial equations (Eqs. (1) and (3)) using a simple finite difference method.

### 3. Quantum correction for cylindrical SG-MOSFETs

In Figure 2.(a) we have obtained the electron charge sheet density $Q$ as a function of gate voltage $V_g$ from self-consistent calculation. Being slightly different with its classical counterpart (by solving Poisson’s equation only), quantization of the carrier has effects on both the threshold voltage $V_{th}$ and gate capacitance $C_g$ (the slope of $Q$ vs. $V_g$ curve). Quantum mechanically obtained threshold voltage is higher and gate capacitance is lower than their respective classical solutions. By studying the behavior of these two terminal characteristics, some data can be extracted from self-consistent simulation and they can then be incorporated into the analytical potential model [6, 7] as quantum corrections.

#### 3.1. Threshold Voltage Shift

Based on the $Q$ vs. $V_g$ curve in Fig. 2.(a), the threshold voltage shift $\Delta V_{th}$ is obtained from the $V_g$ shift of the quantum curve with respect to the classical curve for the same $Q$ in subthreshold region. Following the previous work [2], we modeled the trends of the self consistently obtained data by an empirical equation given in Eq. (5)

$$\Delta V_{th} = 0.03001 \ (V) + \frac{0.1187 \times 10^{-18} (V/m^2)}{R^2}. \quad (5)$$

**Figure 2.** (a) Classical and quantum self-consistent mobile charge density $Q$ of cylindrical SG MOSFETs in both linear (right) and logarithmic (left) versus gate voltage. (b) Threshold voltage shift due to quantum effects as a function of silicon radius with $t_{ox} = 1$ nm. Circles were obtained from the self-consistent simulation and the line was calculated from Eq. (5). (c) Inversion charge centroid with $R = 5, 7.5$ and $10$ nm. The self-consistent simulation results were plotted in dots and the line was calculated from Eq. (8).
Comparison between the self consistently obtained data and our empirical fitting in Eq. (5) is shown in Fig. 2.(b). This procedure is quite different with the work by Wang et al. for the DG-MOSFET [4], in which the threshold voltage shift can be modeled only by the lowest subband.

3.2. Gate Capacitance Degradation

As we mentioned before, the quantum mechanically obtained gate capacitance is lower than that calculated under the classical one. In other words, the gate capacitance is degraded due to quantum quantization. For compact modeling purpose, this gate capacitance degradation can be modeled by correcting the oxide capacitance $C_{ox}$. The corrected oxide capacitance was calculated by characterizing the quantum charge distribution in the semiconductor through the determination of the inversion layer centroid which allowed us to account for the oxide interface separation of the inversion charge distribution. To determine the inversion layer centroid, first we defined a $\Delta$ parameter as follows [2]

$$\Delta = \int_0^R n(r)r^2 \, dr \int_0^R n(r) \, dr. \tag{6}$$

Second, the inversion charge centroid $z_l$ calculation was performed as follows [2]

$$z_l = R - \Delta, \tag{7}$$

where $R$ is the radius of the silicon wire. This calculation can be performed in the simulator and the results are shown in Fig. 2.(c). It can be seen that its value decreases as the inversion charge increases since the charge distribution shifts towards the silicon/oxide interface.

In order to model these centroid data, we have used the following empirical equation [2]

$$\frac{1}{z_l} = \frac{1}{a + 2bR} + \frac{1}{z_{10}} \left( \frac{Q}{qN_{10}} \right)^n, \tag{8}$$

where $a = 0.55 \, \text{nm}$, $b = 0.198$, $z_{10} = 5.1 \, \text{nm}$, $N_{10} = 7 \times 10^{16} - 4.9 \times 10^{24} \, \text{R/m}$, and $n = 0.75$ are constants. It is shown in Fig. 2.(c) that this empirical formulation fitted well for the radii of 5, 7.5, and 10 nm.

To incorporate the effects of $z_l$ for the evaluation of the inversion charge concentration in Eq. (4), the classical oxide capacitance $C_{ox}$ was replaced in our model by another capacitance, corrected oxide capacitance $C_{ox}^*$. This corrected oxide capacitance are the capacitance of the oxide in series with a “centroid capacitance,” which is the capacitance of a silicon layer, the thickness of which corresponding to the value of the inversion charge centroid, i.e., [2]

$$\frac{1}{C_{ox}^*} = \frac{1}{C_{ox}} + \frac{1}{C_{centroid}}, \tag{9}$$

where $C_{centroid}$ is calculated as follows [2]

$$C_{centroid} = \frac{\varepsilon_{st}}{(R - z_l) \ln \left( 1 + \frac{z_l}{R - z_l} \right)} \tag{10}$$
4. Implementation of quantum correction for SG-MOSFETs

The quantum mechanical correction factors are implemented in a classical analytic potential compact model for SG MOSFETs. In the analytic potential model, Poisson’s equation is rigorously solved to obtain an analytical expression for potential in the silicon film [6, 7]

\[
\psi(r) = V - \frac{2kT}{q} \ln \left[ \frac{R}{2} \sqrt{\frac{q^2 n_i}{2\varepsilon_{si} kT(1-\alpha)}} \left(1 - \frac{(1-\alpha)r^2}{R^2}\right)\right],
\]

where \(V\) is the electron quasi-Fermi potential at a point along the channel, \(n_i\) is the intrinsic carrier density, and the dimensionless parameter \(\alpha\) which is a function of \(V\) to be determined from the boundary condition in Eq. (4) with \(V_g\) replaced by \(V_g - V\). Substituting Eq. (11) into Eq. (4) leads to

\[
\frac{1}{2} \ln(1-\alpha) - \ln \alpha + \frac{s}{\alpha} = \frac{q(V_g - \Delta\phi - V)}{2kT} - \ln \left(\frac{2}{R} \sqrt{\frac{2\varepsilon_{si} kT}{q^2 n_i}}\right),
\]

where \(s = 2\varepsilon_{si}/RC_{\alpha}\).

From Gauss’s law, the classical charge density is \(Q = \varepsilon_{si}(d\psi/dr)_{r=R}\), which is simply

\[
Q = \frac{4\varepsilon_{si} kT(1-\alpha)}{qR}.
\]

To incorporate the quantization effects into the above analytical potential model, the following procedure was performed:

(a). Implement the threshold voltage shift by changing the gate work function in Eq. (12) from \(\Delta\phi\) to \(\Delta\phi + \Delta V_{th}\), with \(\Delta V_{th}\) is given by Eq. (5), then solve Eq. (12) to find \(\alpha\). A simple explicit procedure to calculate \(\alpha\) can be found in Ref. [7].

Figure 3. (a) Mobile charge density \(Q\) and (b) gate capacitance obtained by analytical model without correction (solid line), analytical model with correction (dashed line) and self-consistent simulation data (dot)
(b). Compute the inversion charge density \( Q \) by substituting \( \alpha \) into Eq. (13).
(c). Compute the inversion layer centroid \( z_I \) by putting \( Q \) found in (b) into Eq. (8) then find the corrected oxide capacitance \( C_{ox}^* \) by substituting \( z_I \) into Eq. (10) and then Eq. (9).
(d). Put this new corrected oxide capacitance into Eq. (12) then compute the second value of \( \alpha \) as step (a). We name this \( \alpha \) as \( \alpha_{QM} \) since its value determines all quantum-mechanically corrected parameters.
(e). Compute the corrected inversion charge density by substituting \( \alpha_{QM} \) into Eq. (13). A good result with respective self-consistent simulation of the corrected \( Q \) and its derivative \( C_g \) is shown in Figs. 3.(a) and (b).

In Fig. 3 we have compared our model final result of inversion charge density with those obtained from self-consistent calculation for both logarithmic and normal scale to show the accuracy of the model. It is also shown that our model of inversion charge density fitted well for some variation of silicon radii.

5. Conclusion
An analytic compact model with quantum corrections has been developed for cylindrical surrounding-gate MOSFETs. Two distinctive quantum effects have been extracted from numerical solutions obtained from a 1-D Poisson- Schrödinger solver in the cylindrical coordinate system. First, the threshold voltage shift as a function of silicon radius has been implemented as an effective change in the gate work function. Second, quantum degradation of the gate capacitance has been expressed as a correction to the oxide capacitance by introduction of quantum inversion layer centroid. Those two quantum effects are then incorporated into an analytic potential SG compact model by a simple procedure. Inversion charge density versus gate voltage curves generated by compact model with quantum modifications were in excellent agreement with the self-consistent Poisson- Schrödinger simulation.

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References
[1] ITRS 2013 Ed, available at www.itrs.net/Links/2013ITRS/Home2013.htm
[2] J. B. Roldan, A. Godoy, F. Gamiz, and M. Balaguer 2008 IEEE T. Electron Dev. 55(1), 411
[3] B. Iniguez, D. Jimenez, J. Roig, H. A. Hamid, L. F. Marsal, and J. Pallares 2005 IEEE T. Electron Dev. 52(8), 1868
[4] W. Wang, H. Lu, J Song, S.-H. Lo, and Y. Taur 2010 Microelectr. J. 41(10), 688
[5] Y. Taur, X. Liang, W. Wang, and H. Lu 2004 IEEE Electr. Device L. 25(2), 107-109
[6] D. Jimenez, B. Iniguez, J. Su, L F. Marsal, J. Pallars, J. Roig, and D. Flores 2004 IEEE Electr. Device L. 25(7), 571
[7] B. Yu, H. Lu, M. Liu, and Y. Taur 2007 IEEE T. Electron Dev. 54(10), 2715
[8] B. Yu, W.-Y. Lu, H. Lu, and Y. Taur 2007 IEEE T. Electron Dev. 54(3), 492