Compact Quantum Modeling Framework for Nanoscale Double-Gate MOSFET

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ABSTRACT

A quantum mechanical modeling framework for ultra-thin body (UTB) device operating in the subthreshold and near-threshold regime is presented. For subthreshold conditions, we have assumed that the electrostatics is dominated by capacitive coupling between the body electrodes. Hence, the charge is neglected in Poisson equation, thus decoupling the quantum effects and electrostatics in the body. The potential is obtained as a solution of the 2D Laplace equation with the help of conformal mapping techniques. In the near-threshold regime, we have solved Poisson’s equation using the quantum charge density along the gate-to-gate symmetry line to calculate the total potential. We find that the classical approach underestimates the total potential inside the device body. Finally, the current in subthreshold is modeled assuming drift-diffusion transport with electron density calculated quantum mechanically.

Keywords: short-channel MOSFET, double-gate, quasi-Fermi potential, conformal mapping, quantum modeling.

1 INTRODUCTION

Precise classical models for the electrostatics, drain current and capacitance of short-channel, nanoscale double-gate (DG) and gate-all-around (GAA) MOSFETs have been previously presented. [1-9]. we have used conformal mapping techniques to model the inter-electrode potential in subthreshold regime [7,8].

In subthreshold, the potential is maximum at the center and minimum at the silicon-insulator interface. This corresponding energy well is similar to a harmonic oscillator in a box, and hence the Schrödinger equation can be expressed in terms of standard equation of parabolic cylindrical functions. Near and above threshold, the influence of the electronic charge on the electrostatics is taken into account in a precise, self-consistent manner by combining suitable model expressions with Poisson’s equation [7].

The DG device considered has gate length $L = 25$ nm, insulator thickness $t_{ox} = 1.6$ nm, and insulator relative dielectric constant $\varepsilon_{ox} = 7$. The doping density of the p-type silicon body is $10^{15}$ cm$^{-3}$. As gate material, we selected a near-midgap metal with the work function 4.53 eV.

Idealized Schottky contacts with a work function of 4.17 eV (corresponding to that of n+ silicon) are assumed for the source and drain. This ensures equipotential surfaces on all the device contacts. To simplify the modeling, we replace the insulator by an electrostatically equivalent silicon layer with thickness of $t'_{ox} = t_{ox}\varepsilon_{si}/\varepsilon_{ox}$ where $\varepsilon_{si}$ is the relative permittivity of silicon.

We’ve considered the $x$-axis along the channel length of the device and the $y$-axis along gate-to-gate symmetry line.

2 QUANTUM MECHANICAL MODELING

A parabolic potential distribution in the $y$-direction has been shown to be a good approximation in subthreshold [8], the potential can be represented as:

$$\phi(x, y) \approx \phi_c(x) \left[1-\left(\frac{2y}{H}\right)^2\right] + V_{gs} - V_{fb}$$

where $\phi_c(x)$ is the difference between the potential at position $x$ on the D-S symmetry line and the effective gate voltage, $V_{gs}$ is the gate-source potential, and $V_{fb}$ is the flat-band voltage of the gate. To simplify the expression we shift the axis along the $y$-direction, such that the device center is at $y=0$. The potential energy in this can be represented as:

$$P(x, y) = \frac{q\phi_c(x) + V_{gs} - V_{fb}}{2}$$

where:

$$b = \frac{q\phi_c}{\sqrt{(t_{ox}/2 + t'_{ox})}}$$

The corresponding Schrodinger equation can be expressed into the standard equation of parabolic cylinder functions [10,11] given as:

$$\frac{d^2\psi(t)}{dv^2} - \left(\frac{\alpha^2}{4} + v}\right)\psi(t) = 0$$

where:

$$t = \alpha y, \alpha = (8m^*_f b / \hbar^2)^{1/4}, \beta = \hbar^{1/4}(2b / m^*_f), E = \beta v$$
where \( m^*_{L,T} \) is the electron effective mass and \( E \) is the eigenvalue of the corresponding Schrödinger equation. The equation (5) has both even and odd solutions [10], as the potential is symmetric about \( y=0 \), the wavefunction must have a definite parity and thus \( \psi(t) \) is given by two different polynomials with even and odd terms:

\[
\psi_{en}(t) = A_e(1 + \sum_{n=0}^{\infty} c_n t^n / n!), A_o(1 + \sum_{n=1}^{\infty} c_n t^n / n!)
\]

where \( A_e \) and \( A_o \) are normalization constants and the coefficients \( c_n \) are determined from recursive relation given in [10]. The eigenvalues can be determined by truncating the above polynomials to some higher term and then finding the numerical solution. As only the first few subbands are important in the actual calculation of charge, the analytical solution can be obtained by making an assumption that \( v<1 \) and then truncating the polynomial to second term. The even parity wavefunction gives lower subbands and the odd function gives higher subbands for same effective mass. The eigenfunction and the eigenvalue corresponding to the first unprimed subband are given as:

\[
\psi(y) = \frac{15}{8a} \left( 1 - \frac{4y^2}{a^2} \right)
\]

\[
E_{i} = \frac{4\hbar^2}{m^*_i}
\]

### 3 QUASI-FERMI POTENTIAL MODELING IN SUBTHRESHOLD

Starting with the differential form of drift-diffusion equation, we obtain the following expression for quasi-Fermi potential:

\[
V_F(x) = C_1 - eV_{th} \left[ \frac{C_2}{V_{th}} - \sqrt{\frac{2\pi}{V_{th}}} \text{Erf} \left( \frac{2x}{V_{th}} \right) \right]
\]

where \( C_1 \) and \( C_2 \) are determined from the boundary conditions and the parameter depends \( k \) upon \( V_{th} \), for UTBs, a value of \( k=0.26 \) (for \( V_{th}<0.25 V \)) and 0.19 (for \( V_{th}>0.25 V \)) gives sufficient accuracy. The above expression is evaluated for two different regions \( x_m \leq x \), where \( x_m \) is the position of top of the barrier calculated using conformal-mapping of the extended rectangular device body. In the transformed \((u,v)\)-plane, \((u_m, v)\) represents the position of barrier maximum.

\[
u_m = \frac{(1+k)\nu_{th}}{2k(2\nu_{th} + \nu_{th} - 2\nu_{th} + 2\nu_{th})}
\]

where \( k \) is the shape parameter expressed in terms of the \( L/H \) ratio of the extended device body. To evaluate (9) completely, we have to evaluate \( V_{th} \), the value of quasi-Fermi potential at the top of the barrier, given as [8]

\[
V_{th} = -\frac{e}{\hbar} \ln \left[ 1 - \frac{1 - e^{-\frac{V_{th}}{eV}}}{\frac{dV}{dx}} \right] \int_{-\infty}^{\infty} n_o(x) dx
\]

where \( n_o(x) \) is the charge-sheet density along \( x \)-axis with quasi-Fermi level set to zero. The inverse of charge-sheet density follows a normal distribution with maxima at top of the barrier and is almost symmetric at \( x_m \), and thus covers approximately half of the total area. The value of \( V_{th} \) can thus be approximated as:

\[
V_{th} = \ln \left[ 1 + \left( \frac{e^{\nu_m}}{e^{\nu_m} - 1} \right) \left( \frac{e^{\nu_m}}{e^{\nu_m} + 1} \right) \right]
\]

Figure 1 shows the modeled quasi-Fermi level, compared with numerical simulations for \( V_{gs} = -0.2 V \).

![Figure 1: Comparison of modeled and numerically quasi-Fermi potential with gate voltage \( V_{gs} = -0.2 V \).](image)

### 4 CHARGE AND POTENTIAL MODELING

The electron density along \( y \)-axis is given as:

\[
n(y) = \sum_{\text{valleys}} \sum_{j} N_{2D} \ln \left[ 1 + e^{-\frac{(E_j-E_F)}{kT}} \right] \left| \psi(y) \right|^2
\]

where \( N_{2D} \) is 2D effective density of states and \( E_j - E_F \) is given as:

\[
E_j + E_g / 2 + q \left[ \phi_{b} - \phi_{a} + \phi_{F}(x) \right]
\]
where $\varphi_b$ is the potential difference between the Fermi level of intrinsic silicon and doped silicon, $\varphi_i$ represents shift in intrinsic Fermi level which emerges from difference in electron and hole density states and $\varphi(0)$ is the center potential. In actual calculation only the first three subbands are considered. The summation over valleys depends upon the degeneracy. Figure 2 shows the variation of charge density with gate voltage, compared with numerical simulations from ATLAS device simulator. The model shows an excellent agreement with numerical simulation.

As we move near to the threshold, the effect of charge carriers on the device electrostatics become important and thus total potential inside the body near the device center can be written as [7, 8]:

$$\varphi(x, y) \approx \varphi_L(x, y) + \varphi_Q(y)$$

where $\varphi_L$ is potential solution from Laplace equation and $\varphi_Q$ is potential due to charge carriers, $\varphi_Q$ is modeled by solving Poisson equation along the $y$-axis (near the body center we have assumed that lateral electric field is relatively small). Classical treatment of carriers underestimates the total potential and thus we need to solve Poisson equation with charge density calculated quantum mechanically. The equation is given as:

$$\frac{d^2 \varphi_Q(y)}{dy^2} = \frac{q \sum_{valleys} \sum_j N_{j\alpha} \ln \left(1 + e^{\frac{(x_j - E_j)}{kT}}\right) |\psi_j(y)|^2}{\varepsilon_s}$$

Equation (16) is quite complex and thus it’s difficult to obtain an analytical solution from Poisson equation. We thus make some assumptions; firstly we assume that only first subband is occupied. This assumption is quite justified in UTBs because energy difference between different subbands increases as the silicon thickness is reduced. Secondly we assume a non-degenerate carrier statistics at the threshold voltage, at the inset of threshold, the charge density is not high and thus non-degenerate statistics gives negligible error. Using (16) along with the assumptions, the resulting Poisson equation along the $y$-axis at the device center becomes:

$$\frac{d^2 \varphi_Q(y)}{dy^2} = \frac{0 - \left( f_a + t_a / 2 \right) \leq y \leq -t_a / 2}{15 q N_{j\alpha} \alpha e^{\frac{x_j - E_j}{kT}} \left(1 - e^{\frac{4y^2}{t_s^2}} - t_a / 2 \leq y \leq 0\right)}$$

After solving the above equation we get the expression of charge potential at the device center in form of a Lambert function given as:

$$-\varphi_Q(0) = \frac{15 q N_{j\alpha} \alpha e^{\frac{x_j - E_j}{kT}}}{8 \varepsilon_s} \left(1 \ln \frac{2}{t_s^2} + 4t_a \right)$$

For relatively higher thicknesses, the single subband charge density in (19) can be replaced by total charge density including all subbands. Figure 3 shows the total modeled potential at the device center, compared with numerical simulations for $0.2 V \leq V_{gs} \leq 0.36 V$, which corresponds to the near-threshold regime. It’s obvious from the figure that classical potential is lower than the quantum potential.
center potential with gate voltage for 6nm device at $V_{ds}=0V$.

5 CURRENT MODELING

The drain current based on drift-diffusion theory can be expressed as [8]:

$$I_d = \frac{Wq\mu_n kT}{\sqrt{2\pi m*}} \int_{L/2}^{L/2} \left[ 1 - \exp\left( -\frac{V_n}{V_a} \right) \right] dx$$

Here $W$ is the device width, $\mu_n$ is the electron mobility, $V_{ds}$ is the applied drain voltage. In the subthreshold regime, non-degenerate carrier statistics can be assumed and thus $n_{so}(x)$ can be approximated as:

$$n_{so}(x) = \sum_{valleys} \sum_{j} N_{2D} e^{\frac{kT}{h} \sqrt{\frac{E_j}{2} + \phi(x,0) - \phi(0,0)}}$$

where $\phi(x,0)$ is potential along S-D symmetry line, the potential can be approximated by parabolic function given in [8]:

$$Wq\mu_n V_a \left[ 1 - \exp\left( -\frac{V_n}{V_a} \right) \sum_{valleys} \sum_{j} N_{2D} e^{\frac{kT}{h} \sqrt{\frac{E_j}{2} + \phi(x,0) - \phi(0,0)}} \right]$$

The solution of the integral in the denominator comes in form of error function. Fig. 4 shows the modeled current compared with classical and quantum numerical simulations. As expected, classical methodology overestimates the current in ultra-thin body devices.

6 CONCLUSION

We have developed a precise quantum modeling framework for short-channel nanoscale DG MOSFET in subthreshold and near-threshold regime. The eigenfunctions are obtained as a direct solution of Schrodinger equation. A compact model for the quasi-Fermi potential in subthreshold is also presented. It is shown that in the case of ultra-thin body devices the classical potential is lower than quantum potential. The modeled current shows good agreement with simulated results.

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