

Analytical Formulae of Quantum-Mechanical Electron Density in Inversion Layer in Planar MOSFETs

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Analytical formulae for electro-static potential and electron density profile for n-type planar MOSFETs are obtained by solving equations based on the density gradient model using a perturbation theory. Our formulae reproduce exact numerical solutions with excellent accuracy without any fitting parameters or expensive computation time.

I. INTRODUCTION

The electron density in inversion layer in planar MOSFETs are known to differ from that of classical predictions. Up to now several methods to describe such quantum-mechanical electron density have been proposed as summarized in Fig. 1. Exact numerical descriptions can be obtained by solving Schrödinger and Poisson (SP) equations self-consistently. The problem of such rigorous numerical approach is that it requires expensive computation time, and therefore is not suitable for most of the device and circuit simulation needs. An analytical description of the quantum-mechanical electron density has first been made by Stern [1], and Van Dort *et al.* developed the widely-used compact model based on the Stern's work [2]. Although Van Dort's model is efficient enough to be used in device and circuit simulations, the electron density profile as a function of distance from Si/SiO₂ interface shows serious discrepancy from results obtained by SP simulation. The density gradient (DG) model is claimed to give a reasonable trade-off between accuracy and time-efficiency. Numerical solutions to a set of equations based on this model give reasonably accurate results within acceptable computation time. However, it is difficult to obtain good convergence in the numerical calculations, so that it requires highly sophisticated methods. Furthermore, the computation time is not yet short

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enough to be used in circuit simulators.

In this work, we analytically solve the equations based on the density gradient model using a perturbation method. Our analytical solutions successfully reproduce major characteristics of a planar MOSFET without any fitting parameters. With our formulae one can calculate quantum-mechanical electron density instantaneously without any expert knowledge of numerical computation.

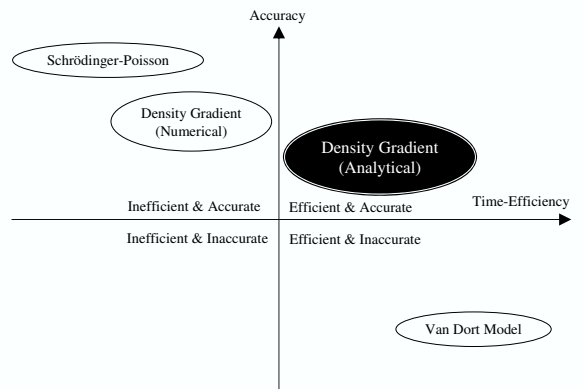


Fig. 1. Map of various modeling methods for quantum-mechanical electron density in inversion layer. Our model presented in this paper is highlighted by black.

II. CALCULATION METHOD AND FORMULAE

In the density gradient model, the following set of equations are solved.

$$\frac{d}{dx} \left[\varepsilon_{\text{si}} \frac{d}{dx} \psi(x) \right] = -e \left[n_i e^{\frac{e}{k_B T} (\phi_p - \psi(x))} - n(x) - N_A \right], \quad (1)$$

$$\phi_n = \psi(x) - \frac{k_B T}{e} \ln \left[\frac{n(x)}{n_i} \right] + 2b_n \left(\frac{\frac{d^2}{dx^2} \sqrt{n(x)}}{\sqrt{n(x)}} \right), \quad (2)$$

where x is the distance from the Si/SiO₂ interface, $\psi(x)$ is the electrostatic potential, ϕ_p is the quasi-Fermi potential for holes, ϵ_{si} is the permittivity for Si, n_i is the intrinsic carrier density, and $k_B T$ is the thermal energy. The coefficient of the quantum potential term, b_n , is a constant defined as $b_n = \gamma_n \hbar^2 / 12 e m_e^*$. For the n-type inversion layer, $\gamma_n = 7.2$ and $m_e^* = 1.084$ (density-of-state effective mass) are used [3]. The perturbation approach decomposes the above equations into a set of simpler ones by expanding the solutions in terms of the small parameter [4], which is b_n in this case. The resulting approximate solutions give results equivalent to those of the numerical approach, with a small error due to neglecting the higher order terms. By exploiting this well-established mathematical method, we successfully obtained approximate analytical solutions to the Eqs. (1) and (2) to the first order in the perturbation expansion. The formulae for the electro-static potential and the electron density as functions of distance from silicon/oxide interface are given in the appendix.

III. COMPARISON WITH NUMERICAL SOLUTIONS

Figs. 2-4 show comparisons of band diagram, electron density, and mobile charge density among classical results (dashed curves), SP calculation results obtained using SCHRED [5] (open circles), and our analytical formulae (solid curves). In the calculations, following values were used: substrate doping density 10^{16} cm^{-3} , gate oxide thickness 2.0nm, gate work function 4.0eV, silicon electron affinity 4.05eV, silicon energy band gap 1.12eV, temperature 300K, and silicon and oxide permittivities 11.9 and 3.9, respectively. Resulting flat-band and threshold voltages are -0.97V and -0.25V , respectively. As shown in these figures, our formulae reproduce exact numerical results with excellent accuracy. Note that the formulae contain no fitting parameters: once above structural/material parameters and bias condition are given, solutions are obtained by just substituting those parameters into the expressions shown in the appendix.

IV. CONCLUSION

We have found analytical expressions for electro-static potential and electron density profile for n-type planar MOSFETs by solving equations based on the density gradient model using a perturbation theory. Our formulae reproduce exact numerical solutions with excellent accuracy without any fitting parameters or expensive computation time. These formulae can be implemented into circuit simulators to improve accuracy on reproducing quantum effects in MOSFETs.

ACKNOWLEDGEMENTS

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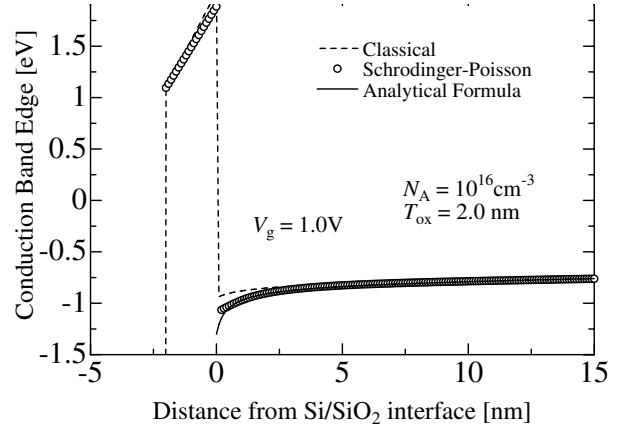


Fig. 2. Conduction band edge obtained using the classical model (dashed curve), SP calculation result obtained using SCHRED [5] (open circles), and our analytical formula (solid curve). Structural/material parameters are given in the text.

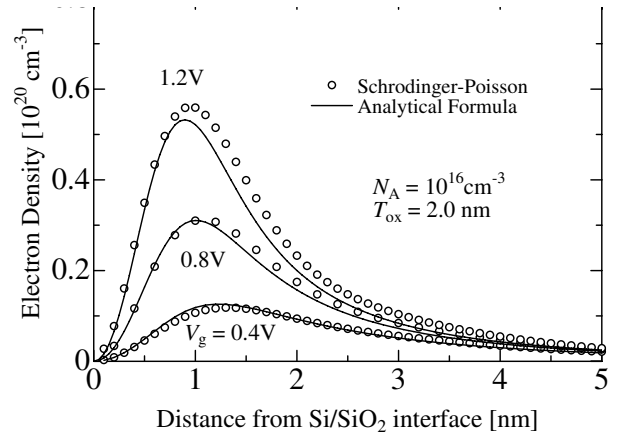


Fig. 3. Quantum-mechanical electron densities for different gate voltages

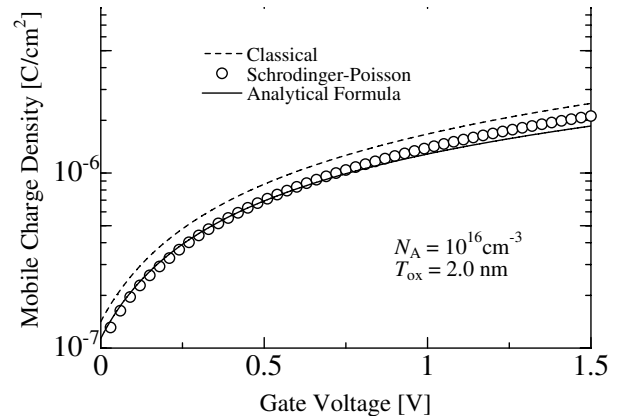


Fig. 4. Mobile charge density as a function of gate voltage. In using our formula, Eq. (8) was numerically integrated over the depth.

V. APPENDIX

The electro-static potential $\psi(x)$ measured from the intrinsic level in the substrate is given by

$$\psi(x) = \phi_n + \frac{k_B T}{e} \left(\ln [\alpha_0^2 \lambda \ln \lambda] - 2 \ln \left[\sinh \left[\frac{\alpha_0}{2} \sqrt{\lambda \ln \lambda} \frac{x}{L_D} + \gamma \right] \right] + \frac{1}{4} \lambda \left(\frac{x}{L_D} \right)^2 + \delta (\ln \lambda) C_1 \coth \left[\frac{\alpha_0}{2} \sqrt{\lambda \ln \lambda} \frac{x}{L_D} + \gamma \right] \right), \quad (3)$$

where ϕ_n is the quasi-Fermi potential for electrons. The parameter λ is defined as $\lambda \equiv N_A/n_i$, and the non-dimensional parameter δ is defined by $\delta \equiv \sqrt{\lambda e b_n / 2 \ln \lambda k_B T L_D^2}$, where $L_D = \sqrt{\varepsilon_{Si} k_B T / 2 e^2 n_i}$ is the intrinsic Debye length. The quantities α_0 and ψ_s are obtained by solving the following set of equations:

$$\alpha_0 \sqrt{\ln \lambda} = \sqrt{\frac{e \phi_n}{k_B T} + \ln [4 \alpha_0^2 \lambda \ln \lambda] - 2 \sinh^{-1} \left[\alpha_0 \sqrt{\exp \left[\frac{-e(\psi_s - \phi_n)}{k_B T} \right] \lambda \ln \lambda} \right] - 1}, \quad (4)$$

$$\psi_s = V_G - V_{FB} - \frac{k_B T}{e} \frac{\varepsilon_{Si} T_{ox}}{\varepsilon_{ox} L_D} \sqrt{\alpha_0^2 \lambda \ln [\lambda] + \exp \left[\frac{e(\psi_s - \phi_n)}{k_B T} \right]}, \quad (5)$$

where V_G and V_{FB} are the gate and the flat band voltages, T_{ox} is the oxide thickness, ε_{ox} is the permittivity of the gate oxide. The constants γ and C_1 are defined, using α_0 and ψ_s , as

$$\gamma = \sinh^{-1} \left[\alpha_0 \sqrt{\exp \left[\frac{e(\phi_n - \psi_s)}{k_B T} \right] \lambda \ln \lambda} \right], \quad (6)$$

$$C_1 = \left(2r_1 - \frac{1}{2} r_1^2 - r_2 \right) \frac{\sqrt{2} T_{ox} \varepsilon_{Si} \exp \left[\frac{e(\psi_s - \phi_n)}{k_B T} \right] \sinh [\gamma]^2}{L_D \varepsilon_{ox} \sqrt{\lambda \ln \lambda} \sinh [2\gamma] + T_{ox} \varepsilon_{Si} \alpha_0 \lambda \ln \lambda}, \quad (7)$$

with $r_1 = 1.2763$ and $r_2 = 0.059199$.

Similarly, electron density profile is given by

$$n(x) = n_i \exp \left[\frac{e(\psi_s - \phi_n)}{k_B T} + 2 \ln \left[S \left(\frac{x}{\delta L_D} \sqrt{\frac{\lambda}{2 \ln \lambda}} \right) \right] + \left(\exp \left[-3 \left(\frac{x}{\delta L_D} \sqrt{\frac{\lambda}{2 \ln \lambda}} - \frac{1}{2} \right) \right] + 1 \right)^{-1} \times \left\{ 2 \ln \left[\frac{\sinh \gamma}{\sinh \left[\frac{\alpha_0}{2} \sqrt{\lambda \ln \lambda} \frac{x}{L_D} + \gamma \right]} \right] + \delta (\ln \lambda) C_1 \left(1 - \exp \left[-\frac{13}{10} \frac{x}{\delta L_D} \sqrt{\frac{\lambda}{2 \ln \lambda}} \right] \right) \coth \left[\frac{\alpha_0}{2} \sqrt{\lambda \ln \lambda} \frac{x}{L_D} + \gamma \right] \right\} \right], \quad (8)$$

where the function $S(X)$ is defined by $X = \int_0^S d\xi [1/2 + \xi^2 (\ln [\xi] - 1/2)]^{-1/2}$.

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