Analytical Solutions to Quantum Drift-Diffusion Equations for Quantum Mechanical Modeling of MOS Structures

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1. Introduction

The quantum drift-diffusion equations, also known as the density-gradient (DG) equations, are a set of equations which model quantum effects in nanostructures such as nano-scale MOS capacitors, MOSFETs, and Double-Gate MOSFETs [1-5]. The complex DG equations are usually solved numerically. However, the numerical calculations require highly sophisticated methods [2, 5] and expensive computation time, so that they are not suitable for circuit simulations. In this work, we solve the DG equations analytically using a perturbation method. Our fully analytical solutions successfully reproduce major characteristics of a MOS structure without any fitting parameters. With these results one reproduce quantum effects can instantaneously without any expert knowledge of numerical computation.

2. Calculation Method

In the DG equations, a quantum correction term is added to the conventional drift-diffusion equations. The coefficient of the quantum correction term contains \hbar , which can be regarded as a small parameter. The perturbation approach decomposes the DG equations into a set of simpler ones by expanding the solutions in terms of the small parameter [6]. The solutions give results equivalent to those of the numerical approach, with a small error due to neglecting the higher order terms.

3. Results

Table 1 summarizes the formulae for the potential, ψ , and electron concentration, *n*, in a MOS capacitor as functions of distance from Si/SiO₂ interface, *x*. Only the 1st order terms of the perturbation expansions are given. Inner solutions are valid only in the vicinity of the Si/SiO₂ interface, and the outer solutions are valid outside the inner region. Uniform solutions can be obtained by analytically blending the inner and outer solutions. The quantity δ is a small parameter containing \hbar , and λ is the doping density divided by the intrinsic carrier density. The potential ψ and quasi-Fermi level ϕ_n are normalized by $\ln[\lambda] k_B T/e$, and distance *x* is

normalized by $L_{\rm D}$ Sqrt[2ln[λ]/ λ], where $L_{\rm D}$ is the intrinsic Debye length. The quantities α_0 and γ_0 are functions of surface potential $\psi_{\rm s}$, which are determined by the equations described in [7, 8]. The constants $\psi_{\rm 1s}$ and C_1 are functions of $\psi_{\rm s}$, λ , α_0 , γ_0 , and other material/structural parameters.

Figures. 1, 2, 3, and 4 show the potential profile, electron

density profile, and the mobile charge density obtained from our analytical solutions (thick solid curves) and Schrödinger-Poisson (SP) self-consistent solutions (open circles). The value of the quantum correction coefficient was taken from [2]. Classical solutions (dashed curves) and SP solutions were calculated using SCHRED [9]. These figures show excellent agreement between the SP solutions and our analytical solutions. Similar accuracy was found at other oxide thickness and doping densities. It is important to note that no fitting parameter is used in our calculation; our formulae are fully analytical descriptions of the solutions to the DG equations. For this reason, DG calculations can be easily done much faster than the numerical approach, while maintaining excellent agreement with SP solutions.

4. Conclusion

We have found analytical solutions to the quantum drift-diffusion (density-gradient) equations in MOS capacitors, which successfully reproduce Schrödinger-Poisson solutions without any fitting parameter. Our analytical solutions dramatically reduce the calculation time of device/circuit simulators. The same method can be used to model other structures, e.g. planar and double-gate MOSFETs, and these devices will be addressed in future work.

Acknowledgements

The authors would like to thank Hitachi Cambridge Laboratory for its support on device simulation. Dr. S. Uno was supported by a Fellowship from I. S. I. MOSIS Service.

Reference

[1] M. G. Ancona, et. al. Phys. Rev. B, vol. 39, p. 9536, (1989).

[2] A. Wettstein, *et. al., IEEE Trans., Electron Devices*, vol. 48, no. 2, p. 279 (2001).

[3] C. S. Rafferty, et. al. Proc. SISPAD, 1998, p. 137.

[4] A. Asenov, *et. al., IEEE Trans., Electron Devices*, vol. 50, no. 9, p. 1837 (2003).

[5] S. Odanaka, *IEEE Trans., Computer-Aided Design*, vol. 23, no. 6, p. 837 (2004).

[6] Bender and Orszag "Advanced Mathematical Methods for Scientists and Engineers", Springer-Verlag New York, 1999.

[7] M. J. Ward, et. al., SIAM J. Appl. Math., vol. 50, no. 4, p. 1099 (1990).

[8] E. Cumberbatch, et. al., J. Eng. Math., vol. 39, p. 25 (2001).

[9] SCHRED, http://www.nanohub.org/

Table. 1 Analytical solutions of potential and electron density profiles in a MOS capacitor in the quantum regime. Inner solutions are valid only near the Si/SiO₂ interface, and outer solutions are valid elsewhere. These solutions are smoothly blended to give a uniform solution. The quantity δ is small parameter containing \hbar . The quantity λ is given by N_A/n_i , and α_0 and γ_0 are functions of surface potential ψ_s , as described in [7,8]. Potential and position are normalized by $\ln[\lambda] k_B T/e$, and L_D Sqrt[$2 \ln[\lambda]/\lambda$], respectively, where L_D is the intrinsic Debye length. The constants ψ_{1s} and C_1 are functions of ψ_s , λ , α_0 , γ_0 , and other material/structural parameters.

Potential	Inner	$\psi_{inner}(x) = \psi_s + \delta \psi_{1s} - \sqrt{2}\alpha_0 \coth[\gamma_0] x$
	Outer	$\psi_{outer}(x) = 1 + \phi_n + \frac{1}{\ln[\lambda]} \ln\left[\alpha_0^2 \ln[\lambda]\right] - \frac{2}{\ln[\lambda]} \ln\left[\sinh\left[\frac{\alpha_0}{\sqrt{2}}\ln[\lambda]x + \gamma_0\right]\right] + \delta C_1 \coth\left[\gamma_0 + \frac{\alpha_0\ln[\lambda]}{\sqrt{2}}x\right]$
Carrier Density	Inner	$n_{inner}(x) = \lambda n_i e^{(\psi_s - \phi_n - 1)\ln[\lambda]} \{ S_0(x/\delta) \}^2, \text{ where } S_0(X) \text{ is given by } X = \int_0^{S_0} \left(\frac{1}{2} + \xi^2 \left(\ln[\xi] - \frac{1}{2} \right) \right)^{-1/2} d\xi$
	Outer	$n_{outer}(x) = \lambda n_i \left(\alpha_0 \sqrt{\ln[\lambda]} \sinh\left[\gamma_0 + \frac{\alpha_0 \ln[\lambda]}{\sqrt{2}} x \right]^{-1} + \delta C_1 \frac{1}{2} \alpha_0 \ln[\lambda]^{3/2} \sinh\left[\gamma_0 + \frac{\alpha_0 \ln[\lambda]}{\sqrt{2}} x \right]^{-1} \coth\left[\gamma_0 + \frac{\alpha_0 \ln[\lambda]}{\sqrt{2}} x \right] \right)^2$



Distance from Si/SiO2 interface [nm]

Fig. 1 Potential profile calculated using classical model, Schrödinger-Poisson solver SCHRED [9], and our analytical solutions. Parameters used are shown in the figure.



Fig. 3 Log plot of the electron density profiles at $V_g = 0.4$, 1.0, and 1.8V, showing excellent agreement at wide range of gate voltages.



Fig. 2 Electron density profile at $V_g = 1.0V$. The values of parameters were same as those used in Fig. 1



Fig. 4 Mobile charge density as a function of gate voltage, which is obtained by integrating the electron density in the inversion layer. This quantity corresponds to the source/drain current in MOSFETs.