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A SPICE-Compatible Model for Nanoscale MOSFET Capacitor Simulation Under the Inversion Condition

Ting-wei Tang, *Fellow, IEEE,* and Yiming Li, *Member, IEEE*

***Abstract*—A SPICE-compatible charge model for nanoscale MOSFETs is proposed. Based on the solution of Schrödinger–Poisson (S-P) equations, the developed compact charge model is optimized with respect to: 1) the position of the charge concentration peak; 2) the maximum of the charge concentration; 3) the total inversion charge sheet density; and 4) the average inversion charge depth, respectively. This model can predict inversion layer electron density for various oxide thicknesses and applied voltages. Compared to the S-P results, our model prediction is within 5% of accuracy. Application of this charge quantization model to the *C–V* measurement produces an excellent agreement. This compact model has continuous derivatives and is therefore amenable to a device simulator. It can also be easily incorporated into circuit simulator for modeling ultrathin oxide MOSFET *C–V* characteristics.**

***Index Terms*—*C–V* curve, compact charge model, device and circuit simulation, MOSFETs, quantum correction, Schrödinger–Poisson.**

I. Introduction

As THE feature size of MOS devices shrinks for higher density and performance, the thickness of silicon oxide also scales down. In aggressively scaled MOSFETs, the thickness of oxide in a MOS capacitor can be as thin as 0.8 nm [1] prevented only by the leakage tunneling current. For the oxide thickness ($T_{\rm ox}$) of $1 \sim 3$ nm and the applied gate voltage (V_G) of $0.5 \sim 1.5$ V, the displacement of the inversion carrier density away from the Si–SiO_2 interface due to the quantization effect cannot be neglected [2]. Thus, any accurate calculation of the inversion-layer capacitance must take this quantization effect into consideration.

The most accurate way of incorporating the quantum effect in the inversion layer is to solve the coupled Schrödinger–Poisson (S-P) equations subject to an appropriate boundary condition at the Si–SiO_2 interface [3]. This can be done without difficulties in solving the S-P equations in one dimension, but the S-P approach is not amenable to a realistic device simulator such as a simple compact model used in the SPICE. Other approaches such as the density gradient method [3], [4] and the effective potential method [5], [6] also suffer from the same disadvantage—computationally it is still excessive and physically the method is not very transparent.

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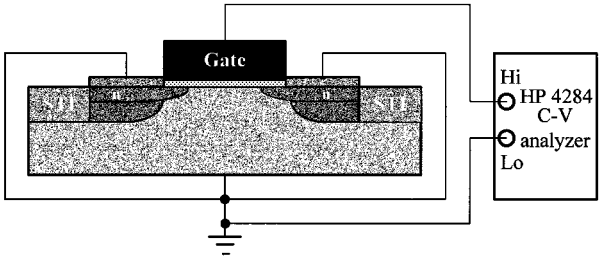

Fig. 1. Cross-section view of the nanoscale MOSFET and *C–V* curves measurement configuration.

In this paper, we have successfully developed a SPICE-compatible model feasible for nanoscale MOSFET capacitor simulation. The model is a generalization of an analytical model proposed by Hänsch *et al.* many years ago [7]. The solution of S-P equations is utilized to construct the model, where four optimization constraints: 1) the position of the charge concentration peak; 2) the maximum of the charge concentration; 3) the total inversion charge sheet density; and 4) the average inversion charge depth are used as criteria for the model parameter extraction. The model parameters are expressed as a function of $T_{\rm ox}$ and V_G for the purpose of simulating nanoscale MOSFET capacitances. For other applications, they can be also expressed in terms of the surface electric field and the oxide thickness.

II. Model Construction and Result

First, a poly-oxide-silicon system as shown in Fig. 1 is simulated using the drift-diffusion (D-D) approximation [8], [9]. The D-D equations are solved self-consistently with the S-P equations. The S-P equations are assumed to have no wave penetration at the Si–SiO_2 interface [10]. The S-P equations are discretized by the finite difference method (the so-called box method). After the discretization, the corresponding matrix eigenvalue problem and the system of nonlinear algebraic equations are solved iteratively to obtain a self-consistent solution. More than 16 subbands are used in the Schrödinger equation solver. The chosen $T_{\rm ox}$ varies from 1 to 3 nm and the applied V_G ranges from 0.2 to 2 V. The calculated inversion-layer charge densities are then cast into the form

$$n_{\rm QM} = n_{\rm CL} a_0 \left[1 - \exp\left(-a_1\left(\frac{x}{\lambda_{\rm th}}\right)^2 + a_2\left(\frac{x}{\lambda_{\rm th}}\right)^4 - a_3\left(\frac{x}{\lambda_{\rm th}}\right)^6\right)\right] \quad (1)$$

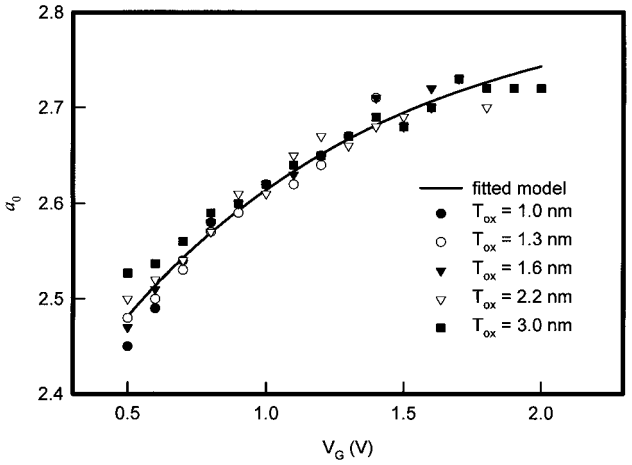

Fig. 2. Plot of the optimal value for the parameter a_0 and its fitting formula for various $T_{\rm ox}$ and different V_G.

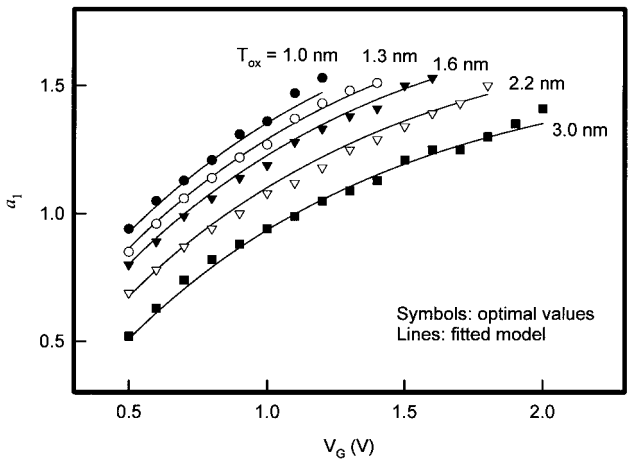

Fig. 3. Plot of the optimal value for the parameter a_1 and its fitting formula for various $T_{\rm ox}$ and different V_G.

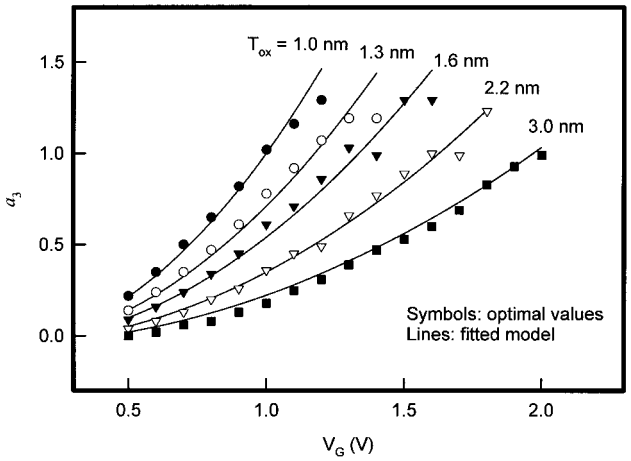

Fig. 4. Plot of the optimal value for the parameter a_3 and its fitting formula for various $T_{\rm ox}$ and different V_G.

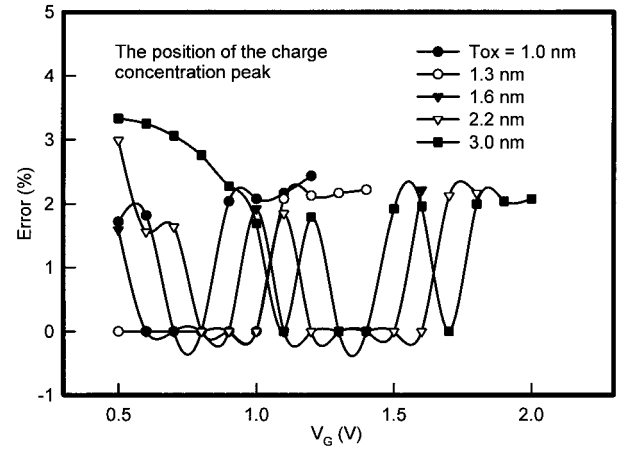

Fig. 5. Error plots of the position of the charge concentration peak versus V_G for various $T_{\rm ox}$.

where $n_{\rm CL}$ is the classical electron density solved from the Poisson equation and $\lambda_{\rm th} = (\hbar/2m^*k_BT)^{1/2}$ is the thermal wavelength. Using a generic algorithm, the four model parameters a_0, a_1, a_2, and a_3 are optimized to best fit the self-consistent S-P solution for all $T_{\rm ox}$'s and V_G's. The fitting accuracy of these parameters is based on the optimization with respect to the aforementioned four constraints. The average inversion charge depth is defined as

$$\langle x\rangle = \frac{\int_0^\infty xn(x)dx}{\int_0^\infty n(x)dx}. \tag{2}$$

The results of these parameters fittings are shown in Figs. 2–4. As seen in Fig. 2, the plots of a_0's versus V_G are almost independent of $T_{\rm ox}$. Fig. 3 shows that the dependence of a_1's on V_G for different $T_{\rm ox}$ is similar; all have a decreasing slope. Note that a_1 increases as $T_{\rm ox}$ is decreased. Not shown are plots of a_2's which are for all practical purpose nearly zero. Shown in Fig. 4 are plots of a_3's versus V_G, all having an increasing slope opposite to the shape of a_1's. Also noticed is that all a_3's converge to zero at a very low V_G, implying that a_3 is only associated with a higher-order quantum correction.

After optimization, these parameters are empirically fitted as a function of V_G and $T_{\rm ox}$ as follows:

$$a_0 = 2.82 - 0.555\exp(-V_G) \tag{3}$$

$$a_1 = 2.22 - 1.79\exp(-V_G) - 0.21T_{\rm ox} \tag{4}$$

$$a_3 = -0.004\,67 + 1.048\frac{V_G^2}{T_{\rm ox}^{1.23}} \tag{5}$$

where V_G is in volts and $T_{\rm ox}$ is in nanometers. The model parameters given in (3)–(5) are based on a p-type substrate with $N_A = 10^{17}$ cm^{-3}. For other substrate dopings, V_G should be adjusted by an amount equal to a shift in the threshold voltage due to the change in N_A. However, this adjustment is usually very small (< 0.13 V). The accuracy of the model inversion-layer charge density given by (1), (3) – (5) compared to the S-P solution is very good. In terms of the four criteria mentioned above, the accuracy is within 5%.

Shown in Figs. 5–8 are, respectively, errors between the fitted a's formula and the S-P solution against V_G for each optimization criterion. In Figs. 5 and 6, it is shown that the error of the position of the charge concentration peak is less than 3.5% and the error of the maximum of the charge concentration is less than 3%, respectively. Fig. 7 shows that the error of the total inversion charge sheet density between our model and the S-P equation is

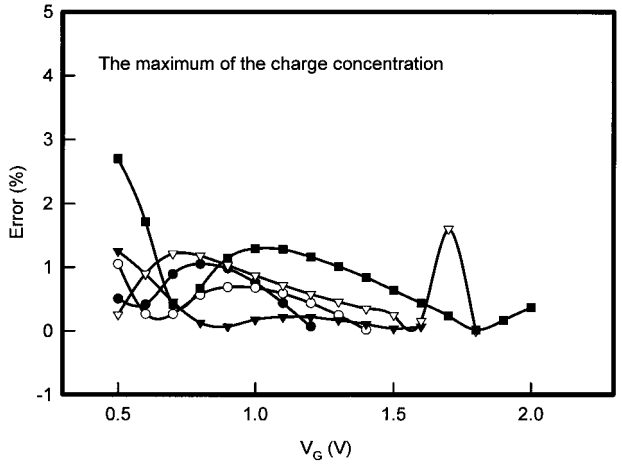

Fig. 6. Error plots of the maximum of the charge concentration versus V_G for various $T_{\rm ox}$.

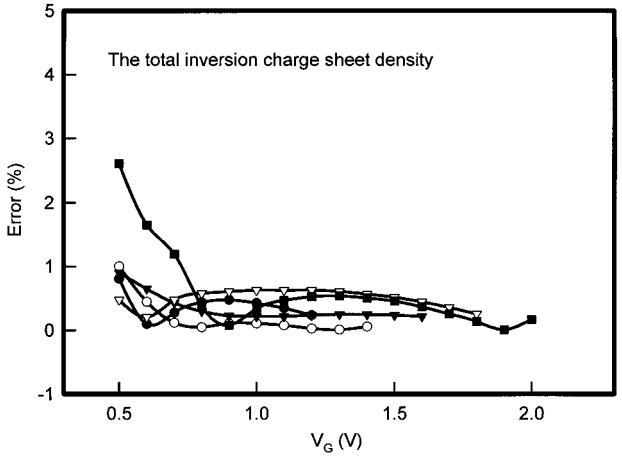

Fig. 7. Error plots of the total inversion charge sheet density versus V_G for various $T_{\rm ox}$.

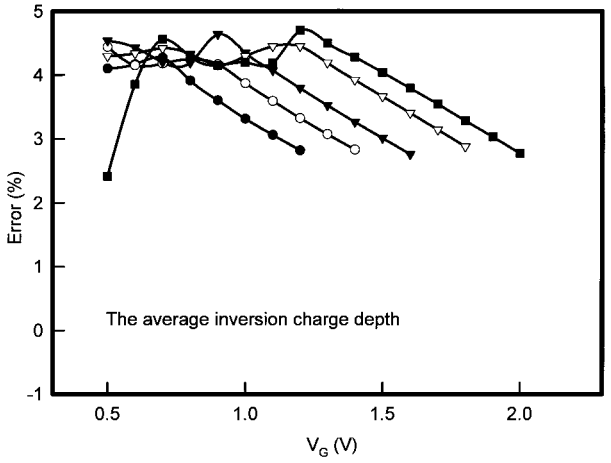

Fig. 8. Error plots of the average inversion charge depth versus V_G for various $T_{\rm ox}$.

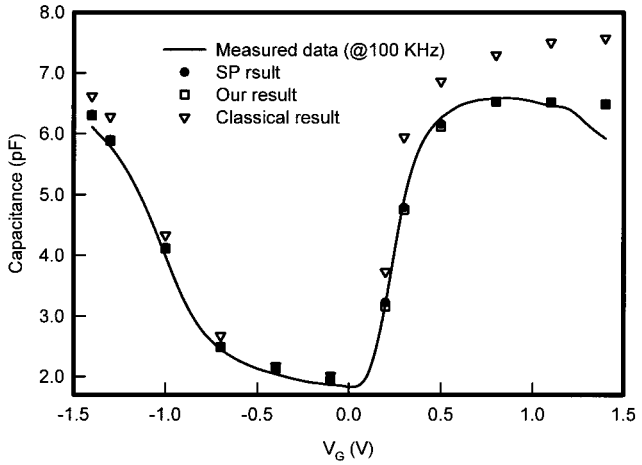

Fig. 9. Comparison of the simulated and measured *C–V* curves for the proposed SPICE-compatible model and the S-P model.

less than 3%. Fig. 8 shows that the error of the average inversion charge depth is within 2%–5%. For the doping concentration N_A varying from 10^{16} cm^{-3} to 10^{18} cm^{-3}, the four errors versus V_G are also estimated with the same fitted a's formula. We have found that the variation of errors are all within 6% and this maximum error of the average inversion charge depth occurred at $N_A = 10^{16}$ cm^{-3}, $T_{\rm ox} = 3.0$ nm, and $V_G = 0.5$ V. For a MOSFET with the Gaussian and low–high doping profiles, we have also found that the error trend is similar to that of uniform doping and that the largest error fluctuation (6.7% for Gaussian doping profile) occurs under low doping level ($N_A = 10^{16}$ cm^{-3}), thicker oxide thickness ($T_{\rm ox} = 3.0$ nm), and low gate bias ($V_G = 0.5$ V) conditions.

Finally, for other applications such as a two-dimensional (2-D) simulation, it is more conventient to express the coefficients: a_0, a_1, and a_3 in terms of the surface electric field E_s and the oxide thickness $T_{\rm ox}$

$$a_0 = 2.11 + 1.3 \times 10^{-6} E_s^{2/3} + 0.085 T_{\rm ox} \tag{6}$$

$$a_1 = -0.96 + 4.2 \times 10^{-3} E_s^{1/3} \tag{7}$$

$$a_3 = 2.13 \times 10^{-8} \left(E_s^{1/2} - 6500 \right)^2 \tag{8}$$

where the $T_{\rm ox}$ is in nm and the E_s in kV/cm is self-consistently computed with the D-D model.

III. Application to Prediction of *C–V* Characteristics

As an application, we have applied our compact quantum correction model for the inversion charge to the calculation of *C–V* curves. A 20×20 μm^2 N-MOSFET with $T_{\rm ox} = 1.6$ nm is fabricated and is measured for the *C–V* curve. The developed model is used to analyze the *C–V* data of the MOSFET sample at a frequency of 100 kHz as shown in Fig. 1. The total capacitance consists of three components in series connection, the poly-gate capacitance ($C_{\rm poly}$), the gate-oxide capacitance ($C_{\rm OX} = \epsilon_{\rm ox}/T_{\rm ox}$, where $\epsilon_{\rm ox}$ is oxide dielectric constant), and the surface capacitance ($C_{\rm surf}$). The total capacitance C is thus given by [11], [12]

$$C = \left(\frac{1}{C_{\rm poly}} + \frac{1}{C_{\rm ox}} + \frac{1}{C_{\rm surf}} \right)^{-1}. \tag{9}$$

The surface capacitance $C_{\rm surf} = \partial Q_{\rm surf}/\partial \phi_s$, where ϕ_s is the surface potential, is computed by the Poisson equation. The surface charge $Q_{\rm surf}$ consists of the inversion and depletion charge, and the computed $n_{\rm QM}$ from (1) is integrated over the entire inversion layer to obtain the inversion charge sheet density. For the sample with 1.6-nm oxide thickness, the doping profile of the device is simulated and calibrated in our *C–V* curve calculation. The experimentally measured data is shown together with the classical and S-P results in Fig. 9. Our result almost coincides

with that of the S-P model as should be. The agreement with the experimental data is excellent except for $V_G \geq 1.0$ V. This is expected as we have assumed zero penetration of the wavefunction into the oxide in our S-P equation solver. The deviation of the calculated result from the measured data indicates that there is a substantial tunneling through the oxide taking place at $V_G \geq 1.0$ V.

IV. Conclusion

Based on the S-P solutions, we have developed a compact model for correcting the classical inversion-layer charge distribution which agrees with the S-P solution within 5%. By inputting the classical charge density from the series expansion solution of Poisson's equation [13], [14] or the D-D-based simulator, together with the device oxide thickness and gate voltage, the proposed inversion-layer charge correction model calculates nanoscale MOSFET inversion charge explicitly, taking into consideration of the quantum effect. The application of this SPICE compatible model to the *C–V* measurement produces an excellent agreement. This inversion-layer charge correction model has continuous derivatives and therefore is amenable to a device simulator. It can also be easily incorporated into circuit simulator for modeling ultrathin oxide MOSFET *C–V* characteristics without impact on the computational time and data storage. We are currently extending this model to include leakage tunneling currents at high gate voltages.

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