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# A unified quantum correction model for nanoscale single- and double-gate MOSFETs under inversion conditions

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Received 16 January 2004

Published 18 June 2004

Online at [stacks.iop.org/Nano/15/1009](http://stacks.iop.org/Nano/15/1009)

doi:10.1088/0957-4484/15/8/026

## Abstract

In this paper a unified quantum correction charge model for nanoscale single- and double-gate MOS structures is presented. Based on the numerical solution of Schrödinger–Poisson equations, the developed quantum correction charge model is mainly optimized with respect to (i) the left and right positions of the charge concentration peak, (ii) the maximum of the charge concentration, (iii) the total inversion charge sheet density, and (iv) the average inversion charge depth, respectively. For nanoscale single- and double-gate MOS structures, this model predicts inversion layer electron density for various oxide thicknesses, silicon film thicknesses, and applied voltages. Compared to the Schrödinger–Poisson results, our model prediction is within 2.5% of accuracy for both the single- and double gate MOS structures on average. This quantum correction model has continuous derivatives and is therefore amenable to a device simulator.

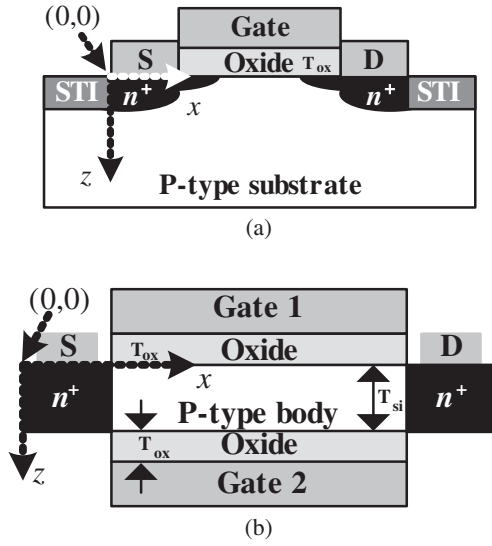
## 1. Introduction

The study of nanoscale single- and double-gate (SG and DG) MOSFETs has been of great interest in recent years [1–11]. As the dimensions of MOSFETs are aggressively scaled into the nanoscale regime, it is quite necessary to take the quantum mechanical effects into consideration in device modelling and simulation. Various approaches have been proposed to investigate the device's quantization effects in the inversion conditions [1, 4, 12–22]. For an oxide thickness ( $T_{ox}$ ) of 1–3 nm, a silicon film thickness ( $T_{si}$ ) of 5–100 nm, and an applied gate voltage ( $V_G$ ) of 0.5–1.5 V, the inversion carrier density shifts away from the interfaces of SiO<sub>2</sub>/Si due to the quantization effect [12]. The Schrödinger–Poisson (SP) equations subject to an appropriate boundary condition at the Si/SiO<sub>2</sub> interfaces have been applied to study such a quantum

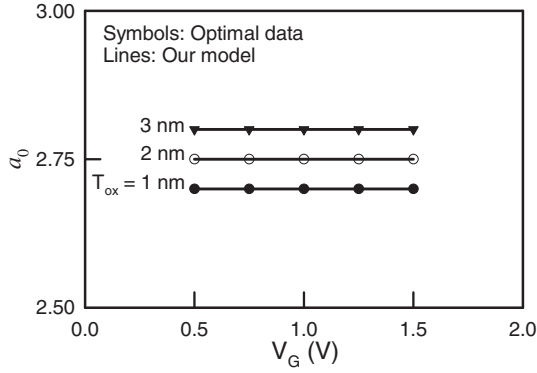
effect [13–15], but it is a time-consuming task in realistic device simulation and characterization.

In this paper, we have successfully developed a unified quantum correction model feasible for nanoscale SG and symmetric and asymmetric DG (SDG and ADG) MOSFETs simulation simultaneously. This unified model for both the SG and DG MOS structures is a generalization of the analytical model proposed by us [16] recently. The numerical solution of SP equations is utilized to construct the model, where there are four physically based optimization constraints: (i) the left and right positions of the charge concentration peak, (ii) the maximum of the charge concentration, (iii) the total inversion charge sheet density, and (iv) the average inversion charge depth; these are considered as criteria for the parameter formulation. All parameters of the unified model are expressed as a function of  $T_{ox}$ ,  $T_{si}$ , and  $V_G$ . For a 2D nanodevice simulation, they can also be in terms of  $T_{ox}$ ,  $T_{si}$ , and surface electric field  $E_s$ . The developed model is

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**Figure 1.** Cross-section views of the nanoscale (a) single-gate MOSFET and (b) double-gate MOSFETs.



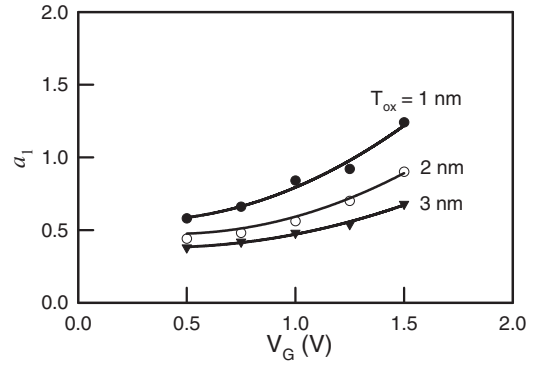
**Figure 2.** Plot of the optimal value for the parameter  $a_0$  and its formula for the SG MOS structure with different  $T_{ox}$  and  $V_G$ .

firstly compared with four well established quantum correction models, i.e., the Hänisch model [17], the modified local density approximation (MLDA) model [18], the density gradient (DG) model [14, 19, 20], and the effective potential (EP) model [21], in terms of accuracy for predicting the inversion layer charge distribution of the SG and DG MOS structures. Application of this charge quantization model to the  $C$ - $V$  measurement of an ultra-thin oxide MOSFET produces an excellent agreement. We have also applied it to the simulation of a 20 nm SDG MOSFET's  $I$ - $V$  curves with a hydrodynamic (HD) device simulator.

This paper is organized as follows. Section 2 introduces the model formulation. Section 3 describes the calculated results illustrating the preliminary model accuracy and different simulation cases. Section 4 draws the conclusions.

## 2. A unified quantum correction model

As shown in figure 1, poly-oxide-silicon (figure 1(a)) and poly-oxide-silicon-oxide-poly (figure 1(b)) are simulated [15, 16, 22]. The coupled Schrödinger and Poisson equations are solved self-consistently along the longitudinal  $z$ -direction under the gate. First of all the Poisson equation

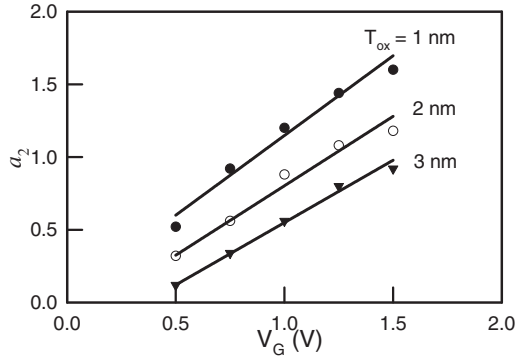


**Figure 3.** Plot of the optimal value for the parameter  $a_1$  and its formula for the SG MOS structure with different  $T_{ox}$  and  $V_G$ .

is solved to obtain the potential distribution. It is then used in the solution of the Schrödinger equation. With the two-dimensional electron gas formula [23, 24], the charge density can be calculated with the solved wavefunctions and energy levels from the Schrödinger equation. Once the new charge density is obtained, it is plugged into the Poisson equation to solve the new potential. The potential is then updated and the Schrödinger equation is solved again. These steps are repeated iteratively until the convergence criterion is reached [13–15]. For simplicity in the model construction, the SP equations considered here are only assumed to have no wave penetration at the Si/SiO<sub>2</sub> interface [13–15]. The SP 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 [13–15]. More than 32 sub-bands are calculated in the Schrödinger equation solver. For the DG MOS structures, the chosen  $T_{ox}$  varies from 1 to 3 nm,  $T_{si}$  varies from 5 to 100 nm, and the applied  $V_G$  ranges from 0.5 to 1.5 V [1–11]. For the SG MOS structures under inversion we consider the electron density from the interface of SiO<sub>2</sub>/Si to silicon bulk completely. For both the SDG and ADG MOS structures, it is sufficient to consider the modelling from the left (or right) interface of SiO<sub>2</sub>/Si to  $T_{si}/2$ . The proposed explicit formula of the calculated inversion-layer charge densities for both the SG and DG MOS structures are

$$n_{QM} = a_0 n_{CL} \left( 1 - \exp \left( -a_1 \xi^2 \left( 1 - \frac{1}{2} \left( \frac{\xi}{\xi_0} \right)^2 \right) - a_2 \xi^3 \right) \right), \quad (1)$$

where  $n_{CL}$  is the classical electron density solved from the Poisson equation.  $\xi = z/\lambda_{th}$  and  $\lambda_{th} = (\frac{\hbar^2}{2m_0 k_B T})^{1/2}$  is the thermal wavelength,  $\hbar$  is the reduced Planck constant,  $m_0$  is the electron rest mass,  $k_B$  is the Boltzmann constant, and  $T$  is the absolute temperature. For the SG MOS structure,  $\xi_0$  is chosen to be the bulk thickness. Physically, the bulk thickness is at infinity where the gradient of potential vanishes. The potential is calculated with the classical Poisson equation. Numerically, it is effectively taken far enough so that it does not significantly affect the results. For example, the bulk thickness used in our modelling and simulation is taken as 100 nm.  $\xi_0 = T_{si}/2\lambda_{th}$  is for both the SDG and ADG MOS structures. The mathematical derivation of (1) is based on an approximate solution of the Schrödinger equation as well as the two-dimensional electron



**Figure 4.** Plot of the optimal value for the parameter  $a_2$  and its formula for the SG MOS structure with different  $T_{ox}$  and  $V_G$ .

gas formulation for the electron density near the interfaces of  $\text{SiO}_2/\text{Si}$  [17, 23, 24]. Using a generic algorithm [25], the three model parameters  $a_0$ ,  $a_1$ , and  $a_2$  are systematically optimized to best fit the self-consistent SP solution with respect to the values of  $T_{ox}$ ,  $T_{si}$ , and  $V_G$  for both the SG and DG MOS structures. The model accuracy of these parameters is based on the optimization with respect to the aforementioned four constraints. The average inversion charge depth is defined as  $\langle z \rangle = \int_0^{T_{si}} zn(z) dz / \int_0^{T_{si}} n(z) dz$ .

The results of these parameters for the SG MOS structures are shown in figures 2–4. As seen in figure 2, the plots of  $a_0$  versus  $V_G$  are horizontal lines and are independent of  $V_G$ . Figure 3 shows that the dependence of the  $a_1$  on  $V_G$  for different  $T_{ox}$  is similar; all have a positive slope when  $V_G \geq 0.2T_{ox}$ . Shown in figure 4 are plots of  $a_2$  versus  $V_G$ , all having a positive slope when  $T_{ox} \leq 10$  nm. For a fixed  $V_G$ , we note that  $a_1$  and  $a_2$  decrease as  $T_{ox}$  increases. Similarly, figures 5–7 show the results of these parameters for the SDG and ADG MOS structures with  $T_{si} = 5$  nm for example. As seen in figure 5, the plots of  $a_0$  versus  $V_G$  are quadric functions of  $V_{G1}$  and  $V_{G2}$ . It is found that  $a_0$  is independent of  $T_{si}$  when  $T_{si}$  approaches infinity. Figure 6 shows that the dependence of the  $a_1$  on  $V_G$  for fixed  $T_{si}$  and different  $T_{ox}$  is similar; all almost have a positive slope. Shown in figure 7 are plots of  $a_2$  versus  $V_G$ , all having a positive slope similar to the cases of SG MOS structure shown in figure 4. It is found that  $a_1$  and  $a_2$  depend only on  $T_{si}$  and  $T_{ox}$  at a very low  $V_{G1}$ . Both  $a_1$  and  $a_2$  are independent of  $T_{si}$  exponentially when  $T_{si}$  approaches infinity. For a fixed  $V_G$ , we note that  $a_0$ ,  $a_1$ , and  $a_2$  decrease as  $T_{ox}$  is increased.

After optimization, a set of these parameters for the SG MOS structure is expressed as a function of  $V_G$  and  $T_{ox}$ :

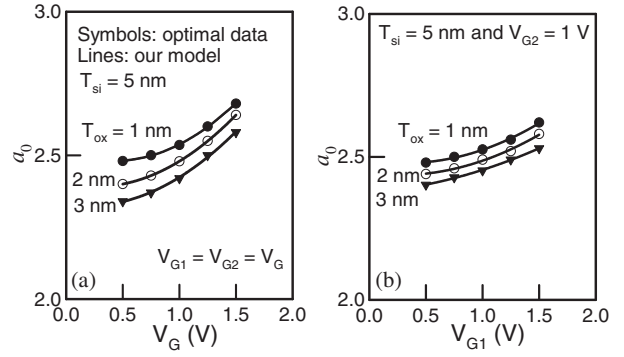
$$a_0 = 2.65 + 0.05T_{ox}, \quad (2)$$

$$a_1 = 0.549 - 0.0152T_{ox} - 0.159T_{ox}V_G + 0.398V_G^2, \quad (3)$$

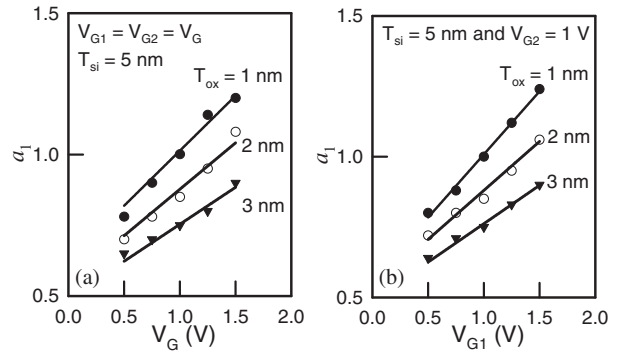
$$a_2 = 0.252 - 0.172T_{ox} + 1.104V_G - 0.1T_{ox}V_G, \quad (4)$$

where  $V_G$  is in volts and  $T_{ox}$  is in nanometres. With variables of  $V_{G1}$ ,  $V_{G2}$ ,  $T_{si}$ , and  $T_{ox}$ , the parameters for both the SDG and ADG MOS structures are

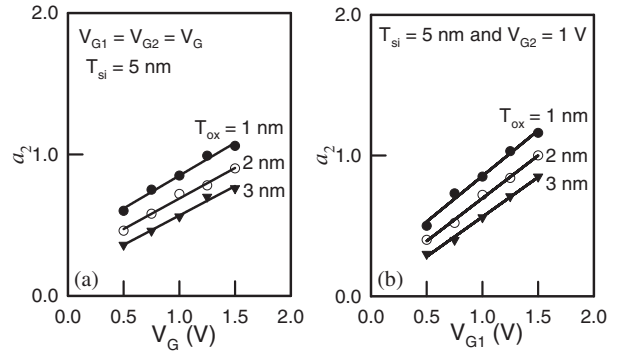
$$a_0 = 1.456 + \frac{0.314}{T_{ox}} + \frac{3.980}{T_{si}} - \frac{0.502(V_{G1} + V_{G2})}{T_{ox}T_{si}} + 0.0427(V_{G1} + V_{G2})^2, \quad (5)$$



**Figure 5.** Plot of the optimal value for the parameter  $a_0$  and its formula for the (a) SDG and (b) ADG MOS structures with different  $T_{ox}$  and  $V_G$ , where  $V_{G2}$  is fixed at 1 V for the case of ADG.



**Figure 6.** Plot of the optimal value for the parameter  $a_1$  and its formula for the (a) SDG and (b) ADG MOS structures with different  $T_{ox}$  and  $V_G$ , where  $V_{G2}$  is fixed at 1 V for the case of ADG.

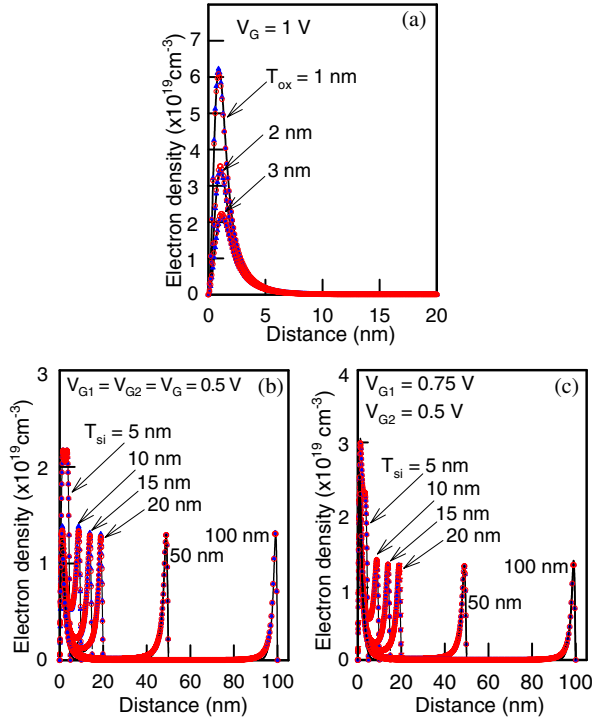


**Figure 7.** Plot of the optimal value for the parameter  $a_2$  and its formula for the (a) SDG and (b) ADG MOS structures with different  $T_{ox}$  and  $V_G$ , where  $V_{G2}$  is fixed at 1 V for the case of ADG.

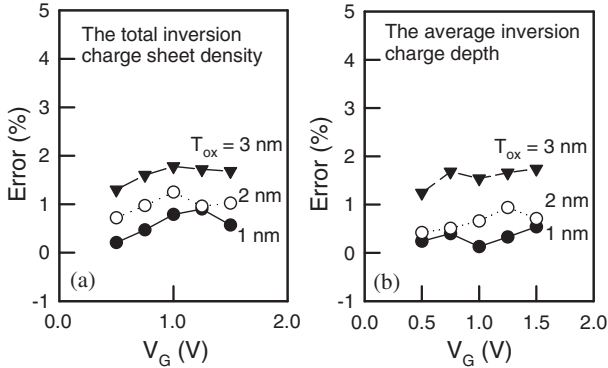
$$a_1 = 0.087 - 60.881 \exp(-T_{si}) + \frac{0.916}{T_{ox}} + 0.909V_{G1} - \frac{102.121 \exp(-T_{si})V_{G1}}{T_{ox}} + \frac{0.341V_{G1}^2}{(V_{G1} + V_{G2})}, \quad (6)$$

$$a_2 = 0.011 + 52.041 \exp(-T_{si}) - \frac{0.0421}{T_{ox}} - 0.115V_{G1} + \frac{86.036 \exp(-T_{si})V_{G1}}{T_{ox}} + \frac{0.244V_{G1}^2}{(V_{G1} + V_{G2})}, \quad (7)$$

where  $V_{G1}$  and  $V_{G2}$  are in volts, and  $T_{si}$  and  $T_{ox}$  are in nanometres. The two sets of the model parameters given



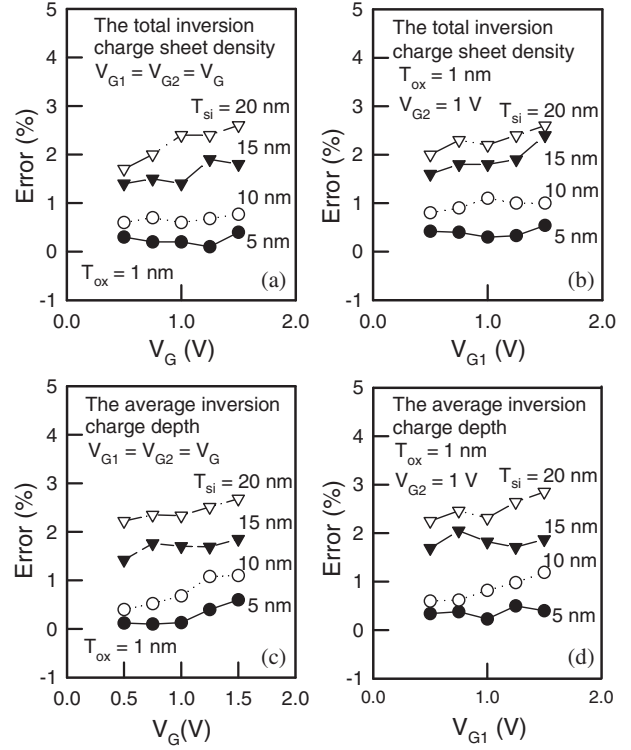
**Figure 8.** Electron density with the SP (curves) model, the optimal value (triangles), and our model (circles) for the (a) SG, (b) SDG, and (c) ADG MOS structures.



**Figure 9.** Errors of (a) the total inversion charge sheet density and (b) the average inversion charge depth versus  $V_G$  for the case of an SG with different  $T_{ox}$ .

in (2)–(4) and (5)–(7) are based on a p-type silicon body with  $N_A = 10^{17} \text{ cm}^{-3}$ . For other doping concentrations,  $V_G$  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 ( $\sim 0.1 \text{ V}$ ). The accuracy of the model inversion-layer charge density given by (1), (2)–(4), and (5)–(7) compared to the SP solution is very good. In terms of the four criteria mentioned above, the accuracy is within 2.5%.

Shown in figures 8(a)–(c) are the electron densities between our results (symbols) and the SP solutions (lines) against distance for the SG, SDG, and ADG MOS structures, respectively. A uniform doping profile with  $N_A = 10^{17} \text{ cm}^{-3}$  is used for the simulations. Shown in figures 9, 10 respectively are the errors between the established  $a$  formula and the SP solution against  $V_G$  for each optimization criterion in the SG and DG MOS structures. For the SG MOS structure, as shown



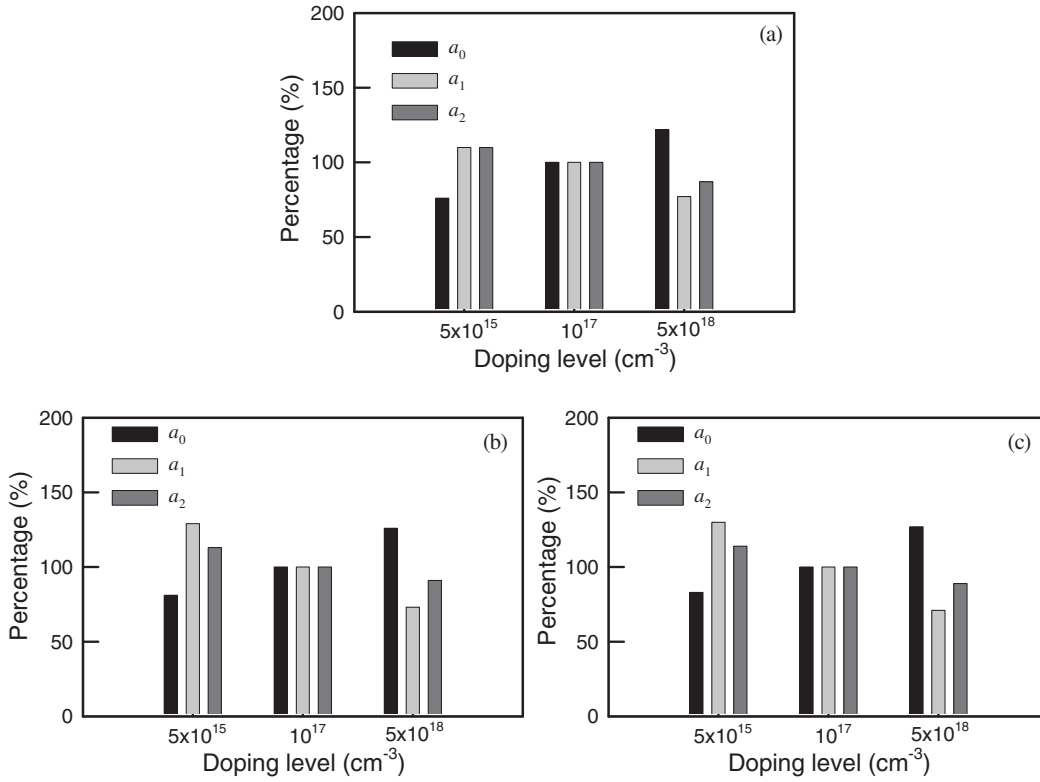
**Figure 10.** Errors of the total inversion charge sheet density versus  $V_G$  for both the (a) SDG and (b) ADG. Errors of the average inversion charge depth versus  $V_G$  for both the (c) SDG and (d) ADG with different  $T_{si}$ .

in figures 9(a) and (b), the errors of the total inversion charge sheet density and the average inversion charge depth between our model and the SP equation are all less than 1.8%. The error of the position of the charge concentration peak and the error of the maximum of the charge concentration are both less than 1%. For both the SDG and ADG MOS structures, figures 10(a) and (b) show that the error of the total inversion charge sheet density between our model and the SP equation is less than 2.6%. Figures 10(c) and (d) show that the error of the average inversion charge depth is within 2.7%. The error of the left and right positions of the charge concentration peak is less than 2.1%, and the error of the maximum of the charge concentration is less than 1.8%, respectively. For the SG and DG MOS structures with different doping profiles, i.e., Gaussian doping profiles and low-high doping profiles, and concentration  $N_A$  varying from  $10^{16}$  to  $10^{18} \text{ cm}^{-3}$ , the four errors versus  $V_G$  are also theoretically estimated with the same  $a$  formula. We have found that the error fluctuations are all less than 4.8%, and this maximum error occurred at the SDG MOS structure with the Gaussian doping profiles with  $N_A = 10^{16} \text{ cm}^{-3}$ ,  $T_{ox} = 3.0 \text{ nm}$ ,  $T_{si} = 100 \text{ nm}$  and  $V_G = 0.5 \text{ V}$ . We have expressed the coefficients  $a_0$ ,  $a_1$ , and  $a_2$  in terms of the surface electric field  $E_s$  and the oxide thickness  $T_{ox}$  for applications to a two-dimensional (2D) simulation. For the SG MOS structure, the formulae are

$$a_0 = 2.65 + 0.05T_{ox}, \quad (8)$$

$$a_1 = 0.222 + 0.220E_s + 0.0652E_s^2, \quad (9)$$

$$a_2 = -0.5137 + 1.329E_s - 0.212E_s^2, \quad (10)$$



**Figure 11.** The variation percentage of the modelled parameters  $a_0$ ,  $a_1$ , and  $a_2$  versus the uniform doping level. (a) The result of the SG MOS structure with  $V_G = 1.5$  V,  $T_{ox} = 1$  nm, (b) the plot of the SDG MOS structure with  $V_{G1} = V_{G2} = 1.5$  V,  $T_{ox} = 1$  nm, and  $T_{si} = 5$  nm, and (c) the plot of the ADG MOS structure with  $V_{G1} = 1.5$  V,  $V_{G2} = 1.0$  V, and  $T_{ox} = 1$  nm.

and for the DG MOS structures the formulae are

$$a_0 = 1.639 + \frac{0.0598}{T_{ox}} + \frac{3.905}{T_{si}} - \frac{0.333(E_{S1} + E_{S2})}{T_{ox}T_{si}} + 0.0202(E_{S1} + E_{S2})^2, \quad (11)$$

$$a_1 = 0.694 - 81.93 \exp(-T_{si}) - \frac{0.256}{T_{ox}} + 0.773E_{S1} - \frac{50.99 \exp(-T_{si})E_{S1}}{T_{ox}} + \frac{0.259E_{S1}^2}{E_{S1} + E_{S2}}, \quad (12)$$

$$a_2 = 0.0247 + 96.02 \exp(-T_{si})E_{S1} + \frac{0.0628}{T_{ox}} - 0.148E_{S1} - \frac{28.6 \exp(-T_{si})E_{S1}}{T_{ox}} + \frac{0.189E_{S1}^2}{E_{S1} + E_{S2}}, \quad (13)$$

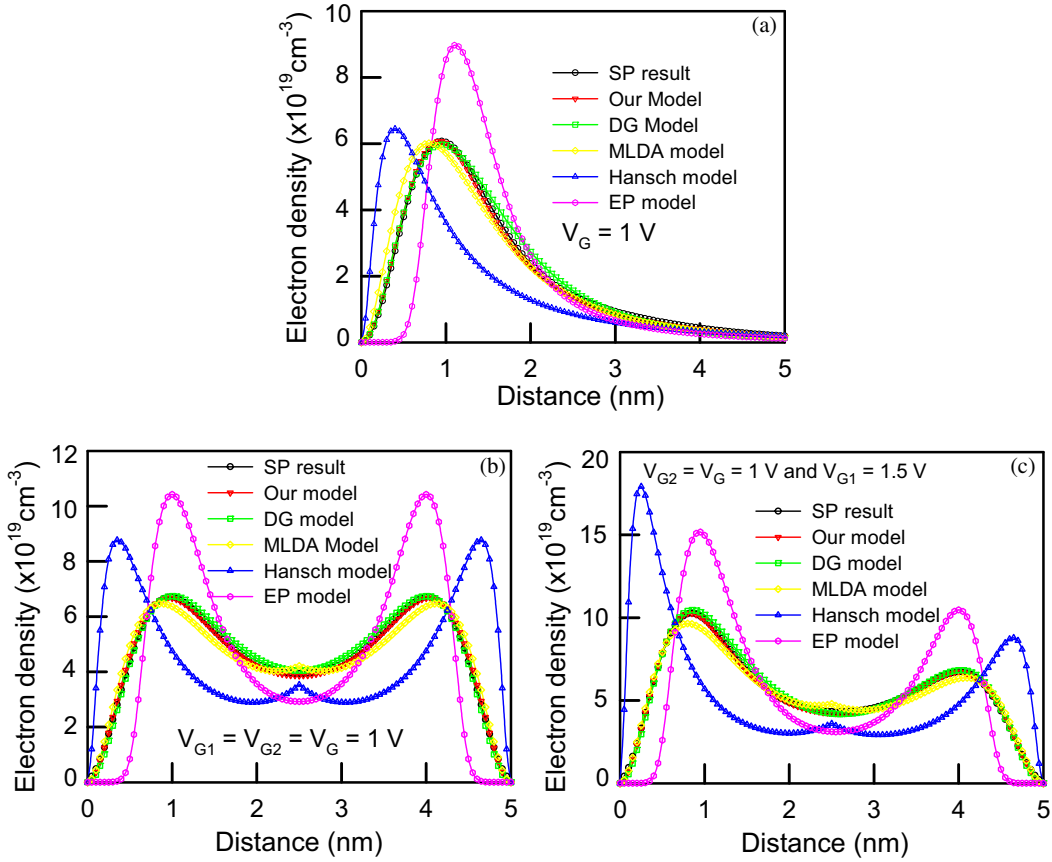
where  $T_{ox}$  is in nm and the  $E_s$  in  $\text{MV cm}^{-1}$  is self-consistently computed with the DD model. If the silicon film thickness of the DG MOS structure becomes very thick, i.e.,  $T_{si}$  approaches infinity in (5)–(7) and (11)–(13), the models of  $a$  are independent of  $T_{si}$ .

The model parameters  $a_0$ ,  $a_1$ , and  $a_2$  discussed above are mainly based on the doping level  $N_A = 10^{17} \text{ cm}^{-3}$ . To assess the validity of the proposed model, the variation of the modelled parameters  $a_0$ ,  $a_1$ , and  $a_2$  with respect to the doping level is further examined. For the aforementioned four constraints under the same error criteria above, the variation is calculated for all  $V_G$ ,  $T_{ox}$ , and  $T_{si}$ . For both the SG and DG MOS structures with uniform doping profile, the modelled parameter  $a_0$  increases when the doping level varies from  $5 \times 10^{15}$  to  $5 \times 10^{18} \text{ cm}^{-3}$ . Both the modelled parameters  $a_1$  and  $a_2$  decrease when the doping level changes from  $5 \times 10^{15}$

to  $5 \times 10^{18} \text{ cm}^{-3}$ . For example, under a set of fixed  $V_G$ ,  $T_{ox}$ , and  $T_{si}$ , figures 11(a)–(c) show the variation of the modelled parameters  $a_0$ ,  $a_1$ , and  $a_2$  versus the doping level, respectively. Based on our numerical calculations, it is found that the variation of the three modelled parameters  $a_0$ ,  $a_1$ , and  $a_2$  is within 25% for all  $V_G$ ,  $T_{ox}$ , and  $T_{si}$ .

### 3. Results and discussion

Figures 12(a)–(c) are comparisons of the inversion layer charge distribution for the SG, SDG, and ADG MOS structures among the Hänsch model [17], the MLDA model [18], the EP model [21], the DG model [14, 19, 20], and our model. A uniform doping profile with  $N_A = 10^{17} \text{ cm}^{-3}$  and  $T_{ox} = 1$  nm are assumed for the SG and DG MOS structures.  $T_{si} = 5$  nm is for the cases of SDG and ADG. The parameter  $m_k$  appearing in the first four well known quantum correction models are optimally determined by calibrating with the SP solutions [22, 26]. More than 32 subbands are calculated in the Schrödinger equation solver. For the SG MOS structure, the optimized  $m_k$  is  $0.36 m_0$  ( $m_0 = 9.11 \times 10^{-31} \text{ kg}$ ),  $0.41$ ,  $0.283$ , and  $1.22 m_0$  corresponding to the Hänsch, the MLDA, the EP, and the DG models, respectively. The optimized  $m_k$  in the SDG MOS structure is  $0.32$ ,  $0.45$ ,  $0.315$ , and  $1.41 m_0$  (similarly, the optimized  $m_k$  in the ADG MOS structure is  $0.27$ ,  $0.41$ ,  $0.291$ , and  $1.34 m_0$ ) for the Hänsch, the MLDA, the EP, and the DG models, respectively. Among these simulations we find that the agreement of our result with the SP data is excellent in the prediction of the inversion layer charge distributions. The

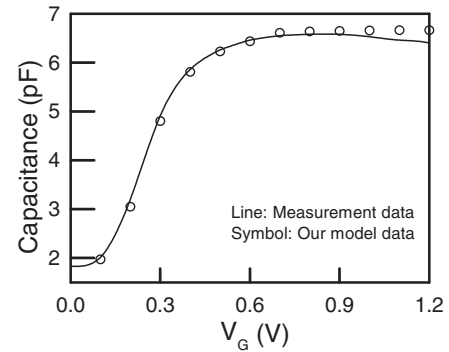


**Figure 12.** Electron density with different models for the (a) SG, (b) SDG, and (c) ADG MOS structures.

Hansch and MLDA models are found to have non-physical kinks in the DG MOS simulation which are sensitive to the selection of parameter  $m_k$  and depend on  $T_{si}$  and  $V_{G1}$  and  $V_{G2}$ , as seen in figures 12(b) and (c).

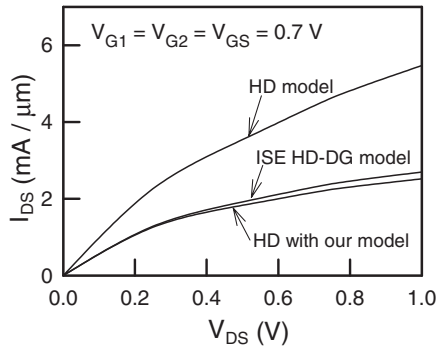
As applications, we apply our quantum correction model, equations (1) and (2)–(4), for the inversion charge to the calculation of  $C$ – $V$  curves. A  $20 \times 20 \mu\text{m}^2$  N-MOSFET with  $T_{ox} = 1.6 \text{ nm}$  is considered for investigating the  $C$ – $V$  curves. The details of the calculation of  $C$ – $V$  curves as well as the experimental measurement setting were discussed in [16]. As shown in figure 13, the agreement of our result with the measurement is acceptable except for  $V_G \geq 1.0 \text{ V}$ . The difference between simulated and measured  $C$ – $V$  curves is due to the assumption of zero wavefunction penetration in the SP equations.

Application to a 2D DG MOSFET simulation is performed with the quantum correction model in terms of  $E_s$ ,  $T_{ox}$ , and  $T_{si}$ . The drain current ( $I_{DS}$ ) of the 20 nm SDG N-MOSFET is computed using the conventional HD model together with equations (1) and (11)–(13). The device in our simulation is with  $T_{si} = 10 \text{ nm}$  and  $T_{ox} = 2 \text{ nm}$ . We assume the source and drain doping concentration  $N_D = 10^{20} \text{ cm}^{-3}$ . The device has a uniform channel doping profile  $N_A = 10^{17} \text{ cm}^{-3}$ . The mobility model is crucial to nanoscale device simulation. In this simulation a field dependent mobility is adopted [11, 27]. However, different surface mobility models lead to different drain current also in the linear region. Therefore, advanced studies and experimental calibration are necessary to enable a sound model for practical nanoscale



**Figure 13.** Comparison of  $C$ – $V$  curves between our model and the SP model for a  $20 \times 20 \mu\text{m}^2$  N-MOSFET with  $T_{ox} = 1.6 \text{ nm}$ .

MOSFETs simulation. Numerical solution of the 2D classical HD with and without a quantum correction model is achieved by using an adaptive mesh refinement technique [28, 29]. Error estimation is performed on the computed results, and therefore the simulation mesh is refined to locate the sharp variations of electrostatic potential and electron density near the channel surfaces and drain side. Figure 14 shows the computed  $I_{DS}$  versus drain voltage ( $V_{DS}$ ) for the 20 nm SDG MOSFETs at gate voltage  $V_{G1} = V_{G2} = 0.7 \text{ V}$ . Due to the overestimation of the current density at both surfaces of the device channel, the classical HD simulation yields higher drain current levels ( $>40\%$  at  $V_{DS} = 1 \text{ V}$ ) than the quantum mechanical simulation [30–32]. To verify the validity of our



**Figure 14.** The simulated drain current of the 20 nm SDG N-MOSFET using the classical HD with and without the quantum correction model.

simulation, we have performed the same simulation by using an ISE DESSIS device simulator (version 8.5), where the 2D HD together with the density-gradient (DG) model is simulated. As shown in figure 14, it is found that the result obtained with our proposed model has demonstrated its accuracy in comparison to the results calculated with the HD-DG model. However, for including complete transport phenomena, such as the short channel effect for multi-dimensional application, a set of 2D SP equations should be further considered in the model formulation.

#### 4. Conclusions

We have successfully developed a unified quantum correction model for correcting the classical inversion-layer charge distribution which agrees with the SP solution within 2.5%. By using the classical charge density from the solution of the DD/HD based device simulator, together with the device oxide thickness, silicon film thickness, and gate voltage (or surface electric field), the proposed inversion-layer charge correction model calculates nanoscale single- and double-gate MOSFET inversion charge explicitly, taking into consideration the quantum effect. Comparisons among the four well known quantum correction models suggest that the proposed model is attractive to the modelling of nanoscale MOSFETs. The application of this model to the  $C-V$  measurement has produced an excellent agreement. Our preliminary 2D HD simulation shows that this inversion-layer charge correction model is computationally cost-effective and amenable to a device simulator for industrial application.

#### Acknowledgments

This work is supported in part by the National Science Council of TAIWAN under contract No. NSC-92-2112-M-429-001 and by the grant of the Ministry of Economic Affairs, Taiwan under contract No. PSOC 92-EC-17-A-07-S1-0011.

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