

# A Comparison of Quantum Correction Models for the Three-Dimensional Simulation of FinFET Structures

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## Abstract

For the prediction of the device performance of FinFET structures three-dimensional device simulation is inevitable. Due to the strong quantum mechanical confinement in the channel, quantum correction models need to be applied. Two of these models, where one is based on the correction of the density-of-states in a pre-processing step and the other calculates a correction for the band edge energy, have been implemented in the device simulator Minimos-NT. The models have been applied to the simulation of double- and triple-gate FinFET structures. However, while the drive current reduction can be reproduced, the carrier concentration in the fin shows only poor agreement with rigorous quantum mechanical simulation.

*Keywords:* three-dimensional device simulation, FinFET, quantum correction models

## Introduction

CMOS device technology is undergoing a constant shrinking process. According to the International Technology Roadmap for Semiconductor Devices 2003 [1] the printed gate length will scale down to 28 nm until 2009. With this perspective in mind fully-depleted devices such as FinFETs are very promising candidates due to their immunity against short-channel effects. FinFET devices with a gate width of only 6.5 nm have already been reported [2]. In contrast to bulk MOSFETs, these devices inherently require three-dimensional investigations [3, 4]. Unfortunately, with shrinking device dimensions classical device simulation becomes more and more inaccurate. A rigorous Schrödinger-Poisson solver would be necessary to accurately describe the device behaviour. As such simulations are computationally extremely demanding, due to the large number of grid points in three-dimensional problems, they are normally not appropriate. Instead, classical device simulations with additional quantum correction models can be used. However, the validity of these models for ultra thin silicon layers is currently under heavy discussion.

## Quantum Correction Models

The drift-diffusion model estimates an exponential increase of the carrier concentration towards the Si/SiO<sub>2</sub> interface. Quantum mechanical simulations show, however, that the charge centroid is located several angstroms away from the interface. Therefore, several quantum confinement models have been proposed.

### Density-of-States Correction

In classical device simulation the density-of-states (DOS) in homogenous materials is modeled as a constant value throughout the device. In order to describe the quantum mechanical confinement a distance-dependent reduction of the DOS at the Si/SiO<sub>2</sub> interface has been proposed [5, 6]

$$h_{\text{corr}} = 1 - \exp\left(-\frac{(z+z_0)^2}{\zeta^2 \lambda_{\text{TH}}^2}\right), \quad (1)$$

where  $z$  is the distance to the Si/SiO<sub>2</sub> interface, the parameter  $z_0$  moves the whole function relative to the interface, and  $\zeta$  is a newly introduced parameter which enables the variation of  $\lambda_{\text{TH}}$  for fitting purposes. The symbol  $\lambda_{\text{TH}}$  denotes the thermal wavelength which is given by

$$\lambda_{\text{TH}} = \frac{\hbar}{\sqrt{2mk_{\text{B}}T}}. \quad (2)$$

The resulting DOS  $N_{\text{c}}$  is then calculated from the classical DOS  $N_{\text{c},0}$  with the correction factor  $h_{\text{corr}}$  as

$$N_{\text{c}} = N_{\text{c},0} h_{\text{corr}}. \quad (3)$$

The interplay of the different parameters and the distance to the Si/SiO<sub>2</sub> interface can be seen in Figure 1. The parameter  $z_0$  is important, because with  $z_0 = 0$  the DOS at the interface becomes zero. This leads to convergence problems of the numerical solver. The value of  $\zeta \lambda_{\text{TH}}$  defines the effective depth of the correction. A high value which can be achieved with  $\zeta > 1$ , leads to a reduction of the DOS even deep in the substrate.

Note that the correction factor does not depend on the bias, and the band edge energies are not influenced. Hence, the model can be evaluated in a pre-processing step and does not impose any additional computational burden during iteration steps.

### Band Edge Energy Correction

An alternative approach is based on  $\mathcal{E}_0$ , the first eigenvalue of the triangular energy well seen in Figure 2. This model was proposed by van Dort [7]

$$\Delta\mathcal{E}_g = \mathcal{E}_0 - \mathcal{E}_c(0) = \frac{13}{9}\beta\left(\frac{\kappa_{si}}{4qk_B T}\right)^{\frac{1}{3}}|E_n|^{\frac{2}{3}}, \quad (4)$$

where  $\beta = 4.1 \times 10^{-8}$  eVcm is an empirically determined constant,  $\kappa_{si}$  is the permittivity of silicon, and  $E_n$  is the electric field at the Si/SiO<sub>2</sub> interface perpendicular to the interface.

The value of  $\Delta\mathcal{E}_g$  is multiplied with a distance-dependent weight function which has been introduced in [8] for the modeling of surface roughness scattering in MOSFETs. The function is of the following form:

$$F(z) = \frac{2 \exp(-(z/z_{ref})^2)}{1 + \exp(-2(z/z_{ref})^2)}, \quad (5)$$

where  $z_{ref}$  is the scaling factor for the interface distance. The resulting band gap energy with van Dort's quantum correction reads as follows:

$$\mathcal{E}_c = \mathcal{E}_{class} + F(z)\Delta\mathcal{E}_g. \quad (6)$$

Figure 2 depicts the distance dependent weight function  $F$  and the band edge energy for both, the classical approach and after quantum correction with van Dort's method.

### FinFET Simulation

For the evaluation of the quantum correction models a state-of-the-art three-dimensional FinFET device structure was chosen. The device geometry can be seen in Figure 3. The silicon fin has a size of  $6 \times 10 \text{ nm}^2$ . The gate length is 20 nm with a gate oxide thickness of 1.5 nm. The source and drain regions are heavily n-type doped whereas the channel itself remains undoped.

The contour lines of the electron concentration as a two-dimensional cut through the silicon fin can be seen in Figure 4. The gates are biased at 0.9 V and the source and drain contacts are unbiased.

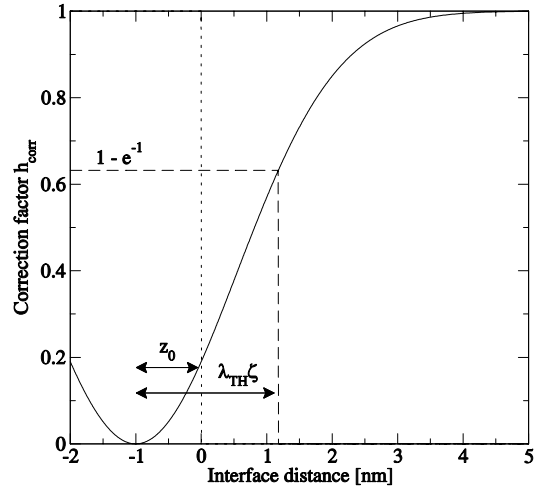


Fig. 1: Plot of the DOS correction factor  $h_{corr}$  for  $z_0 = 1$  nm and  $z = 1$  at  $T = 300$  K.

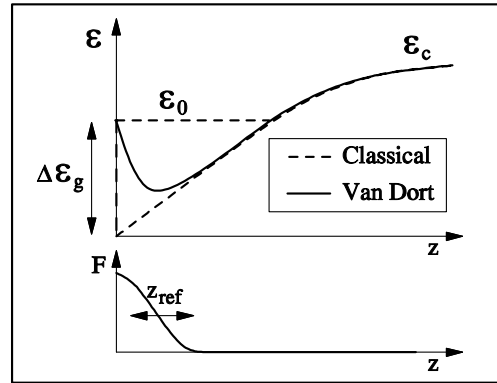


Fig. 2: Band edge bending at the Si/SiO<sub>2</sub> interface. The classical band edge is corrected by the factor  $\Delta\mathcal{E}_g F(z)$ .

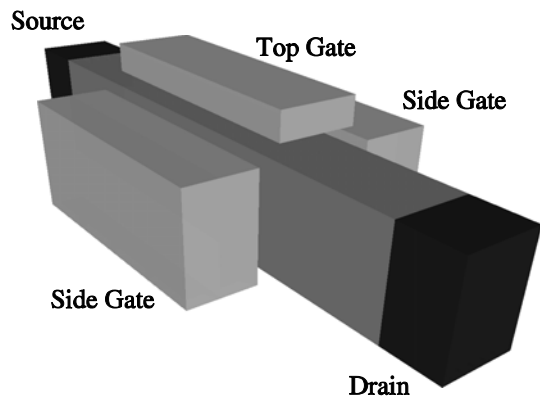


Fig. 3: Device geometry of a triple-gate FinFET structure

The picture shows a comparison of a classical simulation with a simulation using the DOS correction model with the maximum electron concentration at the inside of the fin.

Figure 5 depicts the electron concentration across the silicon fin for a gate voltage of 0.9 V and unbiased source and drain contacts. The classical simulation shows the maximum of the electron concentration at the Si/SiO<sub>2</sub> interface whereas the quantum correction models move the peak to the inside.

A comparison of FinFETs with different fin widths can be seen in Figure 6. It shows the electron concentration across the fin simulated with both, the classical drift-diffusion model and a Schrödinger solver, respectively. The fin widths are 6, 12, and 18 nm. At a fin width of 6 nm the electron concentration has its maximum in the center of the fin. This shape of the carrier concentration cannot be reproduced by the quantum correction models. With larger widths the maximum moves to the interfaces enabling a better fit of the correction models.

The channels in the silicon fin are displaced from the surface to the inside of the silicon and thus the drive current is reduced. Figure 7 depicts the drain current for a gate voltage of 0.9 V and different quantum correction mechanisms. Additionally to the triple-gate device the simulation has been performed with a double-gate structure, where the top gate from Figure 3 has been replaced with SiO<sub>2</sub>. Simulation of the double-gate structure show a reduced output current by a factor of approximately 20 % which can be explained by the channel geometry.

### Conclusion

We have presented a comparison of different quantum correction models and applied them to a state-of-the-art three-dimensional device structure. Quantum correction leads to a considerable reduction of the saturation current. The DOS correction model yields reasonable results, but since it does not account for the band bending it must be calibrated for each bias point. Van Dort's model completely fails to reproduce the carrier concentration in the channel which may be due to the assumption of a triangular energy well, which does not hold for extremely thin channels. Therefore, these models cannot be used to describe effects which depend on the shape of the carrier concentration in the channel.

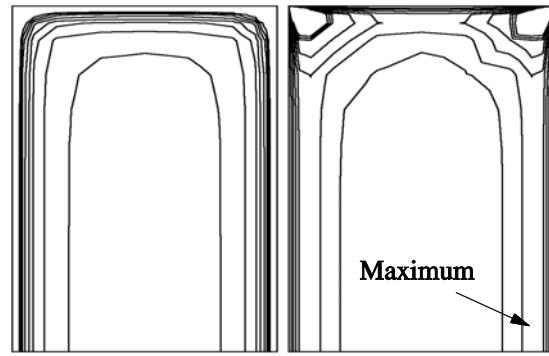


Fig. 4: Electron concentration in a triple-gate FinFET for classical simulation (left) and with the DOS correction model.

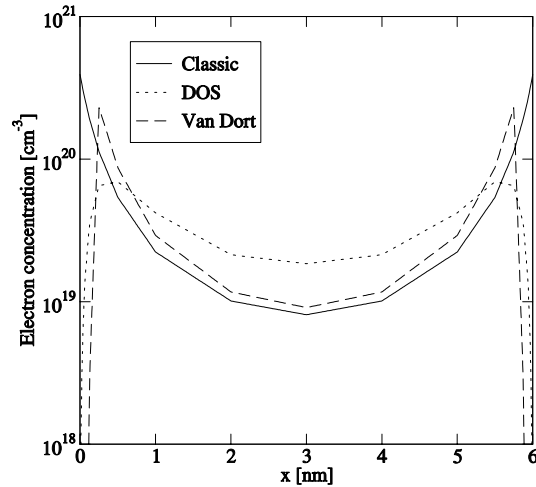


Fig. 5: Electron concentration across the fin applying different correction models

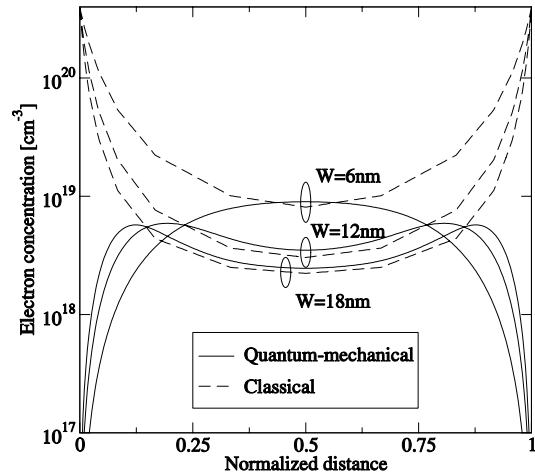


Fig. 6: Comparison of classical and quantum mechanical carrier concentrations for different fin widths

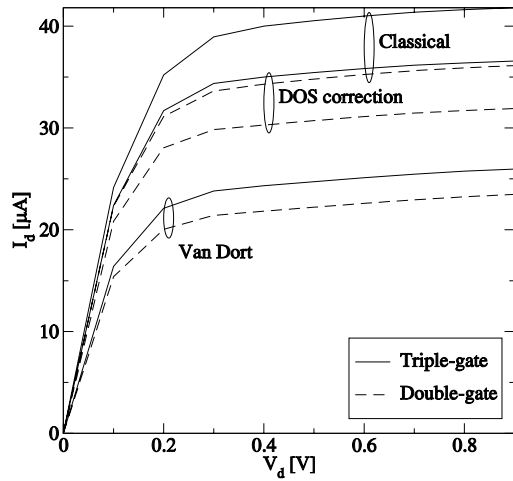


Fig. 7: Comparison of the output characteristics of double- and triple-gate FinFETs at a gate voltage of 0.9 V

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