Quantum Correction Models for Modern Semiconductor Devices

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ABSTRACT: Due to the strong quantum mechanical impact on the characteristics of modern semiconductor devices, classical device simulators have to be adapted. In this work several quantum correction models developed in order to improve device simulation results are compared to self-consistent Schrödinger Poisson solutions. Furthermore, we judge their applicability to conventional and upcoming technology nodes.

INTRODUCTION

The continously shrinking size of device structures increases the influence of quantum mechanical effects. Besides tunneling, the effect of quantum confinement highly affects the characteristics of bulk, SOI, and double gate (DG) MOSFET devices under inversion conditions. Classical simulation predicts an exponential shape of the carrier concentration near the gate oxide. However, due to quantum confinement, which affects the local density of states, the carrier concentration near the gate oxide decreases. To modify classical simulations, several correction models have been proposed.

Schrödinger Poisson (SP) solvers, which deliver a self consistent solution of a quantum mechanically calculated carrier density and the Poisson equation, provide accurate results. However, since the evaluation of the quantum mechanical electron density is based on the calculation of the eigenstates of a Hamiltonian, which is computationally very demanding, the application of SP solvers is impractical. Since classical simulation can not cover quantum mechanical effects, proper correction models have to be applied.

QUANTUM CORRECTION MODELS

One of the early published quantum correction models is based on the local density approximation (LDA) suitable for band edges in an inversion layer, called the modified LDA [1, 2, 3].

While the effective density-of-states (DOS) N_c is constant in classical device simulation, the modified local density approximation (MLDA) models the quantum mechanical impact

near the gate oxide as a local correction of the effective DOS with the characteristic thermal wavelength

$$N_\mathrm{c} = N_\mathrm{c,0}\Big(1 - \exp\Big(-\frac{\big(z+z_0\big)^2}{\zeta^2\lambda_{th}^2}\Big)\Big), \qquad \lambda_{th} = \frac{\hbar}{\sqrt{2m_\mathrm{e}\mathrm{k_B}T}}.$$

The parameter ζ is used for fitting purposes. Since a DOS value of zero at the gate interface would lead to convergence problems of the solver, the distance to the gate oxide interface z is increased by z_0. As an advantage of this method, no solution variable is used as parameter, so the model can be implemented as a preprocessing step and has only a minor effect on the overall CPU time.

A different approach was proposed by Van Dort [4]. The confinement of minority carriers in the inversion layer is modeled as a local effective bandgap widening

$$\Delta\mathcal{E}_\mathrm{g} = \frac{13}{9}\beta\Big(\frac{\kappa_\mathrm{Si}}{4\mathrm{qk_B}T}\Big)^{1/3}|E_\perp|^{2/3}, \qquad F(z) = \frac{2\exp\big(-\big(z/z_\mathrm{ref}\big)^2\big)}{1+\exp\big(-2\big(z/z_\mathrm{ref}\big)^2\big)}.$$

An empirical correction accounting for the perpendicular electric field $E_\perp$ is applied. The correction decays as a function of the distance to the interface $F(z)$. This finally leads to a corrected conduction band edge $\mathcal{E}_\mathrm{c} = \mathcal{E}_\mathrm{class} + F(z)\Delta\mathcal{E}_\mathrm{g}$. However, this model depends on the potential, which is a solution variable, and therefore it has to be calculated after each iteration which results in a higher computational effort and occasional convergence problems.

An improved version of the MLDA (IMLDA) was presented in [5, 6] for nMOSFETs where a correction is applied on the conduction band edge energy. As the MLDA and in contrast to the Van Dort correction model, it only depends on the local doping concentration, the local lattice temperature and the distance from the interface, so convergence behavior, robustness and CPU efficiency of classical device simulation are retained. The corrected electron density reads

$$\begin{aligned} n(z) =& n_\mathrm{class}\Big(1 - \frac{2}{3}\exp\big(-(\lambda_\mathrm{t}z)^2\big) - \frac{1}{3}\exp\big(-(\lambda_\mathrm{t}z)^2\big)\Big) = \\ & n_\mathrm{class}\exp\Big(-\frac{\mathrm{q}\Psi_{q,n}(z)}{\mathrm{k_B}T}\Big) \end{aligned}$$

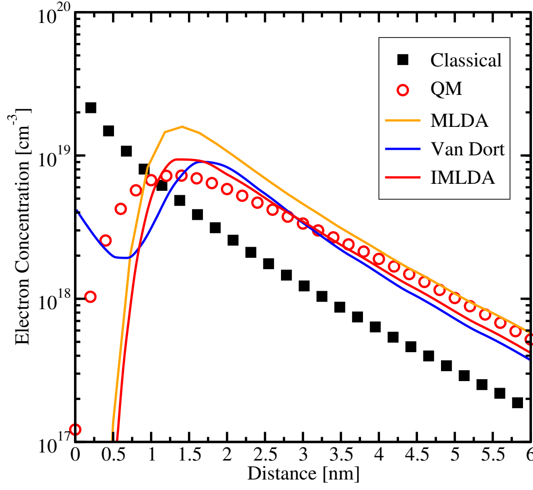

Fig 1: Electron concentration near the Si/SiO_2 interface of a bulk MOSFET with 3 nm oxide thickness.

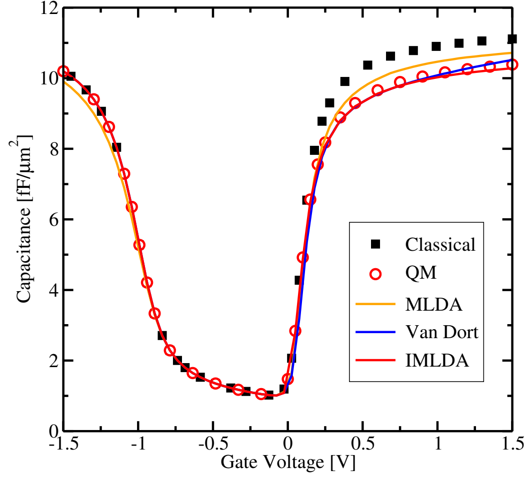

Fig 2: The capacitance voltage characteristics calculated using different quantum correction models.

with the transversal and longitudinal wavelengths $\lambda_{t,l}^2 = \zeta^2 2m_{t,l}k_B T/\hbar^2$. The factor ζ describes the distance dependence of the correction which itself depends on an empirical, doping dependent factor ξ. It is calibrated for a temperature range from 200 K to 500 K and acceptor concentrations up to $5 \times 10^{18}\,\mathrm{cm}^{-3}$.

SIMULATION RESULTS

The models described above were implemented in the device simulator MINIMOS-NT and applied to state-of-the-art single- and double gate MOSFET devices. As a reference, a self-consistent SP solver was used.

Fig. 1 shows the electron concentration near the Si/SiO_2 interface of a single gate MOSFET with 3 nm oxide thickness and a bulk doping of $10^{17}\,\mathrm{cm}^{-3}$ at a bias of 0.5 V. In contrast to the classical distribution of the electron concentration, the QM calculated concentration has a shifted charge centroid. The capacitance voltage characteristics are shown in Fig. 2. In contrast to the MLDA model, which cannot reproduce this CV curve accurately, both the Van Dort and IMLDA model show excellent agreement with the QM derived curve. Furthermore, the MLDA model has an impact in the accumulation regime, which is not physical. Figs. 3 and 4 show the electron concentration within a double gate MOSFET with 3 nm oxide thickness at a bias of 0.5 V. With shrinking device size, the z_0 parameter of the Van Dort model has more impact. All models show an unphysical increase of the concentration in the center of the device at thicknesses of 5 nm and below.

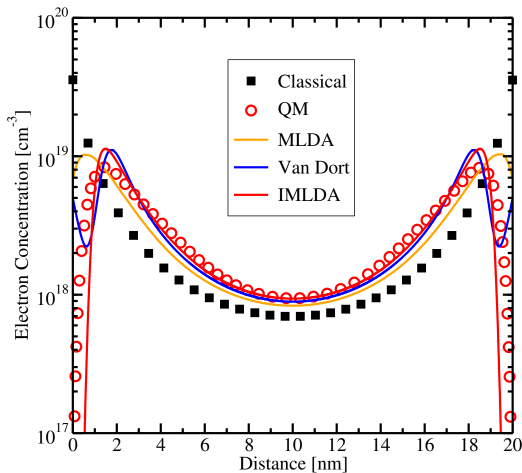

Fig 3: Electron concentration of a 20 nm DG MOSFET.

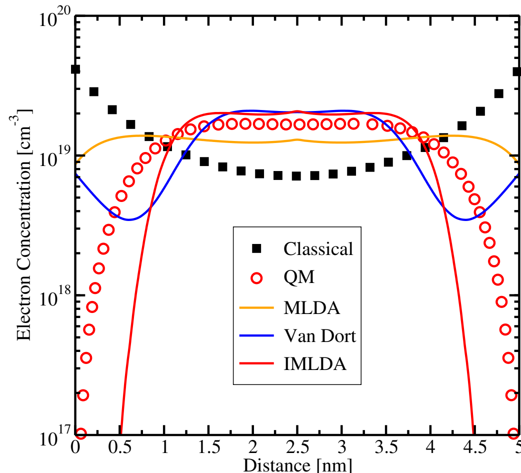

Fig 4: Electron concentration of a 5 nm DG MOSFET.

Summed up, both the Van Dort and the IMLDA model show much better agreement with the QM derived curves than the MLDA model. Both the Van Dort and the IMLDA model are able to accurately reproduce CV curves. While the Van Dort model gives an unphysical increase of the electron concentration close to the oxide interface, the IMLDA model is able to follow this course even at extremely scaled devices like the 5 nm DG MOSFET shown in Fig. 4.

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