Two-Dimensional Modeling of Quantum Mechanical Effects in Ultra-Short CMOS Devices

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Abstract: – Quantum mechanical analysis of the quantum confinement of ultrashort CMOS is numerically very expensive. In this paper we present a macroscopic model, which includes a new approach to match the vertical carrier profile and combines it with a classical model in lateral direction. The simulation results show a significant improvement concerning the accuracy of the carrier profile and the C/V characteristics.

Key-Words: quantum confinement, two-dimensional device modeling, ultrashort CMOS

1 Introduction

It is well known that in consequence of the ever shrinking feature sizes quantum mechanical (QM) effects are getting more important for the performance of state-of-the-art CMOS devices. This issue is widely investigated and understood at physical level, but a full two-dimensional treatment is far from trivial and numerically very expensive.

Up-to-date macroscopic models incorporating QM effects were basically designed to fit the C/V characteristics of the investigated MOS structures [1][2][3] but not for a fully two-dimensional treatment. In this paper a new approach to model the quantum confinement near the channel surface is introduced which does not only match the C/V characteristics but also allows the two-dimensional analysis of advanced CMOS and similar devices. Furthermore the new model is capable to match the vertical carrier profile very accurately, thus offering new insight into the the actual properties of modern devices.

I. The QM Model

Classical device modeling leads to two significant inaccuracies concerning the carrier concentration near the channel surface.

First, the splitting of the conduction band into several discrete eigenvalues is not considered. This leads to an overestimation of the surface charge, as the energy difference between these discrete eigenvalues and the Fermi-level is bigger than the one from the bottom of the conduction band to the Fermi-level. Second, classical models do not consider that the shape of the wave functions reduces the carrier concentration near the surface as well. Consequently, a rigorous approach to simulate the carrier concentration has to take care of both effects, by offering approximations for the wave function and the actual band structure.

A. Approximation of the Wave Function

We model the first of these effects by a reduction of the density of states N_C near the interface applying an exponential shape function. This follows an approach proposed by Hänsch et al. [1],

$$N_\mathrm{C}(z) = N_\mathrm{C} \cdot \left(1 - e^{-(z+z_0)^2/\lambda_\mathrm{TH}^2}\right), \qquad (1)$$

where z is the distance to the interface and z_0 is an offset to match the nonzero carrier concentration near the surface stemming from the finite barrier height. λ_TH is the thermal wavelength responsible for the reduction of the QM

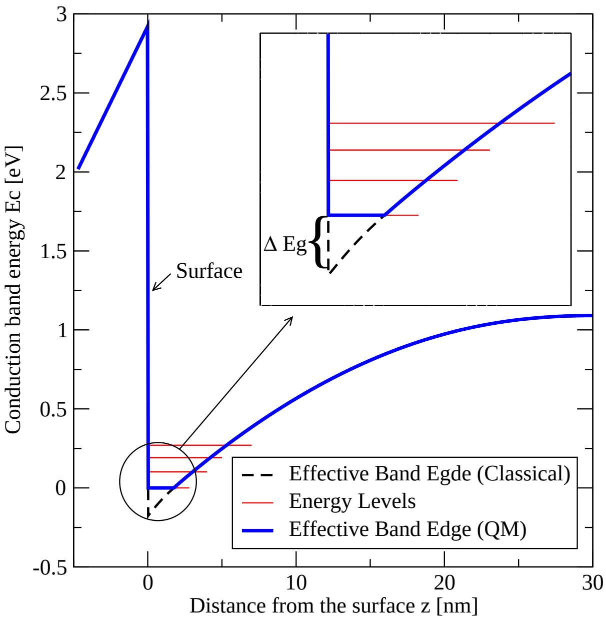

Fig. 1. Band structure near the surface and comparison between the conduction band edge of the classical and the new approach

effect with increasing distance from the interface,

$$\lambda_{\mathrm{TH}} = \frac{\sqrt{2mkT}}{\hbar}. \qquad (2)$$

If this correction is applied the qualitative carrier distribution near the interface in strong inversion is reproduced quite well, but without consideration of band structure effects, this is not the case in the threshold voltage region [3].

B. Approximation of the Energy Band Structure

Fig. 1 shows the actual band structure near the surface of a MOS capacitor, calculated with a self-consistent Schrödinger-Poisson solver working with the effective mass approach [4]. Near the surface the lowest eigenenergy is significancy higher than the band edge, thus causing an overestimation of the charge when the classical simulation approach is applied. The basic idea of our model is to replace the effective band edge by the first discrete energy level (see Fig. 1). This seems reasonable as quantum mechanical calculations show that usually over 90% of the carriers are in this energy band.

We set the band edge at the surface to

$$E_{\mathrm{g,Surface}}^{\mathrm{QM}} = E_{\mathrm{g,Surface}}^{\mathrm{Classical}} + \Delta E_{\mathrm{g}}, \qquad (3)$$

whereas $E_{\mathrm{g,Surface}}^{\mathrm{QM}}$ is the modified bandgap energy which is used in the Boltzmann statistics, $E_{\mathrm{g}}^{\mathrm{Classical}}$ is the bandgap according to the material specification, and ΔE_{g} is the applied correction. Our model pins the band edge $E_{\mathrm{g}}^{\mathrm{QM}}(z)$ inside the device to the value of $E_{\mathrm{g,Surface}}^{\mathrm{QM}}$ as long as $E_{\mathrm{g,Surface}}^{\mathrm{QM}} > E_{\mathrm{g}}^{\mathrm{Classical}}(z)$.

As the exact calculation of the first energy level is numerically expensive and requires the solution of the Schrödinger equation an approximation is used: The offset ΔE_{g} is approximated following a formulation of Van Dort et al. [3], which reads as

$$\Delta E_{\mathrm{g}} = \frac{13}{9} \cdot \beta \cdot \left(\frac{\epsilon}{4qkT}\right)^{1/3} |E_{\mathrm{surf}}|^{2/3}, \qquad (4)$$

whereas $|E_{\mathrm{surf}}|$ is the magnitude of the electric field at the interface and ϵ is the permittivity of the semiconductor. $\beta = 4.1 \times 10^{-8}\mathrm{eVcm}$ is an empirical constant.

II. Simulation Results

The model was implemented into the device simulator MINIMOS-NT [5] and several typical structures were simulated in order to explore its one- and two-dimensional capabilities.

A. Simulation of MOS Capacitors

The one-dimensional capabilities of the new model were checked by simulations of a MOS capacitor. As reference the same structure was simulated using the self-consistent Schrödinger-Poisson solver. Fig. 2 shows a comparison of the C/V characteristics obtained with the new model, the Schrödinger-Poisson solver, and the Hänsch model. An excellent fit between the results from our new model and the quantum mechanical calculations is obtained, especially the onset of inversion is predicted very accurately. The overestimation of the capacity in strong inversion is a well known

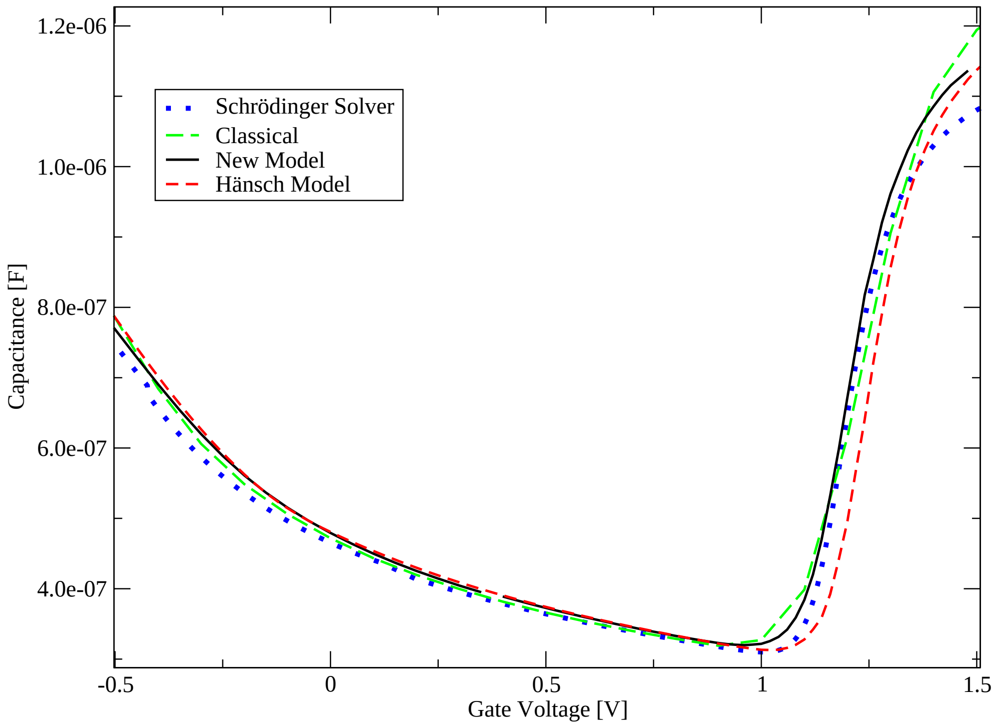

Fig. 2. Comparison of C/V curves of a MOS capacitor obtained with different simulation approaches. The Hänsch model simulations were carried out with optimized offset z_0.

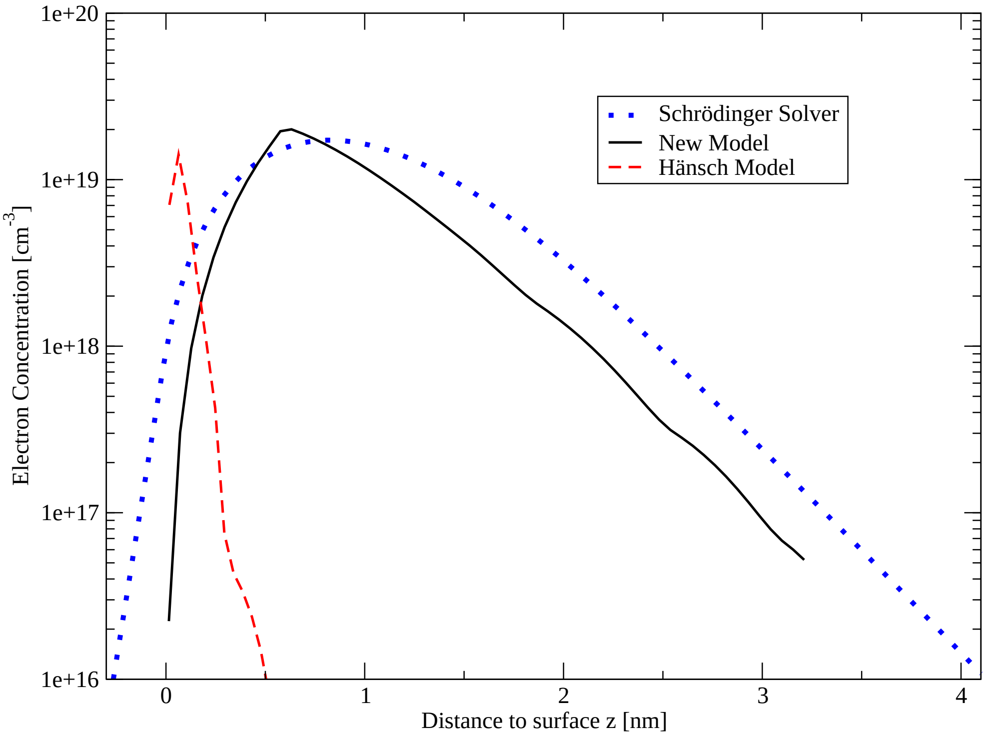

Fig. 3. Comparison of carrier profiles. The operating points for the different models were chosen to obtain similar maximum concentrations. The same parameter sets as for the C/V calculations were applied.

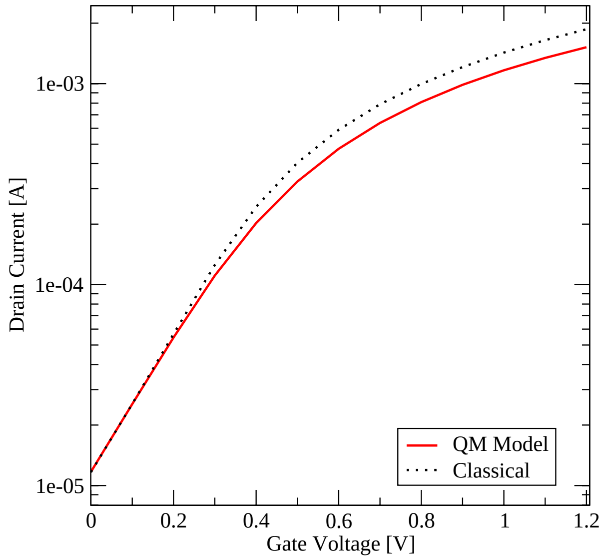

Fig. 4. Transfer characteristics at of a 50nm NMOS at bias $U_{\mathrm{SD}} = 1\mathrm{V}$. The classical approach overestimates the drain current.

effect stemming from the different distribution statistics applied in the Schrödinger solver (Fermi-Dirac) and the device simulator (Boltzmann)(see e.g. [6]).

Fig. 3 shows a comparison of electron concentration profiles. It can be clearly seen that the new model offers a decent fit to the quantum mechanical results. The Hänsch model concentrates the charge closer to the surface, which is a consequence of the comparatively smaller band gap.

B. Simulation of a CMOS Transistor

The ability to reproduce the channel profile opens the door to a precise simulation of state-of-the-art CMOS devices. Fig. 4 shows the results obtained for a device with 50nm gate length using the QM approximation and compares them to a classical simulation. The influence of the quantum confinement, which results in a reduction of the drain current, is clearly visible.

It is remarkable that by introducing our model into the simulator it was not only capable to perform a full two-dimensional analysis of the properties in the channel area but also a significant speed-up and generally better numerical properties were obtained. E.g. for the calculation of a typical CMOS example, discretized at about 5000 nodes, the classical simulation took 55s CPU time per operation point and was reduced to 18s for the QM calculations. This simulations were performed on a Linux machine with a 650MHz Intel Celeron CPU. A possible reason for the speed up can be the smoother distributions when quantum confinement is taken into account.

III. Outlook

In this paper we presented a new macromodel for the simulation of the quantum confinement near the channel surface. A very good fit was obtained for the vertical carrier profile and together with the good numerical properties a deeper insight into the properties of future device generations is possible.

IV. Acknowledgment

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