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On a Simple and Accurate Quantum Correction for Monte Carlo Simulation

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Introduction

Usual quantum corrections to Monte Carlo simulation feature an electron density profile, which tends to vanish at the interface. However, the corresponding formulation of surface roughness scattering and/or the application to realistic MOSFETs is problematic. Using directly or indirectly the Schrödinger equation involves an arbitrary choice of the transition point between bulk and quantization region both in space and in energy, and requires for computational reasons analytical band structure descriptions. The model for surface roughness scattering based on the surface roughness root mean square and correlation length still involves in the full–band versions [1], [2] an effective mass and requires strain–dependent calibration to measurements [1]. In contrast, a combination of specular and diffusive scattering at the interface explicitly involves the strain–dependence via the conservation of energy and parallel–momentum in the specular part. However, this approach necessitates a classical density profile allowing electrons to hit the surface. A possibility to combine this surface scattering model with quantum effects is to use a modification of oxide thickness and work function as obtained from quantum mechanics [3]. It is the aim of this paper to generalize this method to a completely numerical approach, to demonstrate its accuracy and to apply it to process–simulated p– and n–MOSFETs of a 65 nm technology.

Approach and Discussion

Our quantum–correction method consists of reproducing density–gradient (DG) simulations below and around the threshold by a classical drift–diffusion (DD) simulation with modified work function and oxide thickness and to employ these modified values subsequently in full–band Monte Carlo (MC) simulation. First, the increase of the effective oxide thickness in the on–state is computed according to $\Delta t_{ox} = (X_{qm} - X_{cl})\ \epsilon_{ox}/\epsilon_{Si}$. In a 2nd classical DD simulation using this Δt_{ox}, the remaining threshold voltage shift to the DG simulation is extracted and considered as a modified work function in the 3rd DD simulation as well as in the MC simulation.

For the example illustrated by the geometry in Fig. 1 and the roll–off curves in Fig. 2, the logarithmic and linear plots of the transfer characteristics are shown in Figs. 3 and 4. In the subthreshold regime, i.e. in weak inversion, changing only t_{ox} is not sufficient while considering only the threshold voltage shift matches the DG result, whereas both modifications are still significantly away from DG for higher V_{GS}. Only the combined correction reproduces DG up to far above threshold (compare also Fig. 5). In Fig. 6, the results of the different corrections when used in MC simulation are shown for the on–current scaling of n– and p–MOSFET. It can be seen that considering only the total threshold shift still involves a significant difference to the final result based upon the combined correction.

Conclusion

We have presented a quantum–correction scheme for full–band MC simulation which considers the quantum mechanical increase of effective oxide thickness and threshold voltage. In a TCAD environment, this method can be used fully automatical in a workbench project and allows to use consistently diffusive and specular surface roughness scattering and the corresponding stress–dependence.

References

[1] A. T. Pham *et al.*, in *Proc. ESSDERC*, pp. 293–296 (2005).
[2] X.-F. Fan *et al.*, IEEE Trans. Electron Dev. **51**, 962 (2004).
[3] R. Hudé *et al.*, *Proc. ULIS*, pp. 159–162 (2005).

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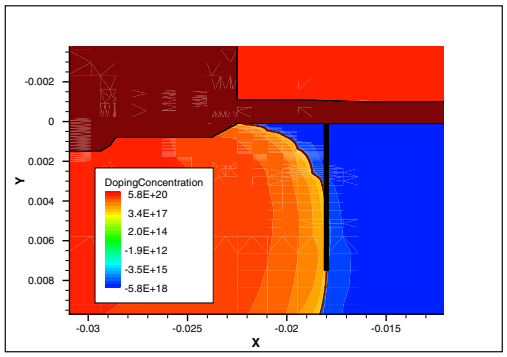

Fig. 1. Cross section of the source side of the channel in a 45 nm nMOSFET. The bold vertical bar shows the position where the charge centroids are calculated from the electron density profiles.

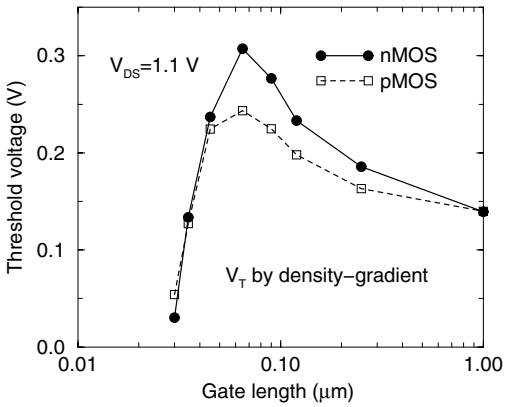

Fig. 2. Saturation threshold voltage roll–off curves of nMOSFET and pMOSFET for a 65 nm node technology according to density–gradient simulations.

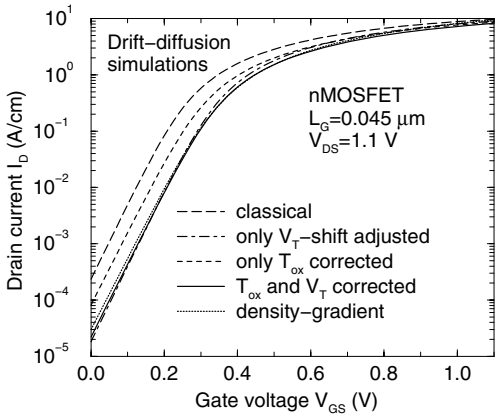

Fig. 3. Logarithmic plot of the transfer characteristics of the 45 nm nMOSFET showing the results of different quantum corrections employed in drift-diffusion simulations.

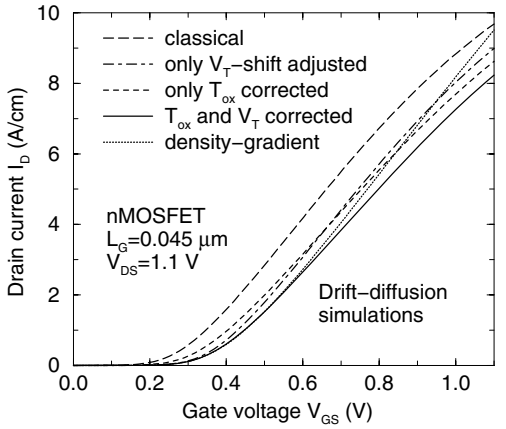

Fig. 4. Linear plot of the transfer characteristics of the 45 nm nMOSFET showing the results of different quantum corrections employed in drift-diffusion simulations.

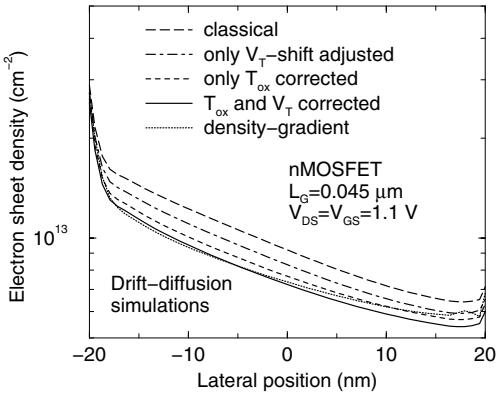

Fig. 5. Electron sheet densities along the channel in the 45 nm nMOSFET as present for different quantum corrections within drift-diffusion simulations.

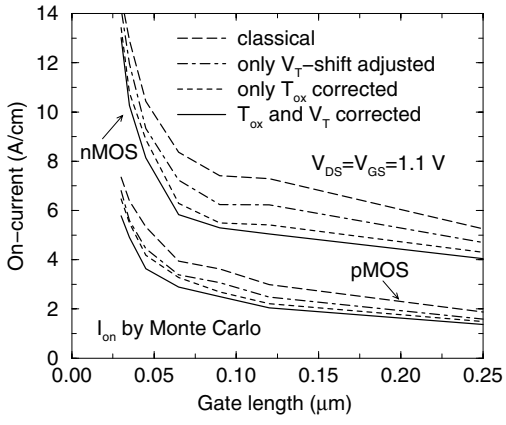

Fig. 6. On–current scaling according to full–band Monte Carlo simulations of nMOSFETs and pMOSFETs using different quantum corrections.