

## Comparison of Monte Carlo and NEGF simulations of Double Gate MOSFETs

Ra Ravishankar, Gulzar Kathawala, Umberto Ravaioli, Sayed Hasan<sup>1</sup> and Mark Lundstrom<sup>1</sup>  
Beckman Institute and Department of Electrical and Computer Engineering, University of  
Illinois at Urbana-Champaign, Urbana, IL 61801, USA.

<sup>1</sup>Department of Electrical Engineering, 1285 Electrical Engineering Building, West Lafayette,  
IN 47907, USA.

email: ravishan@uiuc.edu

The present work compares the simulation results of the two-dimensional full band Monte-Carlo simulator (MoCa) developed at the University of Illinois at Urbana-Champaign and the two-dimensional quantum simulator (NanoMOS) developed at Purdue University. MoCa's semi-classical approach using a quantum correction is known to be accurate for devices as small as a 50nm bulk MOSFET. For smaller devices, we expect its particle-based transport model to be reasonably accurate, but the quantum correction might not capture all the details of the charge distribution. In contrast, NanoMOS's quantum mechanical approach is expected to provide accurate estimates of charge density, but its transport model is not very detailed. In this work, we have sought to ascertain the domain of applicability of the two simulators and envision a super-simulator that would include the best of both approaches.

Double-gate MOSFETs of three body thicknesses —  $t_{Si} = 4\text{nm}$ ,  $3\text{nm}$  and  $2\text{nm}$  — were considered in this study. To ensure a realistic comparison, the source and drain biases in the MoCa simulation were adjusted so that the average conduction band edge in MoCa coincided with that of NanoMOS in the source and drain regions.

For a body thickness of  $4\text{nm}$ , the conduction band profiles and sheet charge densities obtained from MoCa and NanoMOS almost overlap, particularly for high gate and drain-to-source biases. However, as the body thickness is reduced, the agreement becomes progressively worse. This, we believe, is due to MoCa's semi-classical approach (with a quantum correction) that fills all available levels above the conduction band. While this approach might be expected to be reasonably accurate for thicker devices, it is questionable for very small body thicknesses. This is because, in the latter devices, only a few (lower) energy levels would be occupied with electrons while the rest of the levels would have been pushed way higher, so populating all possible levels above a certain energy level (in MoCa, the bottom of the conduction band) might not be a good enough approximation. However, even for thinner devices, MoCa's treatment of transport is expected to be more accurate, particularly at high energies. For all values of  $t_{Si}$  considered in this study, NanoMOS exhibited a very high velocity overshoot, most likely due to the use of parabolic bands which cause electrons to continuously gain energy and acquire an unphysically high velocity.

As device dimensions scale down, surface and interface effects are expected to play a dominant role. We believe that a particle-based, rather than a purely quantum mechanical, approach would be better suited for an accurate treatment of scattering — an inherently granular process. The challenge, therefore, is to better incorporate the quantum mechanical aspects in a particle-based model.

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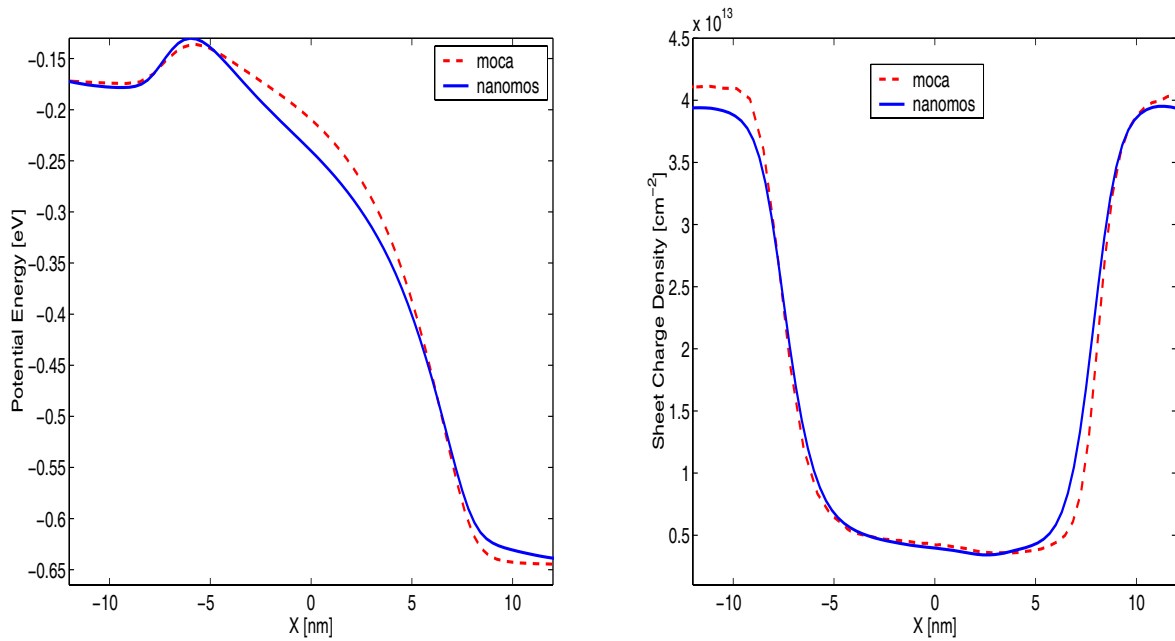


Figure 1: MoCa and NanoMOS profiles of the conduction band edge and sheet charge density for a 4nm thick device at  $V_{ds} = 0.5V$  and  $V_g = 0.5V$ .

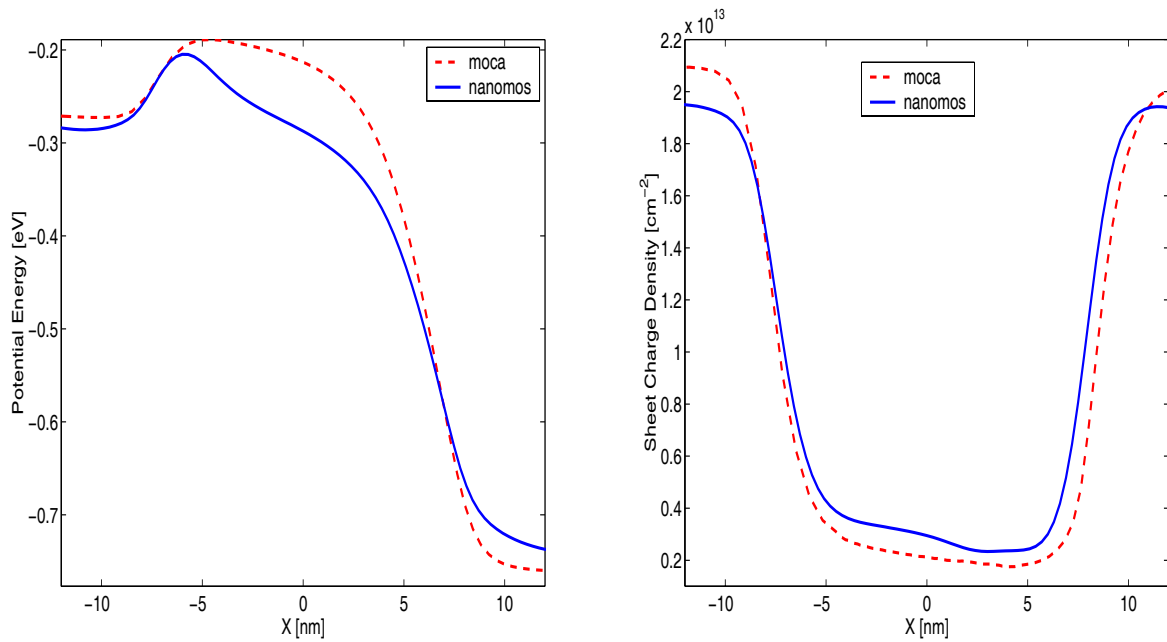


Figure 2: MoCa and NanoMOS profiles of the conduction band edge and sheet charge density for a 2nm thick device at  $V_{ds} = 0.5V$  and  $V_g = 0.5V$ .