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Quantum Corrections to the 'Atomistic' MOSFET Simulation

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The scaling of MOSFETs in integrated circuits is reaching the stage where the granularity of the electric charge and the atomicity of matter start to introduce substantial variation in the characteristics of the individual devices and has to be included in the process/device simulations. The variation in number and position of dopant atoms in the active region of the decanano MOSFETs will make each transistor microscopically different, and introduces significant variations in the device characteristics. At the same time the, thickness of the gate oxide becomes equivalent to several atomic layers with a typical interface roughness of the order of 1-2 atomic layers. This will introduce more than 50% variation in the oxide thickness within an individual transistor and will make the transistors microscopically different in terms of oxide thickness pattern as well. The trapping/detrapping of individual charges at the interface also will have a dramatic effect on the current in such devices.

The statistical variations in the decanano devices shift the paradigm of the numerical device simulations. It is no longer sufficient to simulate a single device with continuous doping distribution, uniform oxide thickness and unified dimensions to represent one macroscopic design [1]. Each device is microscopically different at the level of dopant distribution, oxide thickness and gate pattern, so an ensemble of macroscopically identical but microscopically different devices must be characterised. The aim of the numerical simulation shifts from predicting the characteristics of a single device towards estimating the mean values and the variance of basic design parameters. It must be emphasised that even the mean values obtained, for example, from statistical atomistic simulations are not identical to the values corresponding to continuous charge simulation. The simulation of a single device with random dopants, oxide thickness and gate pattern variation requires essentially a 3D solution with fine grain discretization. The requirement for statistical simulations transforms the problem into a four dimensional one where the fourth dimension is the size of the statistical sample [2].

At the same time the increase in doping concentration and the reduction in the oxide thickness in decanano MOSFETs results in a strong quantization in the inversion layer and a corresponding threshold voltage shift and oxide capacitance degradation. However traditionally the 3D simulation studies of random dopant fluctuation effects [1-4] use a simple drift-diffusion approximation and do not take into account quantum effects. Until recently [5] it was unclear to what extent the quantum effects may enhance or reduce the variations in the device characteristics associated with random dopant, and oxide thickness fluctuation and the effects associated with trapping/detrapping of individual interface charges.

In this paper we study the influence of the quantum effects in the inversion layer on the parameter fluctuation in decanano MOSFETs. The quantum mechanical effects are incorporated in our previously published 3D 'atomistic' simulation approach [1], [2] using a full 3D implementation of the density gradient (DG) formalism. This results in a consistent, fully 3D, quantum mechanical picture which incorporates the vertical inversion layer quantization, lateral confinement effects associated with the current filamentation in the valleys of the potential fluctuation, and tunnelling through the sharp potential barriers associated with individual dopants.

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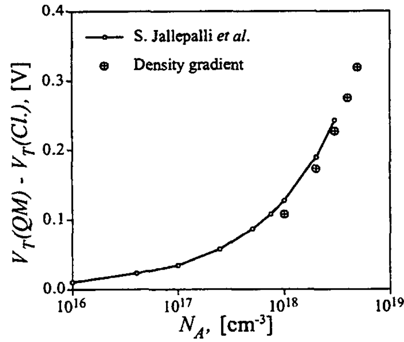

Fig. 1 Quantum mechanical threshold voltage shift as a function of the doping concentration. A comparison between DG and full band Poisson-Schrödinger results for continuous doping distribution.

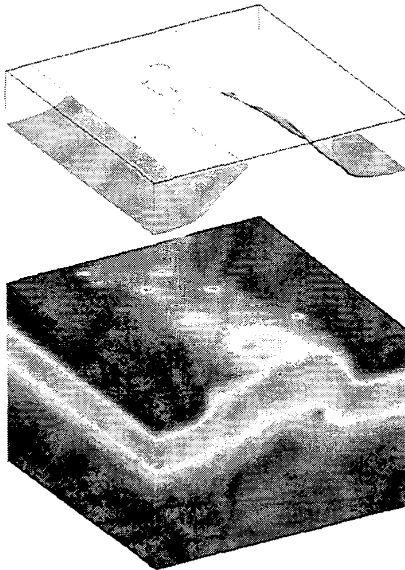

Fig. 2 Potential and equiconcentration distribution at threshold voltage obtained from the 'atomistic' DG simulation of a 30×50nm MOSFET.

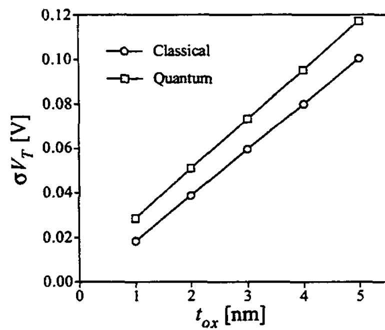

Fig. 3 Dependence of the threshold voltage standard deviation as a function of the oxide thickness for a 50×50 nm MOSFET.

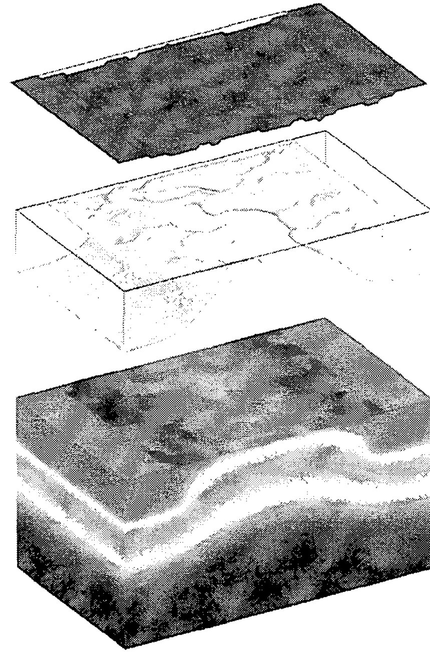

Fig. 4 Effect of the oxide thickness fluctuations (top) on the carrier concentration (middle) and the potential (bottom) distribution in a 30×30 nm MOSFET. Results from 3D DG simulations.

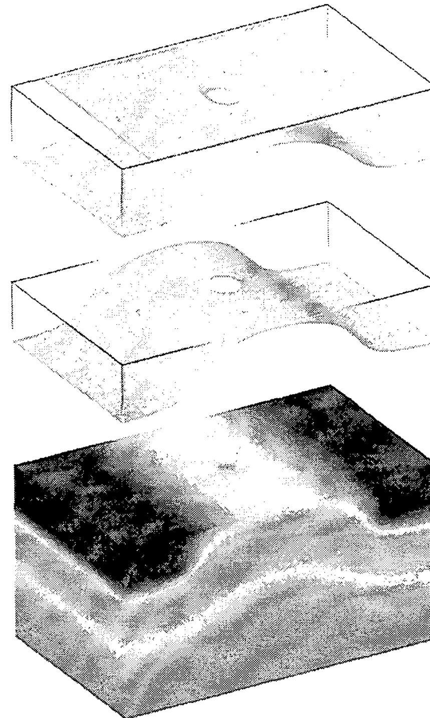

Fig. 5 Effect of the single electron trapping on the potential (bottom) and charge distribution in a 30×30 nm MOSFET. Quantum (top) vs. classical (middle) simulation.