The Use of Quantum Potentials for Confinement in Semiconductor Devices

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ABSTRACT

As MOSFETs are scaled into sub 100 nm (decanano) dimensions, quantum mechanical confinement and tunnelling start to dramatically affect their characteristics. In this paper we describe the introduction of quantum corrections within a 3D drift diffusion simulation framework using quantum potentials. We compare the density gradient (DG) and the effective potential (EP) approaches in term of accuracy and computational efficiency. Their application is illustrated with examples of 3D statistical simulations of intrinsic fluctuation effects in decanano MOSFETs. We also speculate about the capability of the DG formalism to handle source-to-drain tunnelling in sub 10 nm (nano) MOSFETS.

Keywords**:** Numerical simulations, quantum corrections, effective potential, MOSFETs, intrinsic fluctuations

1 INTRODUCTION

MOSFETs scaled down to 15nm gate lengths have been successfully demonstrated [1]. The scaling below these dimensions will require the introduction of new device architectures among which double gate MOSFETs are the most promising candidates [2]. The combination of thin gate oxides and heavy doping in the conventional MOSFETs, and the thin silicon body of the double-gate structures, will result in substantial quantum mechanical (QM) threshold voltage shift and transconductance degradation [3]. Below 10 nm gate-lengths direct source-to-drain tunnelling will rapidly became one of the major limiting factors for scaling [4]. Computationally efficient methods to include QM effects are required for the purpose of practical Computer Aided Design of this generation of devices. First order quantum corrections based on density gradients (DG) have already been introduced in 2-D [5] and 3-D [6] drift-diffusion simulations. Recently a new *Effective Potential* (EP) approach for introducing quantum corrections in classical and semi-classical simulations has been proposed [7] and demonstrated in Monte Carlo MOSFET simulations [8]. In this paper we discuss the implementation of these two quantum correction techniques in a 3-D drift diffusion simulator and compare their accuracy and efficiency. We start with the calibration of the two approaches in respect of a more sophisticated quantum simulator [2]. Then we compare their influence on 3-D 'atomistic' statistical simulations of intrinsic fluctuations, introduced by random discrete dopants, in decanano MOSFETs with conventional architecture. Finally we speculate on the possibility to emulate, at semi-quantitative levels, the source-to-drain tunnelling in sub 10 nm double gate MOSFETs using the DG formalism.

2 QUANTUM POTENTIALS

We are motivated by the need to introduce quantum corrections in our 3D drift-diffusion 'atomistic' simulator widely used to investigate the intrinsic fluctuations in decanano MOSFETs which are introduced by the discreteness of charge and atomicity of matter [6, 9]. The investigation of intrinsic fluctuation effects involves statistical 3-D simulations of large samples of macroscopically identical but microscopically different devices. Therefore the computational efficiency of the quantum correction approach is of great importance and the use of quantum potentials becomes an attractive option.

2.1 The Density Gradient approach

The density gradient approach may be derived from the one particle Wigner function [10]:

$$\frac{\partial f(\mathrm{k},\mathrm{r},t)}{\partial t}+\mathrm{v}.\nabla_{\mathrm{r}} f(\mathrm{k},\mathrm{r},t)-\frac{2}{\hbar}V(\mathrm{r})\sin\left[\frac{\hbar\overleftarrow{\nabla}_{\mathrm{r}}\overrightarrow{\nabla}_{\mathrm{k}}}{2}\right]f(\mathrm{k},\mathrm{r},t)=\left(\frac{\partial f(\mathrm{k},\mathrm{r},t)}{\partial t}\right)_{coll} \quad (1)$$

Quantum effects are included through the inherently non-local driving potential in the third term on the left-hand side. Expanding to first order in $\hbar$, so that only the first non-local quantum term is considered, has been shown to be sufficiently accurate to model non-equilibrium quantum transport and also for the inclusion of tunnelling phenomena in particle based Monte Carlo simulators [11]. The additional, non-classical, quantum correction term may be viewed as a modification to the classical potential and

acts like an additional quantum force term in the particle simulations, similar in spirit to the Bohm interpretation.

The density gradient approximation maybe derived in a manner similar to that for deriving the drift diffusion approximation from the Boltzmann Transport Equation and results in a quantum potential correction term in the standard drift-diffusion flux [5].

$$F_n = n\mu_n \nabla\psi - D_n \nabla n + 2\mu\nabla\left(b_n \frac{\nabla^2 \sqrt{n}}{\sqrt{n}} \right) \qquad (2)$$

where $b_n = \hbar/(12qm_n^*)$, and all other symbols have their usual meaning. To avoid the discretisation of fourth order derivatives in (1) in multidimensional numerical simulations a generalised electron quasi-Fermi potential ϕ_n is introduced as follows:

$$F_n = n\mu_n \nabla\phi_n \qquad (3)$$

Thus the unipolar drift-diffusion system of equations with QM corrections, which in many cases is sufficient for MOSFET simulations, becomes:

$$\nabla \cdot (\varepsilon \nabla \psi) = -q\left(p - n + N_D^+ - N_A^-\right) \qquad (4)$$

$$2b_n \frac{\nabla^2 \sqrt{n}}{\sqrt{n}} = \phi_n - \psi + \frac{kT}{q} \ln \frac{n}{n_i} \qquad (5)$$

$$\nabla \cdot (n\mu_n \nabla \phi_n) = 0 \qquad (6)$$

The system of equations (4) – (6) is solved self-consistently using standard techniques.

2.2 The Effective Potential approach

An alternative approach to the DG formalism for including first order quantum effects is the recently advanced EP approach [7]. In this case the *natural* non-zero size of an electronic wave-packet in the quantised system is used to construct an effective potential. The carriers are considered to be associated with a minimum dispersion Gaussian wavepacket, which is in turn convolved with the classical conduction band profile $V_{Classical}$ (obtained from the solution of Poisson's equation) to obtain an effective potential V_{eff} given by:

$$V_{eff} = \int V_{Classical}(\mathbf{x}+\mathbf{y}) G(\mathbf{y}, a_0) d\mathbf{y} \qquad (1)$$

where G is a Gaussian with standard deviation a_0.

In the implementation of the EP approach we use the Gummel algorithm for solving the semiconductor equations in the drift diffusion approximation. The scenario resembles the standard procedure used to self-consistently solve the Poisson and the Schrödinger equations, using a self-adjusting damping scheme [12] for the potential.

3 RESULTS

3.1 Calibration

We have carefully calibrated both the EP and DG approaches against the results of a 1-D Poisson-Schrödinger solver [2]. Although Poisson-Schrödinger simulations are more sophisticated they are not yet practical for 3-D device simulations. Fig. 1 shows the quantum mechanical threshold voltage shift for DG and EP as a function of substrate doping compared with the results of Jallepalli. Fig. 2 shows typical carrier concentration profiles obtained from the 1-D simulations. All show a peak in the concentration away from the Si/SiO_2 interface, although the effective potential produces a sharper drop-off at the Si/SiO_2 interface.

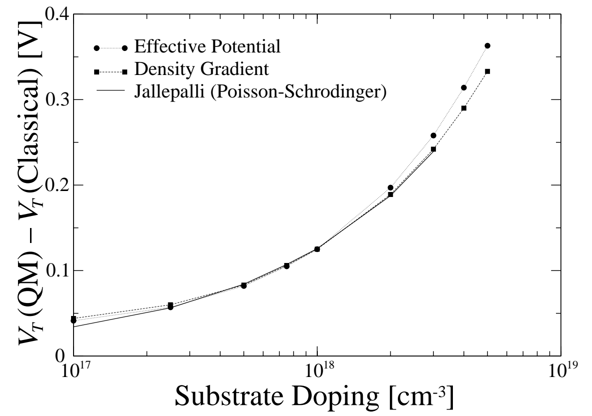

Fig. 1. Threshold voltage shift due to quantum effects versus substrate doping. Results for Density Gradient and Effective Potential are compared to those obtained from Poisson Schrödinger.

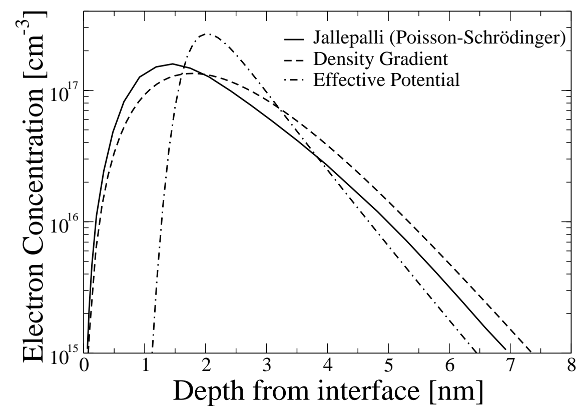

Fig. 2. Electron carrier concentration as a function of distance from the interface, for substrate doping of 5×10^{17}cm^{-3}. All have the same net sheet density.

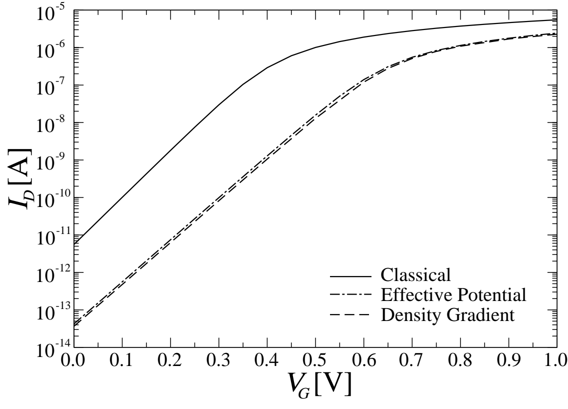

Fig. 3. I_D-V_G characteristic obtained from both classical and quantum simulators for a 30nm×30nm *n*-MOSFET, with V_D=0.01V and a substrate doping of 5×10^{18}cm^{-3}.

Fig. 3, shows an I_D-V_G characteristic for a 30nm×30nm *n*-MOSFET obtained from our 3-D quantum simulator. This demonstrates the threshold voltage shift between the classical and the quantum simulations.

3.2 3-D Atomistic Simulations

Here we compare the impact of the DG and EP quantum corrections on the threshold voltage fluctuations in decanano MOSFETS. Fig. 4, shows a typical equi-concentration contour for a simulated atomistic MOSFET using the EP method.

Simulating 200 atomistic devices we have investigated threshold voltage (Fig. 5) and standard deviation (Fig. 6) at different channel lengths. The EP simulations result in similar average threshold voltages and standard deviations compared to DG.

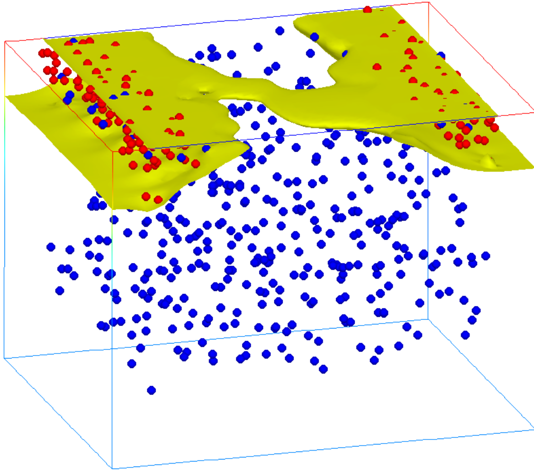

Fig. 4. An equi-concentration contour for a 30×50nm atomistic MOSFET at threshold obtained using our effective potential simulator. Also shown are the individual dopant positions throughout the structure.

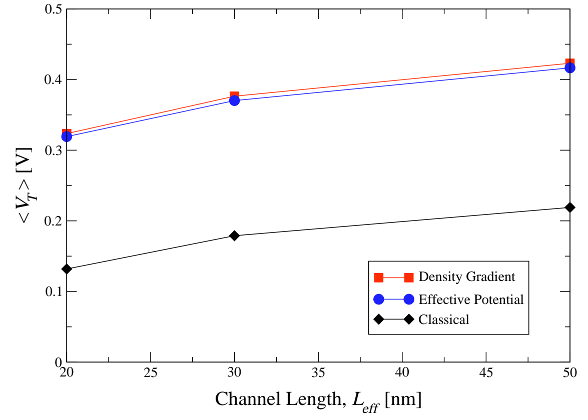

Fig. 5. Average threshold voltage for 50 nm wide atomistic MOSFETs with different channel length, 1.2 nm gate oxide and channel doping 5×10^{18} cm^{-3}. Comparison between classical, density gradient and effective potential simulations

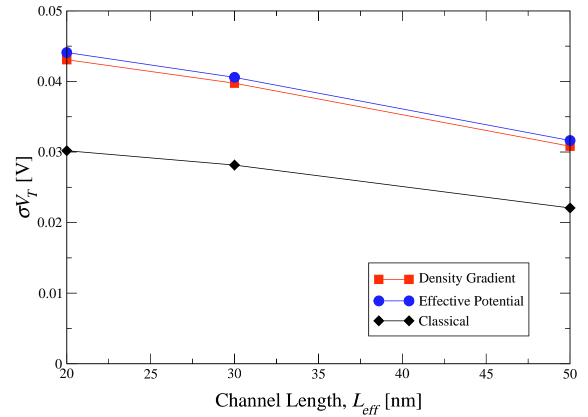

Fig. 6. σV_T for atomistic MOSFETs with different channel length (same parameters as in Fig. 5) Comparison between classical, DG and EP simulations

3.3 Source-to-Drain Tunnelling

It still remains unclear to what extent the approximations involved in deriving the DG approach remove its ability to model the direct source-to-drain tunnelling expected in nanometre channel length MOSFETs. In search of a qualitative answer to this question we simulate a set of double gate MOSFETs with generic structure illustrated in Fig 7. The subthreshold slope in the DG simulations (Fig. 8) degrades significantly as the channel length is decreased, while in the classical simulations the subthreshold slope remains nearly constant with channel length. The degradation in the subthreshold slope in the DG simulations is consistent with the more elaborate quantum mechanical simulations performed by others [13]. These observations provide an indication that source-to-drain tunnelling is included, to some extent, in the DG simulations.

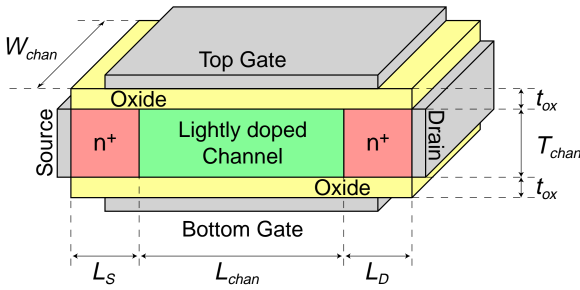

Fig. 7: Schematic representation of the double-gate MOSFET structure considered in this work.

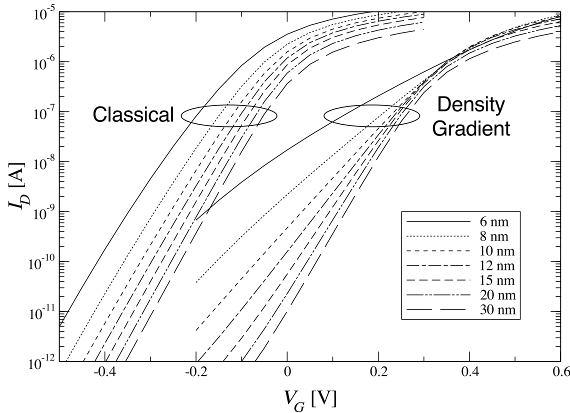

Fig. 8: I_D-V_G characteristics for a double gate structure, with gate lengths ranging from 30nm down to 6nm, obtained from our classical and density gradient simulations. V_D=0.01V and V_G is applied to both top and bottom gate contacts.

4 CONCLUSIONS

The Density Gradient and Effective Potential methods provide efficient means for incorporating quantum corrections in multi dimensional device simulations. Both methods agree well with the available data from Poisson-Schrödinger simulations, although there is a better agreement between Density Gradient and Poisson-Schrödinger calculations in respect of the carrier densities. This, however, appears to have little discernable effect on threshold voltage and current characteristics. Implemented in large scale 3-D statistical 'atomistic' simulations they produce very similar results for the threshold voltage, the threshold voltage lowering and the threshold voltage standard deviation in decanano MOSFETs. The Density Gradient approach implemented in the simulation of sub 10 nm double gate MOSFETs shows behaviour qualitatively consistent with source-to-drain tunnelling.

REFERENCES

[1] S. Thompson, M. Alavi, R. Argavani, A. Brand, R. Bigwood, J. Brandenburg, B. Crew, V. Dubin, M. Hussein, P. Jacob, C. Kenyon, E. Lee, M. Mcintyre, Z. Ma, P. Moon, P. Nguyen, M. Prince, R. Schweinfurth, S. Shvakumar, P. Smith, M. Stettler, S. Tyagi, M. Wei, J. Xu, S. Yang and M. Bohr, "An enhanced 130 nm generation logic technology featuring 60 nm transistors optimised for high performance and low power at 0.7 – 1.4 V", IEDM Tech. Digest, 257-261, 2001.

[2] D. Hisamoto, "FD/DG-SOI MOSFETS – a viable approach to overcoming the device scaling limit", IEDM Tech. Digest, 429-432, 2001.

[3] S. Jallepalli, J. Bude, W. K. Shih, M. R. Pinto, C. M. Maziar, and A. F. Tasch Jr., "Electron and hole quantization and their impact on deep submicron *p*- and *n*-MOSFET characteristics", IEEE Trans. Electron Devices, 44: 297-303, 1997.

[4] Z. Ren, R. Venugopal, S. Datta, M. Lundstrom, D. Jovanovic, and J. Fossum, "Examination of design and manufacturing issues in a 10 nm double gate MOSFET using nonequilibrium Green's function simulation", IEDM Tech. Digest, 107-110, 2001.

[5] C. S. Rafferty, B. Biegel, Z. Yu, M. G. Ancona, J. Bude, and R. W. Dutton, "Multi-dimensional quantum effects simulation using a density gradient model and script-level programming technique", SISPAD'98, Eds De Meyer, and Biesemans, 137-140, 1998.

[6] A. Asenov, G. Slavcheva, A. R. Brown, J. H. Davies, and S. Saini, "Quantum mechanical enhancement of the random dopant induced threshold voltage fluctuations and lowering in sub 0.1μm MOSFETs", IEDM Tech. Digest, 535-538, 1999.

[7] L. Shifren, R. Akis, and D. K. Ferry, "Correspondence between quantum and classical motion: comparing Bohmian mechanics with a smoothed effective potential approach", Physics Letters A, 274: 75-83, 2000

[8] D. K. Ferry, R. Akis, and D. Vasileska, "Quantum Effects in MOSFETs: Use of an effective potential in 3D monte carlo simulation of ultra-short channel devices", IEDM Tech. Digest, 287-290, 2000

[9] A. Asenov, G. Slavcheva, A. R. Brown, J. H. Davies, and S. Saini, "Increase in the random dopant induced threshold fluctuations and lowering in sub-100nm MOSFETs due to quantum effects: a 3-D density gradient simulation study", IEEE Trans. Electron Devices, 48: 722-729, 2001.

[10] P. Carruthers and F. Zachariasen, Review of Modern Physics, 55 pp. 245-284, 1983.

[11] H. Tsuchiya and T. Miyoshi, Superlattices and Microstructures, 27 pp.529-532, 2000.

[12] F. Stern, "Iteration Methods for Calculating Self-Consistent Fields in Semiconductor Inversion Layers", Journal of Computational Physics, 6: 56-67, 1970

[13] Mark Lundstrom, Private Communication, June 2001