Efficient Density Gradient Quantum Corrections for 3D Monte Carlo Simulations

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***Abstract*—An efficient method for including quantum corrections in 3D Ensemble Monte Carlo simulations based on the Density Gradient formalism is presented. The method is used to study the impact of transport on the current variations introduced by the random body thickness pattern in Ultra Thin Body SOI MOSFETs. The resulting increased variability in drive current is studied in comparison between Monte Carlo and Drift Diffusion simulations.**

Keywords-quantum corrections, Monte Carlo, UTB MOSFETs, SOI, double gate, body thickness fluctuations.

I. INTRODUCTION

Quantum mechanical effects play an increasingly important role in the operation of nano-scaled CMOS devices with conventional and novel device architectures. The introduction of quantum corrections in Monte Carlo simulators, widely used for predictive simulations of such devices, is a vibrant area of research. A broad range of quantum correction techniques have been proposed already in the literature and implemented in various Monte Carlo simulators [1]. They range from the simple effective potential approach, which is computationally very efficient but lacks accuracy in predicting the shape of the inversion layer charge [2] to methods based on 1D/2D/3D solution of the Schrödinger equation [3], which gives accurate inversion layer charge distributions at the expense of significant computational efforts. The efficiency of the quantum corrections is particularly important in 3D Monte Carlo simulations, which become a necessity for the wide spectrum of novel device architectures including ultra-thin body (UTB) SOI and multiple gate transistors. The efficiency becomes paramount when using 3D Monte Carlo simulations to study the impact of body thickness variations [4, 5] on the transport and the performance variation in UTB transistors on a statistical scale [6]. Previously such variations introduced by the additional quantum confinement scattering in double gate UTB MOSFETs illustrated in Fig. 1 have been studied only at low drain bias in a frozen field approximation.

In this paper we describe an efficient approach to introduce efficient and accurate quantum corrections in 3D Monte Carlo simulations based on the Density Gradient formalism [7].

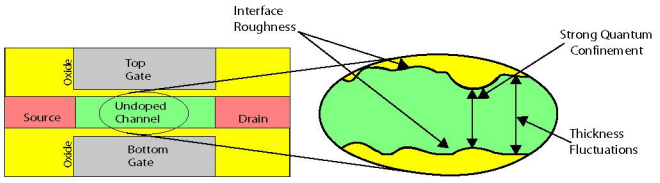

Figure 1. UTB DG MOSFET simulated in this study, showing the sources of the body thickness fluctuations.

II. SIMULATION METHODOLOGY

The use of the Density Gradient approach in the past to define an effective quantum correction potential based directly on the concentration of the particles used to represent the carries in the Monte Carlo simulations has failed due to the high order derivatives involved and the noisy nature of the particle distribution. The method proposed here, which circumvents this difficulty, is very similar to the method based on the solution of the Schrödinger equation advanced in [1, 3]. Instead of using the carrier distribution obtained from the solution of the Schrödinger equation to deduce the effective quantum potential for the quantum corrections, we use the smooth carrier distribution obtained from the solution of the 3D Density Gradient equation. This method is computationally robust and efficient, not requiring the estimate of the eigenvalues of the Schrödinger equation. At the same time, as illustrated in Fig. 2, the carrier distributions obtained from the solution of the carefully calibrated Density Gradient equation can be very close to the ones obtained from the solution of the Schrödinger equation [8].

In our algorithm the 3D MC module is coupled to the Glasgow 3D 'atomistic' Drift Diffusion simulator [9]. Firstly, Drift Diffusion (DD) simulations with Density Gradient (DG) quantum corrections are carried out in order to initialise the MC simulations and to estimate a quantum correction field. The latter is defined as the difference between the 'quantum potential' resulting from the DG solution and the electrostatic potential. This quantum correction field is loaded into the Monte Carlo module along with the resulting carrier distribution, which is used to initialise the particles.

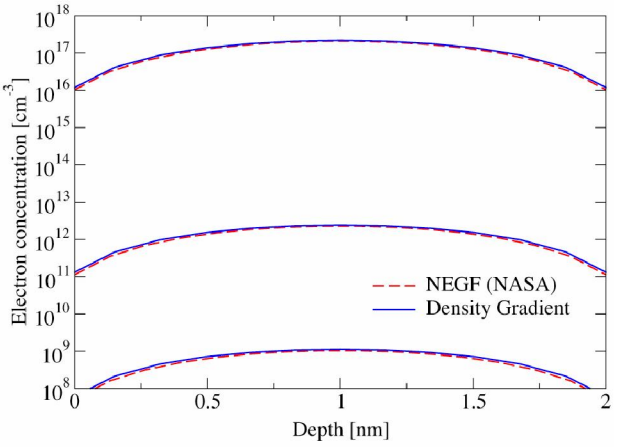

Figure 2. Comparison between carrier distribution obtained from Density Gradient and NEGF simulations showing a good agreement between the two.

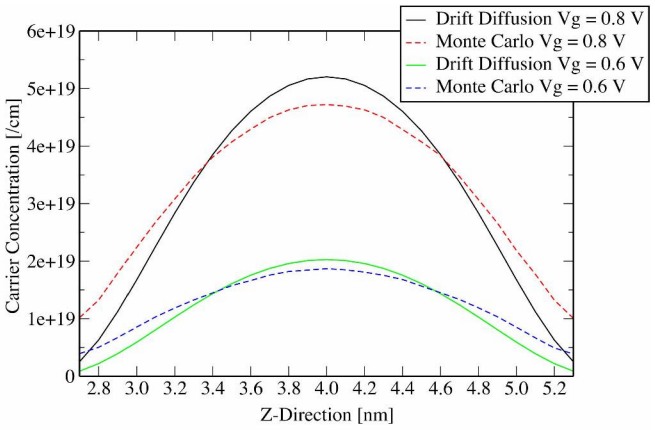

Figure 4. Carrier Distribution running from top to bottom interface from both Drift Diffusion and Monte Carlo showing a good agreement.

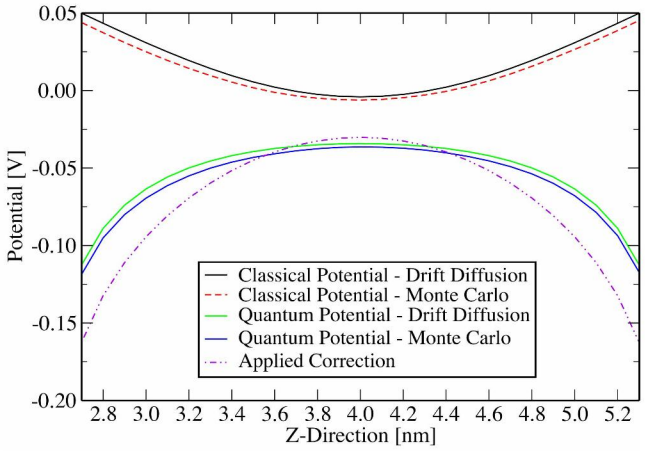

Figure 3. Potential running from top to bottom interfaces from both Drift Diffusion and Monte Carlo showing the correction applied to the classical potential to calculate the quantum potential.

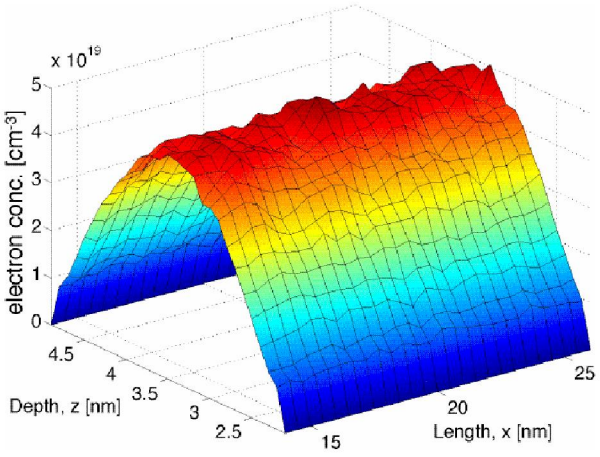

Figure 5. Carrier distribution on a vertical plane in the channel of a UTB double gate MOSFET showing the confinement of carriers in the quantum corrected MC simulation.

After each MC time step the Poisson equation is solved, the quantum correction term added to the electrostatic potential, and the resulting quantum potential is used to calculate the driving force on the particles. At low drain voltage it is sufficient to use the quantum correction term estimated from the initial DD/DG simulations during the whole MC simulation cycle. At high drain voltages and significant channel current it is necessary periodically to estimate the Fermi level from the MC solution and, by using an averaged MC potential distribution, to solve the DG equation and to update the quantum correction field.

In simulating the effect of the body thickness variations in UTB devices the surface roughness patterns present at the top and bottom Si/SiO_2 interfaces are generated and digitized based on the methodology described in [10] and [11]. An exponential auto-correlation function was used [12], with an rms value of 0.3 nm and correlation length of 1.8 nm. The digitised roughness pattern is used to alter the reflective boundaries at the interfaces in the Monte Carlo simulator. This also allows the surface roughness scattering to be included in our simulations through the real space trajectories of the particles in an *ab initio* fashion.

III. Results And Discussion

We have tested our quantum correction approach in the simulation of a UTB Double Gate MOSFET, schematically illustrated in Fig.1. The simulated device has a channel length of 20 nm, body thickness of 2.1 nm and oxide thickness of 1 nm. Fig. 3 compares the electrostatic and the DG quantum potential distribution across the middle of the channel obtained from the 3D DD and the MC simulation of the above transistor at low drain bias of 1 mV and gate voltage 0.8 V. The corresponding quantum correction term is also plotted in the same figure. Fig. 4 compares the carrier distribution across the middle of the channel obtained from the quantum corrected MC and DD/DG simulations, at low drain bias of 1 mV and gate voltages of 0.8 V and 0.6 V. The close match between the two sets of distributions validates our approach. The slight differences can be attributed to differences in the charge assignment schemes used by the two different simulation techniques.

Fig 5 shows the electron distribution in the channel of a uniform UTB double gate MOSFET away from the source and drain obtained from the quantum corrected MC simulation. Fig.

6 shows a comparison of the electrostatic and quantum corrected potentials showing sources of increased scattering captured by the quantum potential. Fig. 7 shows the electron concentration in the channel from the Monte Carlo simulations, and Fig 8 compares the electron distribution in the channel of a similar transistor obtained from DD/DG and the quantum corrected MC simulations. In these cases interface roughness have been introduced at both Si/SiO_2 interfaces resulting in fluctuations in the Si body thickness within the channel. The impact of the body thickness fluctuations can be clearly observed, creating variations in the sub band energy levels along the channel, and in substantial fluctuations in the carrier concentration. The scattering from the corresponding variations in the quantum potential also lead to mobility and drive current degradation which can only be investigated properly using 3D MC transport simulations.

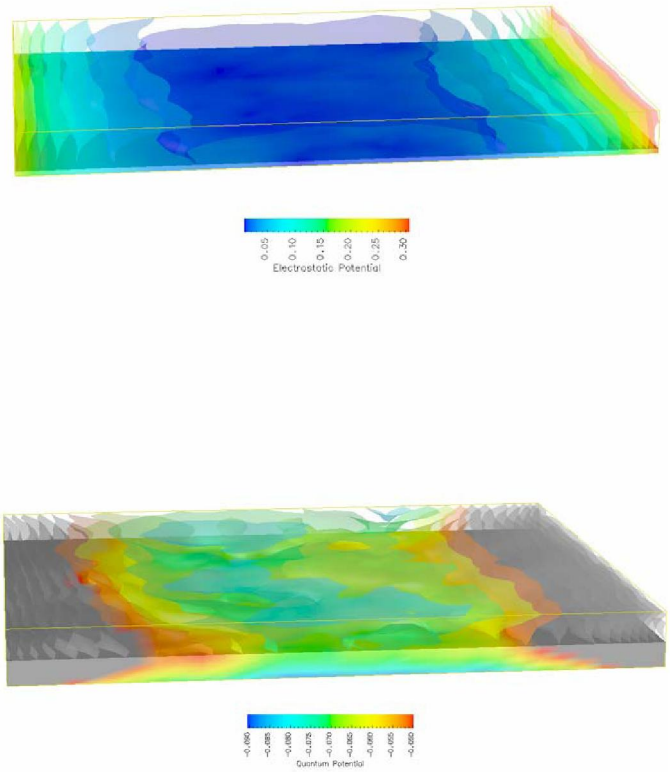

Figure 6. 3D view of the channel running from the source to the drain, showing only the silicon layer. Displays a comparison of (a) electrostatic and (b) quantum corrected potential in MC showing the fluctuations that lead to increased scattering.

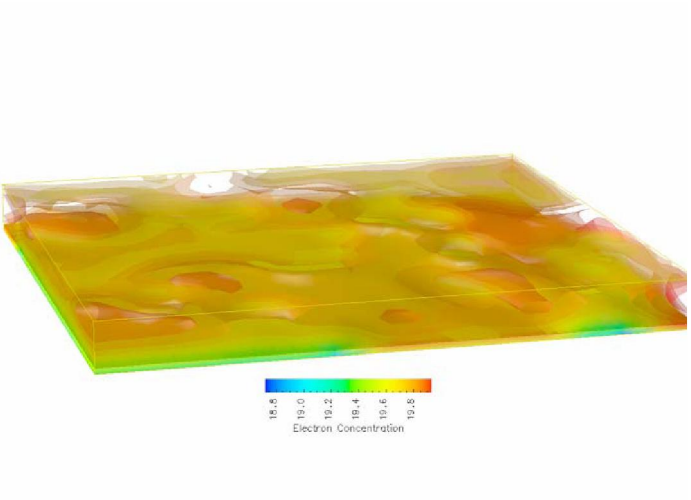

Figure 7. Electron concentration of same region as Fig. 6, showing fluctions resulting from body thickness fluctuations.

A comparison of the I_d-V_g characteristics of the uniform UTB double gate MOSFET obtained using DD/DG, 'frozen field' and self-consistent quantum corrected Monte Carlo simulations are shown in Fig. 9. The simulations are carried out at a low drain bias of 1 mV and a gate voltage of 0.8 V showing a very good agreement. DD/DG and quantum corrected self-consistent MC simulations were carried out for a similar transistor with a rough interface at both high (1 V) and low (1 mV) drain bias in order the quantify the impact of body thickness fluctuations further. The results of these simulations are summarised in Table 1. In the case of MC simulation we see a much greater reduction in the drain current in the case of body thickness fluctuations due to the increased scattering coming from quantum confinement variations. However the reduction is much stronger at low drain voltage when the transport is mobility dominated. At high drain voltage when the degree of balisticity increases the importance of the quantum confinement scattering decreases and the current reduction becomes smaller.

'Frozen field' Monte Carlo simulations of properly scaled single gate UTB Silicon-on-Insulator (SOI) MOSFETs were carried out to investigate the influence of body thickness fluctuations in these devices. The simulated device has silicon body thickness of 2.5 nm, equivalent gate oxide thickness of 0.67 nm and channel length of 10 nm. Fig. 10 compares the percentage reduction in drive current resulting from the inclusion of interface roughness in Drift Diffusion and Monte Carlo simulations of 50 MOSFETs each with unique roughness patterns.

The greater current reduction present in the MC simulations is attributable again to the increased scattering from body thickness fluctuations. It also results in much larger current standard deviation (11.35%) compared to the results of the DD simulations (1.05%).

IV. Conclusions

We have proposed an efficient Density Gradient approach to introduce quantum correction in 3D semi-classical Monte

Carlo transport simulations. This approach was used to study the body thickness fluctuations in UTB MOSFETs with both single and double gate configurations resulting from the unique roughness patterns at the top and bottom Si/SiO_2 interfaces. By comparing DD/DG and quantum corrected MC simulations we were able to demonstrate that the additional scattering resulting from the corresponding body thickness fluctuations significantly degrades the drive current and increases the variability in the studied devices.

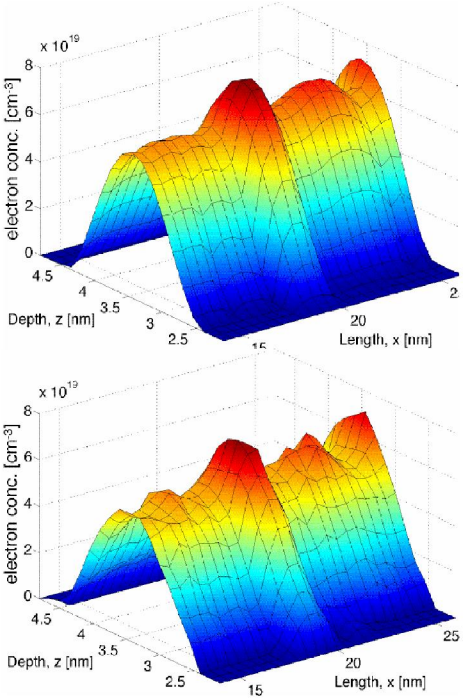

Figure 8. Carrier distribution on a vertical plane in the channel of a UTB double gate MOSFET with interface roughness showing fluctuation in concentration due to the variation in confinement along the channel in (a) the Density Gradient Drift Diffusion and (b) the quantum corrected Monte Carlo simulations.

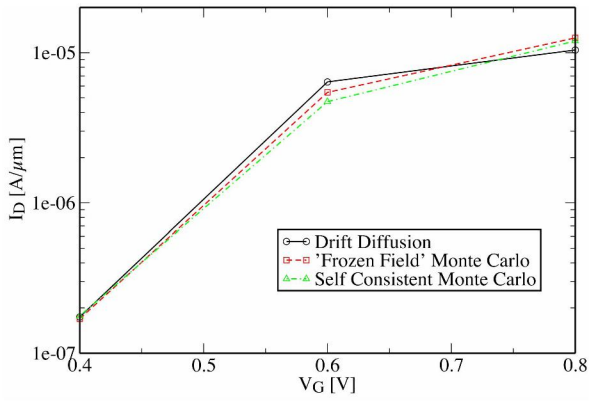

Figure 9. Comparison of I_D-V_G characteristics for Drift Diffusion, 'frozen field' and self-consistent Monte Carlo for a UTB double gate MOSFET showing good agreement.

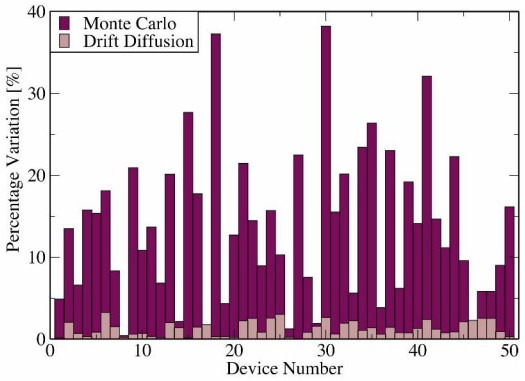

Figure 10. Comparison of percentage variation of drive current in 50 UTB SOI MOSFETs between Drift Diffusion and Monte Carlo simulations, showing a greater variation in Monte Carlo due to the capturing of increased scattering from body thickness fluctuations.

TABLE I COMPAISON OF ON-CURRENT AT LOW AND HIGH DRAIN BIAS IN DRIFT DIFFUSION AND MONTE CARLO.

	Drift Diffusion		**Monte Carlo**	
	1 mV	***1 V***	***1 mV***	***1 V***
Current (smooth interfaces) [A/μm]	1.042e-05	2.21e-03	1.195e-05	1.953e-03
Current (rough interfaces) [A/μm]	9.59e-06	2.043e-03	8.74e-06	1.742e-03
Percentage Reduction [%]	7.92	7.56	26.87	10.8

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