Quantum Corrections in 3-D Drift Diffusion Simulations of Decanano MOSFETs Using an Effective Potential

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Abstract

As MOSFET devices are aggressively scaled into the deep submicron regime quantum mechanical effects become increasingly important. We compare the recently proposed effective potential formalism with the density gradient approach for first order quantum simulations of sub 0.1μm MOSFETs within a modified drift diffusion framework.

1. Introduction

MOSFETs scaled down to 30nm gate lengths have been successfully demonstrated [1]. Further evidence [2] indicates that double gate MOSFET architectures will remain operational down to gate lengths of 10nm and below. However, the combination of thin gate oxides and heavy doping in conventional devices, and the thin silicon body of the double-gate structures, will result in substantial quantum mechanical (QM) threshold voltage shift and transconductance degradation. Computationally efficient methods to include QM effects are required for the purpose of practical Computer Aided Design. First order quantum corrections based on density gradients (DG) have already been introduced in 2-D [3] and 3-D [4] drift-diffusion simulations. Recently a new *Effective Potential* (EP) approach for introducing quantum corrections in classical and semi-classical simulations has been proposed [5] and demonstrated in Monte Carlo MOSFET simulations [6]. This paper investigates the quantum influence on threshold voltage, carrier density profile and I_D-V_G current characteristics within a modified drift diffusion framework. The first section describes the new effective potential formalism. A general and efficient algorithm for including quantum corrections within the self-consistent drift diffusion framework is described in section 3. Results from the new effective potential algorithm are compared with those from the well established density gradient approach in section 4, while section 5 presents our conclusions and discussions.

2. The effective potential formalism

An alternative approach to density gradient for including first order quantum effects is the recently advanced effective potential approach [6] in which, unlike with DG, the electron equation state is not modified directly. Instead 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:

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

where G is a Gaussian with standard deviation a_0.

3. Implementation of quantum corrections within the drift diffusion framework

We use the Gummel algorithm for solving the semiconductor equations in the drift diffusion approximation, introducing quantum corrections to the electron density using either the EP or DG formalism. We have compared two techniques for including the quantum corrections within the standard Gummel algorithm: In the first scenario the EP or DG solution is calculated within each Newton iteration of the non-linear Poisson equation to calculate the electron concentration. The current continuity equation is then solved as normal. However, this approach is computationally expensive. The second scenario resembles the standard procedure used to self-consistently solve the Poisson and the Schrödinger equations, using a self-adjusting damping scheme [7], for the potential. This is motivated by the fact that the DG equation is a partial non-linear equation which closely resembles Schrödinger's equation. In this scheme the quantum correction to the electron concentration is calculated only once per Gummel iteration, either via the effective potential or via a solution of the density gradient equation of state. This is a far less computationally demanding approach, converging in less time over a wide range of bias conditions.

4. Results

We have carefully calibrated both the EP and DG approaches against the results of a 1-D Poisson-Schrödinger solver [8]. 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.

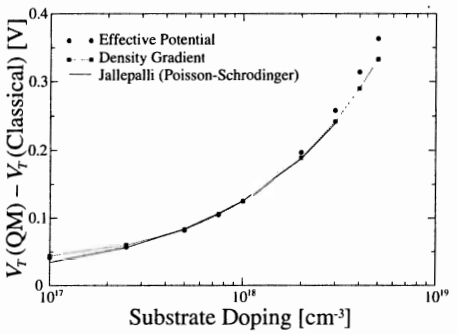

Fig. 1. Threshold voltage shift due to quantum effects versus substrate doping. Results for Density Gradient and Effective Potential are compared to those obtained from Poisson Schrödinger.

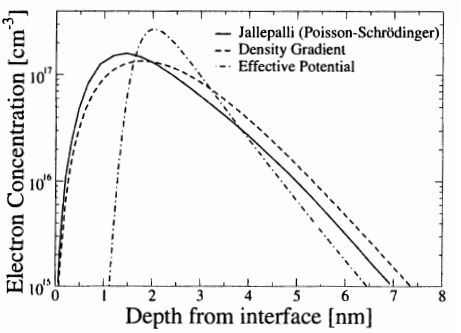

Fig. 2. Electron carrier concentration as a function of distance from the interface, for substrate doping of 5×10^{17}cm^{-3}. All have the same net sheet density.

Fig. 3, 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. We have also investigated the threshold voltage shift as a function of channel length, shown in Fig. 4. The variation with channel length is minimal at least down to 30nm, indicating the well scaled nature of our device structure.

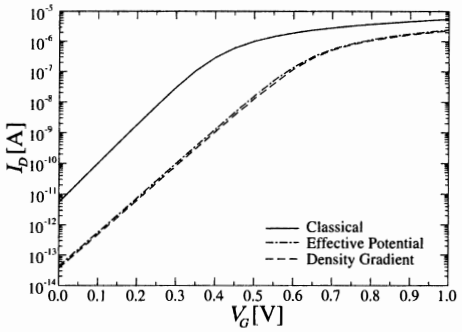

Fig. 3. I_D-V_G characteristic obtained from both classical and quantum simulators for a 30nm×30nm n-MOSFET, with V_D=0.01V and a substrate doping of 5×10^{18}cm^{-3}.

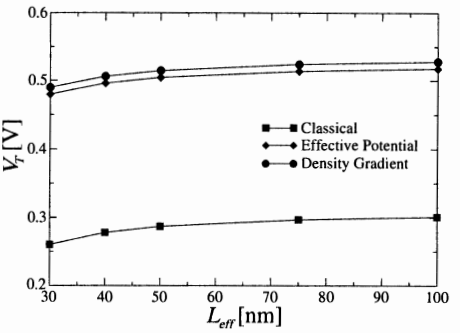

Fig. 4. Dependence of the threshold voltage on the channel length in MOSFETs with W_{eff}=50nm, N_A=5×10^{18}cm^{-3} and t_{ox}=1.3nm. illustrating the quantum mechanical shift in threshold voltage.

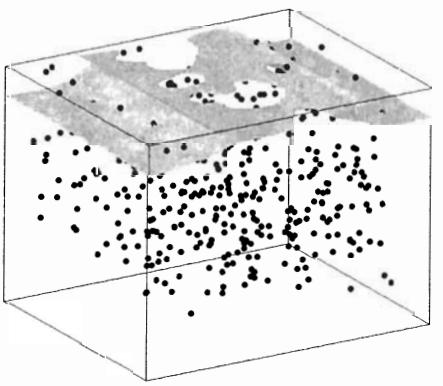

Fig. 5. An equi-concentration contour for a 30×50nm atomistic MOSFET, at threshold obtained using our effective potential simulator. Also shown are the individual acceptor positions throughout the structure.

Table 1. Results of atomistic simulations using classical, DG and EP methods

	Average threshold voltage $<V_T>$			Threshold voltage standard deviation σV_T		
Channel Length	Classical	Density Gradient	Effective Potential	Classical	Density Gradient	Effective Potential
30nm	0.179 V	0.376 V	0.370 V	28.2 mV	39.8 mV	40.6 mV
50nm	0.219 V	0.423 V	0.417 V	22.1 mV	30.8 mV	31.6 mV

We have also performed 3-D atomistic simulations, to compare the influence of EP on threshold voltage fluctuations as compared with DG [9]. Figure 5, shows a typical equi-concentration contour for a simulated atomistic MOSFET. Simulating 200 atomistic devices we have investigated threshold voltage and standard deviation at different channel lengths (Table 1). The EP simulations result in similar average threshold voltages and standard deviations compared to DG.

5. Conclusions

We have included both Density Gradient and Effective Potential quantum corrections within a self-consistent 3-D drift diffusion simulation, which includes a full solution of the current continuity equation. 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. For the simulations presented here we have found that the Density Gradient approach is computationally more efficient due to the numerically intensive nature of the 3-D convolution involved in calculating the effective-potential (V_{eff}). However, it is difficult to make a definitive judgement on which is the most suitable method for including first order quantum effects within device simulations. An important next step is to investigate to what extent, if any, the two methods can cope with source-to-drain tunnelling in decanano MOSFETs.

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