Effect of Oxide Interface Roughness on the Threshold Voltage Fluctuations in Decanano MOSFETs with Ultrathin Gate Oxides

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Abstract- **In this paper we use the Density Gradient (DG) simulation approach to study, in 3-D, the effect of local oxide thickness fluctuations on the threshold voltage of decanano MOSFETs on a statistical scale. The random 2-D surfaces used to represent the interface are constructed using the standard assumptions for the auto-correlation function of the interface. The importance of the Quantum Mechanical effects when studying oxide thickness fluctuations are illustrated in several simulation examples.**

I. INTRODUCTION

In the next generation decanano Si MOSFETs the oxide thickness will reach the few atomic layers limit [1]. As illustrated in Fig. 1 the interface roughness, which is on the scale of 1-2 atomic layers [2], may introduce more than 50% random fluctuations in the oxide thickness of such devices. The unique random pattern of the gate oxide in each decanano MOSFET will affect both the device electrostatics and the surface roughness limited mobility and will introduce random fluctuations in the device characteristics, similar to the fluctuations introduced by random dopants [3]. The proper investigation of the oxide thickness fluctuation effect requires 3-D simulations with fine grain discretisation on a statistical scale. It is also mandatory to include quantum mechanical effects, which shape the actual charge distribution near the interface, and may modify the impact of the surface roughness [4].

In this paper for the first time we use 3-D Density Gradient (DG) simulations [4] to study the effect of the local oxide thickness variations on the threshold voltage fluctuations in decanano MOSFETs with gate oxide thickness in the range of 1 to 2 nm.

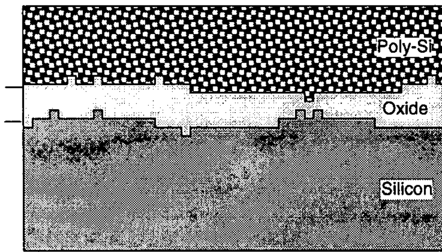

Fig. 1. Schematic illustration of gate oxide with average thickness 12 Å. The step height is approximately 3 Å.

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II. THE DENSITY GRADIENT APPROACH

The DG model [5] is an approximate approach for introducing quantum mechanical (QM) corrections into the macroscopic drift-diffusion (DD) approximation by considering a more general equation of state for the electron gas, depending on the density gradient. The QM corrections introduce an additional term in the carrier flux expression:

$$F_n = n\mu_n \nabla\psi - D_n \nabla n + 2\mu\nabla\left(b_n \frac{\nabla^2 \sqrt{n}}{\sqrt{n}} \right) \quad (1)$$

where $b_n = \hbar / (12 q m_n^*)$ and all other symbols have their usual meaning. In order to avoid the discretisation of fourth order derivatives in the current continuity equation when (1) is considered, a generalised electron quasi-Fermi potential, ϕ_n, was introduced in [4] as $F_n = n\mu_n \nabla\phi_n$. Thus the unipolar DD system of equations with QM corrections, which in many cases is sufficient for MOSFET simulations, becomes:

$$\nabla \cdot (\varepsilon \nabla \psi) = -q\left(p - n + N_D^+ - N_A^-\right) \quad (2)$$

$$2b_n \frac{\nabla^2 \sqrt{n}}{\sqrt{n}} = \phi_n - \psi + \frac{kT}{q} \ln \frac{n}{n_i} \quad (3)$$

$$\nabla \cdot (n\mu_n \nabla \phi_n) = 0 \quad (4)$$

where ψ, ϕ_n and $\sqrt{n}$ are independent variables. It should be pointed out that the simulation of a single device with random local variation of the oxide thickness requires a 3-D solution with fine grain discretisation near the interface. The requirement for statistical interpretation transforms the problem into a four dimensional one where the fourth dimension is the size of the statistical sample. Therefore, similar to [6], in this study we restrict our simulations to low drain voltage which allows us to disentangle (2) and (3) from (4) by considering a quasi-constant quasi-Fermi level. First we solve self-consistently the 3-D Poisson equation (3) for the potential and equation (4), which can be considered as a DG approximation of Schrödinger's equation, for the electron concentration. The boundary conditions are as described in [4]. Knowing the electron concentration from the self-consistent solution of (2) and (3), and following the

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procedure described in [7] we extract the current from the resistance of the MOSFET by solving

$$\nabla \cdot \mu_n n \nabla V = 0 \quad (5)$$

in a thin slab near the Si/SiO_2 interface engulfing the inversion layer charge. Dirichlet boundary conditions are applied for the 'driving' potential, V, at the source and drain contacts with $V = 0$ and $V = V_D$ respectively and Neumann boundary conditions are applied at all other boundaries of the slab. We have demonstrated in [7] that at low drain voltage this approach is in excellent agreement with the full, self-consistent solution of the DD equations.

The DG approach has been carefully calibrated for continuous doping against rigorous 1D full band Poisson-Schrödinger simulations presented in [8]. As illustrated in Fig.2, with an effective mass $m^* = 0.19m_0$ [4] an excellent agreement has been achieved between the DG simulations and the results presented in [8] regarding the QM threshold voltage shift in the doping concentration range relevant to this study. The DG approach also reproduces accurately the spatial charge distribution in the inversion layer [6].

III. Reconstruction of the Interface

The exact details of the Si/SiO_2 interface are still relatively unclear, especially from a physical point of view, despite a constant interest from industry and academe. The main difficulty stems from employing 2-D projection imaging techniques used to study an inherently 3-D and chemically incoherent interface [9]. In addition, sensitivity to the ambient conditions during fabrication, and to the material quality on either side of the interface, can often create further complications.

In line with most experimental and theoretical studies, the random 2-D surfaces used to represent the interface in this work are constructed using the standard assumptions for the auto-correlation function of the interface. Hence, the power spectrum, $S(q)$, of the interface is described by an exponential or Gaussian auto-correlation function with a given correlation length Λ and RMS height Δ [9]. In the Fourier domain we generate a complex $N \times N$ matrix, $\mathbf{A}_{ij}$, representing the height function, with the magnitude of the elements chosen to satisfy the power spectrum, while the phase is selected at random. However, several conditions [10] must be satisfied in order for the corresponding 2D surface in real space, obtained by inverse Fourier transformation, to represent a real function. Examples of random surfaces generated using exponential or Gaussian auto-correlation functions are presented in Fig. 3.

Finally the continuous 'analogue' random surface obtained using this procedure must be quantised in order to take into account the discrete nature of the interface fluctuations caused by random atomic arrangements.

IV. Case Study

In order to illustrate the importance of the QM corrections in respect to the simulation of oxide thickness fluctuations effects a simulation experiment was carried out in a 30x30 nm MOSFET with gate oxide forming a lateral superlattice of thin (1 nm) and thick (1.5 nm) oxide strips in the direction parallel to the channel. The threshold voltage dependence on the period, d, of the superlattice, calculated classically and with QM corrections, is illustrated in Fig. 4. Completely opposite behaviour for the threshold voltage is observed in the two sets of simulations. The classical results show reduction in the threshold voltage as d decreases, while

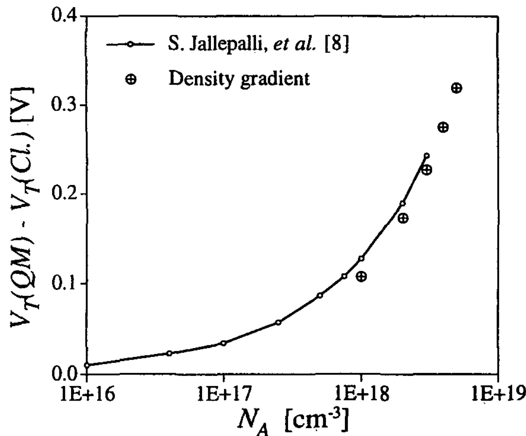

Fig. 2. Quantum mechanical threshold voltage shift as a function of the doping concentration in 1-D DG simulation, oxide thickness $t_{ox} = 4$ nm.

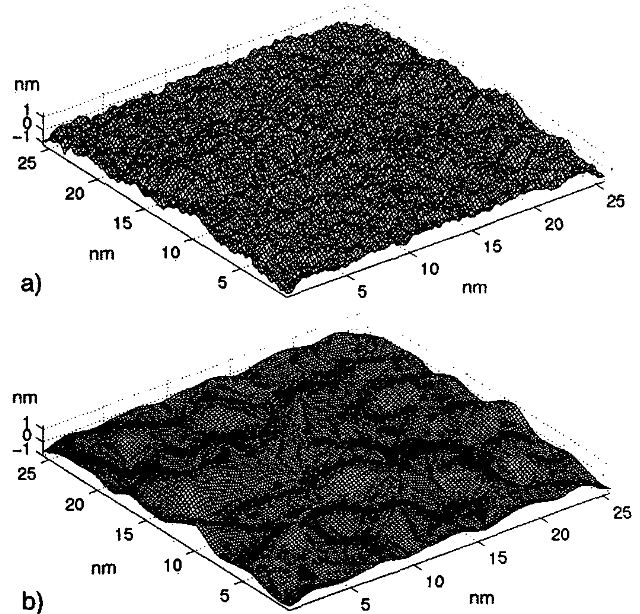

Fig. 3. Random surfaces generated using (a) an exponential or (b) a Gaussian power spectrum

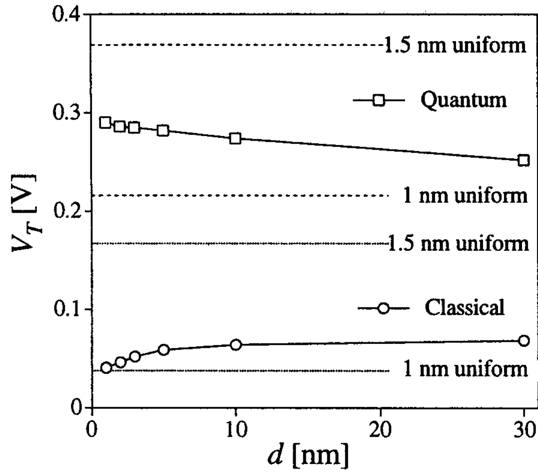

Fig. 4. Threshold voltage as a function of the period of superlattice formed by oxide thickness variation at the interface, aligned with the direction of the channel

the quantum mechanical results show an increase in the threshold voltage.

Fig. 5 offers the explanation of the observed behaviour. The top of the figure illustrates the Si/SiO_2 interface followed by two equiconcentration surfaces obtained from classical and DG simulations and the potential distribution at the bottom. In the classical simulations there is an increase in the carrier concentration near the edges of the well associated with the increase in the potential there. Such increase in the potential near the corners is well known in trench geometries and is the origin of the inverse narrow channel effect in trench isolated devices. The increasing contribution to the current from the corners, when the period of the superlattices decreases, results in a reduction of the threshold voltage in the classical case. However, due to the small depth of the trenches (0.5 nm) the QM charge distribution can not follow the local increase in the potential in the corners and the QM maximum in the charge concentration is in the middle of the wells. This is causing an increase in the threshold voltage when d becomes smaller.

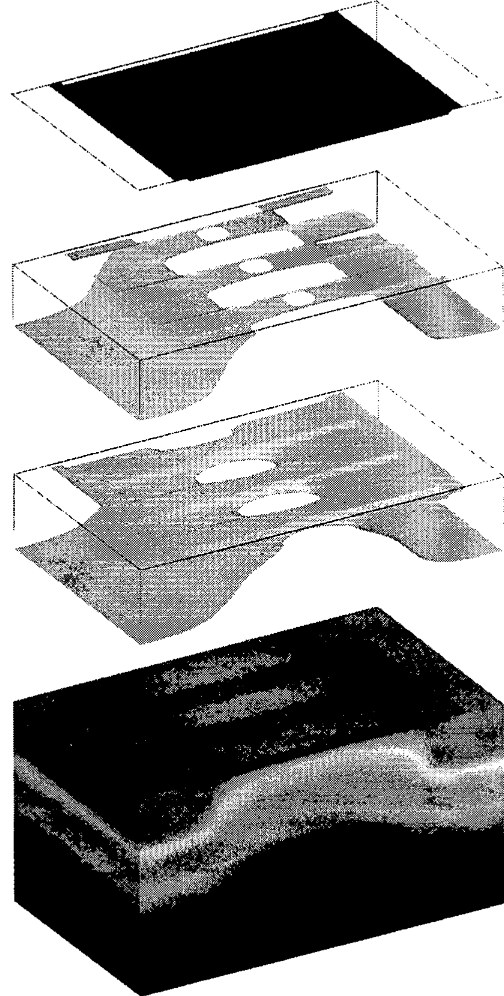

Fig. 5. Profile of the Si/SiO_2 interface in a 30×30 nm gate oxide 'superlatice' MOSFET (top) followed by two equiconcentration surfaces obtained from classical and DG simulations and the potential distribution (bottom).

V. Random Interface Results

Fig. 6 illustrates the potential and the charge distribution in a 30× 30 nm MOSFET with gate oxide which has a dominant random interface oxide roughness on the scale of one interatomic layer (3 Å). The average oxide thickness is 10.5 Å and the doping concentration in the channel region is 5×10^{18} cm^{-2}. The interface has been re-constructed starting from a Gaussian power spectrum. Only the roughness of the Si/SiO_2 interface is introduced in the simulations and the gate/SiO_2 interface is flat. The potential distribution at threshold voltage is shown at the bottom of the same figure. One equiconcentration surface corresponding to electron charge density 10^{17} cm^{-3} is plotted in the top of Fig. 6. The 3D quantum confinement in the thin gate oxide region in the middle of the channel is clearly visible. The oxide thickness fluctuations introduce surface potential fluctuations similar to the fluctuations introduced by random impurities [6].

The dependence of the standard deviation in the threshold voltage, σV_T, as a function of the correlation length Λ of the Si/SiO_2 interface roughness is plotted in Fig. 7 for the 30× 30 nm MOSFET illustrated in Fig. 6. Comparison is made between result obtained from classical and QM DG simulations. First of all σV_T increases with Λ and becomes substantial at correlation lengths above 15 Å which is the typical value reported in the literature today. Secondly, the

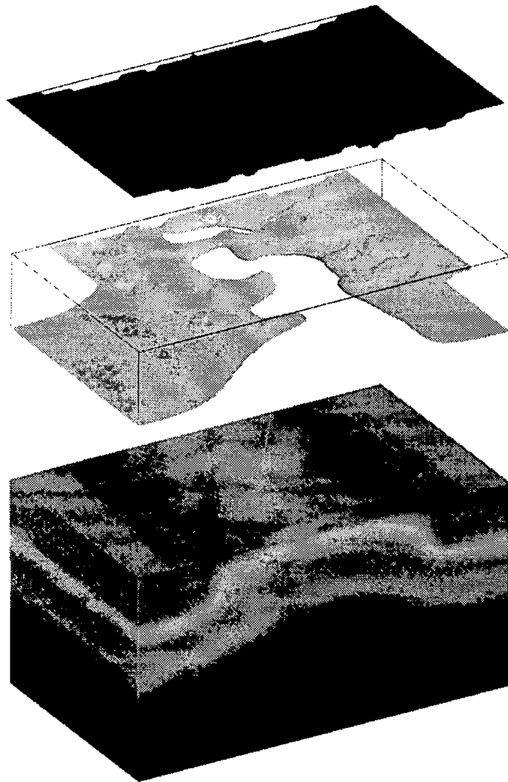

Fig.6. The profile of the random Si/SiO_2 interface in a 30×30 nm MOSFET (top) followed by two equiconcentration surfaces obtained from classical and DG simulations and the potential distribution (bottom).

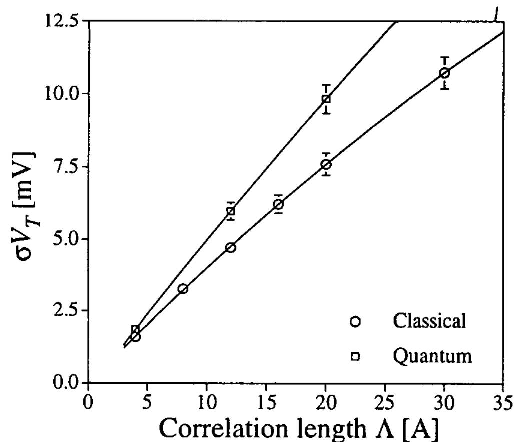

Fig.7. Dependence of the random oxide thickness induced threshold voltage standard deviation on the interface roughness correlation length for the 30×30 nm MOSFET from Fig. 6. Classical vs. DG simulations.

QM corrections result in an enhancement of the threshold voltage fluctuations.

VI. Conclusions

When the size of decanano MOSFETs becomes comparable to the correlation length of the Si/SiO_2 interface the oxide thickness fluctuations start to introduce substantial intrinsic variations in the device characteristics. The Quantum Mechanical confinement effects introduced in our simulations using the Density Gradient algorithm result in enhancement in the oxide thickness fluctuation related intrinsic parameter variations.

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