Analysis of Random Doping and Oxide Thickness Induced Fluctuations in Nanoscale Semiconductor Devices through Poisson-Schrödinger Computations

P. Andrei and I. Mayergoyz

Department of Electrical and Computer Engineering,
College Park, MD 20742, USA
isaak@eng.umd.edu, pandrei@eng.umd.edu

Abstract

The effects of random doping and random oxide thickness fluctuations in ultrasmall semiconductor devices are analyzed by using self-consistent Poisson-Schrödinger computations. A very fast technique based on linearization of the transport equations is presented for the computation of threshold voltage fluctuations. This technique is computationally much more efficient than the traditional Monte-Carlo approach and yields information on the sensitivity of threshold voltage fluctuations to the locations of doping and oxide thickness fluctuations. Hence, it can be used in the design of fluctuation resistant structures of semiconductor devices. Sample simulation results obtained by using our linearization technique are reported and compared with those obtained by using the Monte-Carlo technique.

1 Introduction

Intrinsic parameter variations in ultrasmall semi-conductor devices represent a major problem in the design of ULSI circuits. These variations affect the functionality and yield of many analog and mixed signal circuits that are based on pairs or multiples of nearly identical elements and whose performance depends on the matching properties of their components. In digital circuit applications, parameter variations of individual components have a negative impact on the noise margins and stability of circuits, and thus decrease the reliability of these circuits. The effects of intrinsic parameter variations are even more dramatic in the case of ultrasmall devices, which are becoming pervasive in modern electronics. Therefore, accurate analysis of parameter variations in semiconductor devices and methods for the reduction of these variations are strongly needed for further advances in high speed and low power nanoelectronics.

The effects of random doping and random oxide thickness induced fluctuations have been extensively studied by using classical transport equations [1-3]. Whereas these approaches are appropriate for sufficiently large semiconductor devices, in which quantum induced effects are not important, they cannot be applied to ultrasmall or heavily doped devices. Quantum mechanical (gradient density) approximations have been used to analyze random doping and random geometric dimension fluctuations [4,5]. These approximations provide useful qualitative information, but they fail to produce reliable quantitative results. In the article, we address this problem by

developing a new method for the analysis of fluctuations in semiconductor devices based on self-consistent Poisson-Schrödinger computations.

There are two conceptually different approaches to the analysis of fluctuations in semiconductor devices. The first approach, known as the Monte-Carlo approach, is based on generating numerous realizations of the doping and oxide structures and solving the transport equations for each of such realizations [4]. Statistics of different parameters of interest are then accumulated and used to evaluate the average values and variances of those parameters. The Monte-Carlo approach is computationally very expensive because the same device-level simulations have to be performed many times and the final results are prone to statistical errors. The second approach to the analysis of fluctuations in semiconductor devices is based on linearization of the transport equations and direct computations of variances of fluctuating quantities [5,6]. This approach is computationally much more (orders of magnitude) efficient than the Monte-Carlo technique and is not subject to statistical errors. In addition, it provides information on the sensitivity of parameter variances to the locations random doping and random oxide thickness fluctuations, which makes it instrumental in the design of fluctuation resistant structures. In this paper, both approaches are used to calculate variances of threshold voltages in nanoscale MOSFET devices and the accuracy of these two approaches are compared.

2 Technical discussion and simulation results

The carrier concentration in *n*-type silicon inversion layers is described by the coupled Poisson and "effective mass" Schrödinger equations:

$$\nabla\left(\varepsilon\nabla\varphi\right) = -q\left[p - n + D\right], \tag{1}$$

$$-\frac{\hbar^2}{2}\nabla\left(\frac{1}{m_i^*}\nabla\Psi_{i,n}\right) + \left(\Delta E_c - q\varphi\right)\Psi_{i,n} = E_{i,l}\Psi_{i,n}, \tag{2}$$

where φ is the electrostatic potential, D is the doping concentration, $\psi_{i,n}$ are the "envelope" wave functions associated with the *n*th eigenvalue $E_{i,n}$ in subband *i*, m_i^* is the effective electron mass tensor, ΔE_c is the conduction band off-set, while all other notations have their usual meaning. Any fluctuation of the doping concentration induces fluctuations in the values of electric potential, energy eigenvalues, and energy eigenfunctions. Since most device parameters are directly related to the solution of equations (1)-(2), the values of those parameters will fluctuate. In the first order approximation, the variance of any fluctuating parameter *A* (e.g. threshold voltage, current, cutoff frequency) can be written as:

$$\sigma_A^2 = \sum_i \left(\gamma_A^{D_i}\right)^2 \frac{\left\langle D_i \right\rangle}{\Delta V_i}, \tag{3}$$

where only random doping fluctuations have been considered for simplicity. The summation in (3) is taken over all discretization points of the semiconductor device, and $\left\langle D_i \right\rangle$ is the expected value of the doping concentration at location *i*, and $\gamma_A^{D_i}$ are "superposition coefficients" that shows how sensitive parameter *A* is to the locations of doping fluctuations. The superposition coefficients can be found by using the perturbation theory and the algorithm presented in [7].

Consider the fluctuations of the threshold voltage for 1-D MOS capacitors. The superposition coefficients of the threshold voltage can be written as [7]:

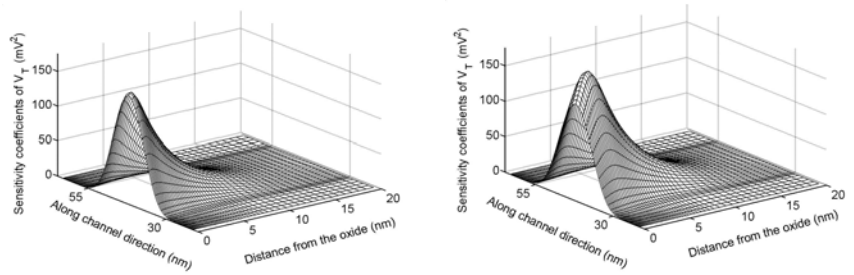
$$\gamma_{V_T}^{D_i} = -\left(\frac{\boldsymbol{g}^t \cdot \hat{\boldsymbol{F}}_{\boldsymbol{D}}}{\boldsymbol{g}^t \cdot \boldsymbol{F}_{V_G}} \right)_i , \tag{4}$$

where $\hat{\boldsymbol{F}}_{\boldsymbol{D}}$ and $\boldsymbol{F}_{V_G}$ are the derivatives of the discretized transport equations with respect to the doping concentration and gate voltage. $\boldsymbol{g}^t$ is the transpose of column vector $\boldsymbol{g}$, which can be found by solving the linear system of equations $\hat{\boldsymbol{J}}^t \boldsymbol{g} = \boldsymbol{a}^t$, where $\hat{\boldsymbol{J}}^t$ denotes the transpose of the Jacobian matrix of the transport equations and $\boldsymbol{a}$ is a vector that depends on the definition of V_T adopted in simulations (e.g. "inversion charge" definition, "current" definition, etc.). More details about the numerical implementation and the efficiency of the algorithm can be found in [7,8].

In the following, we present a few simulation results obtained for 1-D *n*MOS capacitors and 2-D short channel *n*MOSFET devices. The acceptor dopant concentration of both devices decreases from D=5x10^{18} cm^{-3} at y=20 nm from the oxide/semiconductor interface, to D=5x10^{16} cm^{-3} at the interface. For y>20 nm, the doping concentration is constant and equal to its value at y=20 nm. In Table 1 we present the standard deviation of V_T computed by using the Monte-Carlo and the linearization techniques for the 1-D MOS capacitor. One observes a very good agreement between the two techniques. In Figs. 1(a)-(b), we present the "sensitivity coefficients" of V_T computed for the 2-D MOSFET. These coefficients are defined as $\left(\gamma_{V_T}^{D_i} / \Delta V_i\right)^2$ and are computed by using the classical drift-diffusion and self-consistent Poisson-Schrödinger models. Quantum effects result in a slight shift (approximately 1.3 nm) of the maximum of the distribution of "sensitivity coefficients" away from the interface. In Figs. 2(a)-(b), we present the dependence of σ_{V_T} on the average doping concentration in the channel and on the oxide thickness.

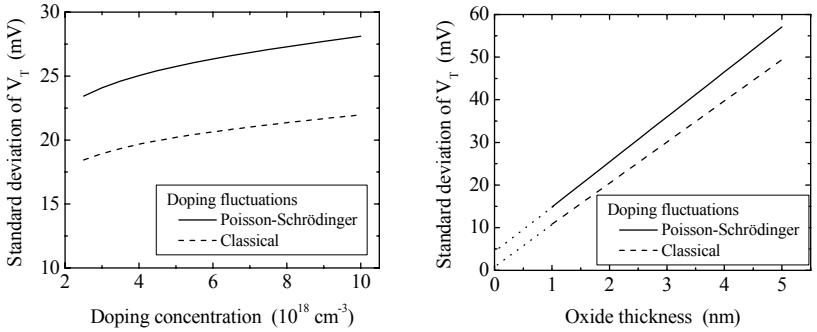
	Doping fluctuations		Oxide thickness fluctuations	
Number of simulations	$\sigma_{V_T} \times \sqrt{LW}$ (mV × μm) Classical	$\sigma_{V_T} \times \sqrt{LW}$ (mV × μm) Poisson-Schrödinger	$\sigma_{V_T} / \sigma_{ox}$ (mV/nm) Classical	$\sigma_{V_T} / \sigma_{ox}$ (mV/nm) Poisson-Schrödinger
100	1.39	1.59	168	171
200	1.43	1.64	166	168
500	1.42	1.62	164	161
1000	1.39	1.60	161	165
Linearization technique	1.41	1.75	159	166

Table 1: Standard deviations of V_T for the *n*MOS capacitor with oxide thickness of 5 nm and retrograde doping profile. L and W denote the length and the width of the device, respectively, while σ_{ox} is the standard deviation of the oxide thickness.



(a) (b)

Figure 1: Sensitivity coefficients of threshold voltage for a MOSFET device: (a) classical computations and (b) quantum computations. The channel length extends from 30 nm to 55 nm in the "along channel" direction. The oxide thickness is 2 nm.



(a) (b)

Figure 2: Standard deviation of V_T for a MOSFET device with $L = W = 25$ nm, and t_{ox} = 2 nm. The doping concentration indicated on the abscissa corresponds to the doping concentration at y=20 nm. Only random doping induced fluctuations are considered.

One can see that the quantum mechanical effects result in the increase of the standard deviation of the threshold voltage by approximately 10-15%. This effect can be detrimental to the scaling of many analog and digital circuits, where the matching properties of the transistors are essential (e.g. differential amplifiers, A/D converters).

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