3D Quantum Corrected Monte Carlo Simulation of n-FinFETs

C. S. Soares, G. F. Furtado[*], A. C. J. Rossetto[**], G. I. Wirth, D. Vasileska[***].

Programa de Pós-Graduação em Microeletrônica Universidade Federal do Rio Grande do Sul Porto Alegre, Brazil.
[*]Silvaco, Porto Alegre, RS, Brazil.
[**]Centro de Desenvolvimento Tecnológico Universidade Federal de Pelotas Pelotas, Brazil
[***]Department of Electrical Engineering Arizona State University Tempe, USA
e-mail: santos.soares@ufrgs.br

A Monte Carlo (MC) device simulator is an efficient tool to analyze the performance and reliability of transistors. However, to adequately model multi-gate transistors, such as n-FinFETs, in which electrons are confined along the fin height and width, a quantum correction (QC) must be included into the MC device simulator.

Previous works have successfully incorporated the Effective Potential model [1] as a QC into MC device simulators of planar devices [2]. In this work, we employ the Effective Potential model as a quantum correction to MC device simulator to consider the quantum confinement of electrons in n-FinFETs.

The Effective Potential approach [1] was developed to model space-quantization effects. The expression for the Effective Potential is derived by employing the density-matrix formalism, that allows one to estimate the potential of a system of electrons, assuming that the electrons are Gaussian wave packets. The Effective Potential is given by

$$V_{eff}(\mathbf{r}) = \int \frac{1}{(2\pi\sigma^2)^{3/2}} V(\mathbf{r}')exp\left(-\frac{|\mathbf{r}-\mathbf{r}'|^2}{2\sigma^2}\right)d\mathbf{r}', \quad (1)$$

where σ is the smoothing parameter of the Effective Potential and $V(\mathbf{r})$ is the Hartree potential. To obtain the smoothing parameter, we employed the fitting method explained in Ref. [3]. From the definition of the Effective Potential, the carriers can be treated as zero-size particles that are exposed to this Effective Potential.

This QC was incorporated into the MC device simulator for n-FinFETs presented in Ref. [4]. In the quantum corrected MC device simulator, the Effective Potential is efficiently calculated using:

$$V_{eff}^{i,j,k} = \frac{1}{(2\pi\sigma^2)^{3/2}}\sum_{l,m,n}\left[\left(x_i,y_j,z_k\right)I_{i,j,k,l,m,n}^1 + \right.$$

$$\left(V(x_l,y_m,z_n) - V(x_i,y_j,z_k)\right)\left(I_{i,j,k,l,m,n}^2 + \right. \quad (2)$$

$$\left. I_{i,j,k,l,m,n}^3 + I_{i,j,k,l,m,n}^4\right)\right],$$

where the index l,m,n refers to the neighbor points around i,j,k, V is the Hartree potential calculated by the Poisson solver, and $I_{i,j,k,l,m,n}^1$, $I_{i,j,k,l,m,n}^2$, $I_{i,j,k,l,m,n}^3$, and $I_{i,j,k,l,m,n}^4$ are error and exponential functions of the mesh spacing. The coefficients of Eq. (2) are calculated ahead of time, thus saving computational time. The flowchart of the simulator is shown in Fig. 1. The force that acts on the electrons in the transport is calculated from the Effective Potential.

The device structure of interest, represented in Fig 2, is an unintentionally doped FinFET with H_{Fin} and W_{Fin} of 42 nm and 8 nm, respectively, with L = 18 nm, and EOT = 1.2 nm. For this device, σ = 0.45 nm. Both semi-classical MC and quantum corrected MC simulators include random distribution of dopants. Fig. 3 shows the conduction band profile for a given dopant distribution. The impact of the random dopant distribution is clearly seen in the transfer characteristics of this device obtained by using the semi-classical MC simulator (Fig. 4) and the quantum corrected MC simulator (Fig. 5). From the semi-classical simulations, we calculate that the average threshold voltage is V_T = 0.4368 V, while the quantum corrected simulation gives V_T = 0.4522 V. The higher V_T obtained by using the QC model is expected due to the quantum-mechanical size quantization effects, that lead to smaller carrier density in the channel (see Fig. 6 for the average line density along the channel length).

In summary, we presented accurate and efficient methodology for studying transport in n-FinFET devices that adequately describes volume inversion in the channel and, at the same time, significantly reduces the computational time as opposed to a full Non-Equilibrium Green Function (NEGF) approach.

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[2] D. Vasileska, et al., *The Role of Quantization Effects on the Operation of 50 nm MOSFETs, 250 nm FIBMOS Devices and Narrow-Width SOI Device Structures*, Journal of Computational Electronics **1**, 453–465 (2002).

[3] C. S. Soares, et al., *Modeling Quantum Confinement in Multi-Gate Transistors with Effective Potential*, 36th SBMICRO Conference, Porto Alegre, Brazil (2022).

[4] G.F. Furtado, et al., *3-D TCAD Monte Carlo Device Simulator: State-of-the-art FinFET Simulation*, Journal of Integrated Circuits and Systems **16**, p. 1 (2021).
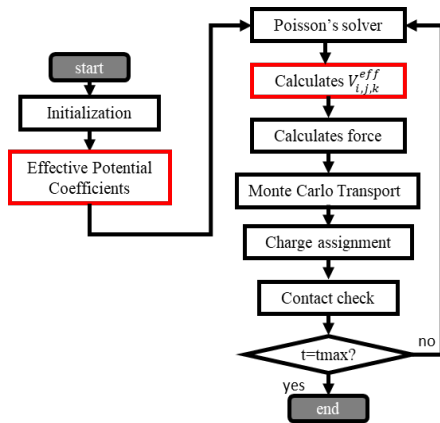
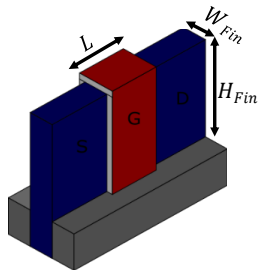Fig. **1**. Flowchart of the quantum corrected MC simulator.

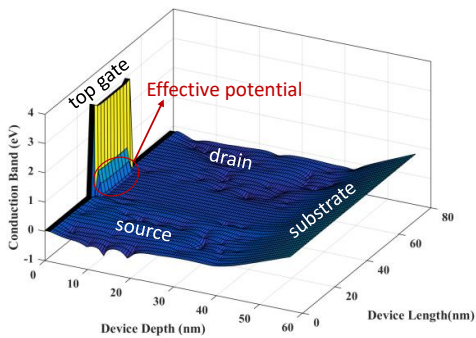Fig. **2**. Structure of the n-FinFET studied in this work.

Fig. **3**. Conduction band along the device length and depth at the middle of W_{FIN}. $V_B = V_S = 0$ V, $V_{DS} = 0.1$ V and $V_{GS} = 0.8$V.
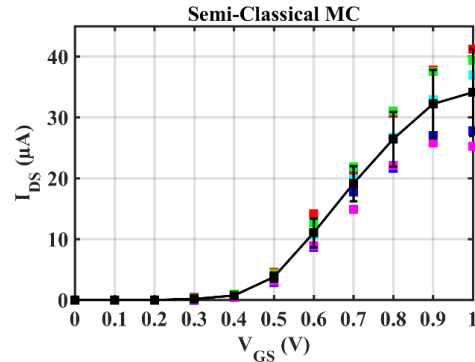

Fig. **4**. Transfer characteristics obtained with semi-classical MC simulator for five devices with different random dopant distribution in the source, drain and channel. The average channel doping is 10^{15}cm^{-3}. Solid line is the averaged characteristic. $V_B = V_S = 0$ V and $V_{DS} = 0.1$ V.
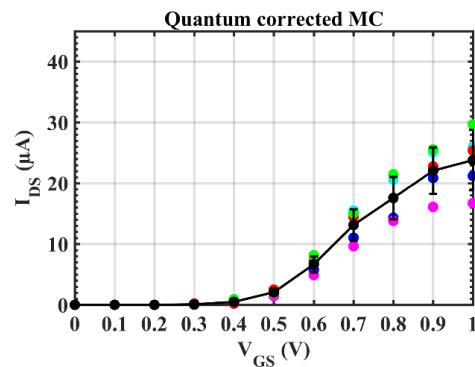

Fig. **5**. Transfer characteristics obtained with the QC MC simulator for five devices with different random dopant distribution in the source, drain and channel. The average channel doping is 10^{15}cm^{-3}. $V_B = V_S = 0$ V and $V_{DS} = 0.1$ V.
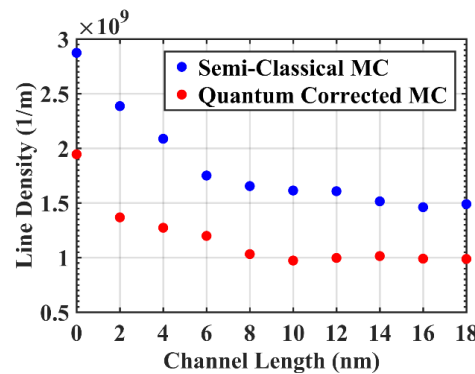

Fig. **6**. Line density calculated using the semi-classical MC device simulator (blue) and quantum corrected MC device simulator (red). $V_B = V_S = 0$ V, $V_{DS} = 0.1$ V and $V_{GS} = 0.8$ V.