Surface Roughness Scattering in NEGF using self-energy formulation

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***Abstract*—The microelectronic industry has moved from matured bulk planar transistor to three-dimensional (3D) architectures with small non-trivial cross-sections and short channel lengths requiring quantum simulation techniques. In addition, novel materials, which enhance the transistor performance, are considered as silicon channel replacement. This necessitates the efficient inclusion of surface roughness scattering in quantum transport simulations. In this work, we report an approximate methodology to include surface roughness scattering in 3D Non-Equilibrium Green's Function (NEGF) simulations using self-energy formulation within the self-consistent Born approximation (SCBA). The method is validated with the well established methodology of treating surface roughness as a variability source. We also extract the mobility from our simulations and then compare with to those reported in the literature.**

***Index Terms*—surface roughness, NEGF, mobility, scattering**

I. Introduction

The progress of the semiconductor industry in the last 50 years has been governed by scaling the physical dimensions of the metal-oxide-semiconductor field effect transistor (MOSFET). In order to continue this scaling trend, the industry has adopted 3D multi-gate architecture [1]. This led to a better control of short channel effects that limit the scaling of the conventional (bulk) MOSFETs. The attention of both industry and academia is also focused on the novel materials to boost the performance of the transistor without scaling of the MOSFETs [2]. These factors make the interface between the oxide and semiconductor even more critical in the working of the MOSFET. Because of these reasons, modeling of surface roughness scattering is important for predicting the performance of the contemporary and future transistors.

The non-equilibrium Green's Function (NEGF) formalism has become the method of choice to model ultra-scaled transistors. NEGF can accurately capture the confinement in the direction normal to the electron transport as well as quantum transport effects, such as source to drain tunneling [3]. However, the efficient modelling of the surface roughness (SR) scattering in NEGF for realistic current simulations has not been addressed yet in the literature [4]. Therefore, in this paper, we report a new approximate methodology to include SR scattering in the 3D NEGF simulation through the inclusion of a self-energy expression for the SCBA. This is implemented in our comprehensive in-house simulation framework, NESS – Nano-Electronic Simulation Software [5].

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II. Methodology

A. Surface Roughness Scattering

Traditionally, SR scattering in the NEGF formalism has been modeled by generating an ensemble of devices with statistically different surface roughness configurations and by performing transport simulation for each one of them [6]–[8]. Then the statistical average of the current is computed for the ensemble in order to estimat the effect of surface roughness scattering. Due to the need of large simulation ensemble to reduce the statistical noise, this method is computationally expensive. In this work, the interface between the semiconductor and oxide is characterized by an auto-correlation function

$$C(r) = \Delta_{rms}^2 e^{-\sqrt{2}r/L_C} \tag{1}$$

where Δ_{rms} is the root mean square of the surface roughness, L_C is the correlation length, and r is the distance between two mesh points.

The electron dynamics in the coupled mode space NEGF implementation is modeled by [9]:

$$\left[E - H_{MS} - \Sigma_{MS}^R\right] G_{MS}^R = I \tag{2}$$

$$G_{MS}^< = G_{MS}^R \Sigma_{MS}^< \left(G_{MS}^R\right)^\dagger \tag{3}$$

where H_{MS} is the Hamiltonian, Σ_{MS}^R and $\Sigma_{MS}^<$ are retarded and lesser self energies (comprising of both the contacts

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and interactions), respectively, and I is the identity matrix. In this work, we have employed parabolic effective mass approximation, which has been shown to give reasonably accurate results when compared to the full-band approach [10]. For elastic interactions, the self-energies [11] can be written as:

$$\Sigma^{<}_{MS} = M^2 G^{<}_{MS} \tag{4}$$

$$\Sigma^{R}_{MS} = \frac{M^2}{2}\left(\Sigma^{>}_{MS} - \Sigma^{<}_{MS}\right) \tag{5}$$

where M is the matrix element. For SR scattering, the ensemble average squared matrix element (using exponential power spectrum of the surface roughness) can be written as [12]:

$$\begin{aligned}\left\langle |M_{m,n}(k,k')|^2 \right\rangle &= |\langle m,k'|H_{pert}|n,k\rangle|^2 \\ &= \frac{e^2 N_E^2(m,n)\Delta_{rms}^2\sqrt{\pi}L_C}{L_x} e^{-\frac{q^2 L_C^2}{4}}\end{aligned} \tag{6}$$

where H_{pert} is the perturbed Hamiltonian (SR), L_x is the normalization length, q is the difference of magnitudes of the wavevectors before and after scattering ($|k_x| - |k'_x|$), m and n are the subband indices. The effective electric field, $N_E(m,n)$, can be calculated as:

$$N_E(m,n) = \int d\mathbf{A}\zeta_n(\mathbf{r})\mathbf{E}_{y,z}(x)\zeta_m(\mathbf{r}) \tag{7}$$

where $\zeta_m(\mathbf{r})$ is the wavefunction corresponding to the m^{th} subband in the cross-section, and $\mathbf{E}_{y,z}$ is the electric field along the confinement directions, which correspond to 'y' and 'z' directions in this work. In the limit $q \to 0$ (and making the self-energies local in real space) makes the matrix element independent of the wave-vector and thus allows us to express the matrix elements in coupled mode space as:

$$\begin{aligned}\left\langle |M_{m,n}(x,x')|^2 \right\rangle &= |\langle m,x'|H_{pert}|n,x\rangle|^2 \\ &= e^2 N_E^2(m,n)\Delta_{rms}^2\sqrt{\pi}L_C\delta(x-x')\end{aligned} \tag{8}$$

B. Mobility Calculation

We simulate three nanowires transistors with gate lengths, L_{G1}, L_{G2} and L_{G3}, and with a very low drain bias (V_{DS} = 1 mV) [13]. Then, using their drain current I_{D1}, I_{D2} and I_{D3}, the mobility (μ) and the necessary condition for the diffusive transport (C_D) can be calculated. The mobility is given by

$$\mu = \frac{L_{G2} - L_{G1}}{R_2 - R_1}\frac{1}{e\rho_{1D}} \tag{9}$$

where $R_1 = V_{DS}/I_{D1}$ and $R_2 = V_{DS}/I_{D2}$ are the resistances of the nanowires, e is the unit electron charge and ρ_{1D} is the 1D charge density evaluated at the center of the device. The diffusive transport condition (variation in the resistance is linearly proportional to the change in the gate length) can be evaluated using

$$C_D = \frac{R_3 - R_2}{L_{G3} - L_{G2}}\frac{L_{G2} - L_{G1}}{R_2 - R_1} \approx 1 \tag{10}$$

where $R_3 = V_{DS}/I_{D3}$.

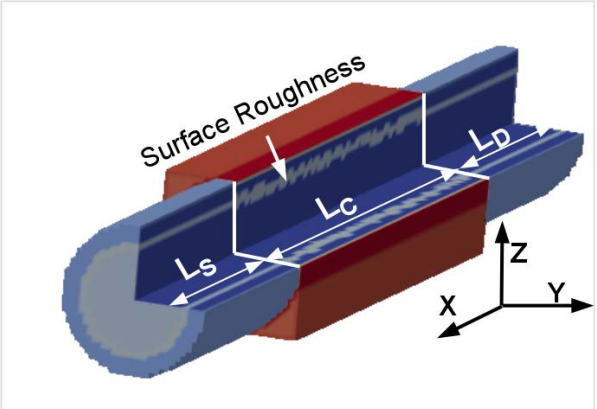

Fig. 1. Schematic of the circular nanowire and illustrating the surface roughness in gated region that is used in the statistical simulations. For the simulation gate length, L_G, was set to 20 nm, and source (L_S) and drain (L_D) length are set to 10 nm. In this study, the diameter, D, of the device was varied.

III. Results

Fig. 1 shows the schematic of the silicon nanowire transistor (NWT) used in the simulations. The transport orientation of the nanowire was [100]. The source and drain doping is 10^{20} cm^{-3} and the channel doping is 10^{15} cm^{-3}. The effective oxide thickness is 0.8 nm. In this work, surface roughness was considered only in the gated region. This is because the electric field normal to the transport direction is highest under the gate and thereby it is expected to dominate the transport. The oxide-semiconductor interface in the source and drain region is assumed to be smooth.

Fig. 2 shows the comparison of the band structure between the tight-binding method (calculated using QuantumATK [14] and parameters published in [15]) and the parabolic effective mass method. The spin-orbit coupling was ignored in the tight-binding band structure calculations as it is expected to have negligible impact on the conduction band. The comparison highlights an excellent agreement between the tight-binding and effective mass (with calibrated effective masses) approximation in the energy range relevant for the MOSFET in terms of the subband minimas and band curvature around the minimas. In this paper, the effective masses for different diameters were calibrated to reproduce the band-structure calculated with the tight-binding method. The effective masses for different cross-sections are reported in [16].

Fig. 3 compares the transfer characteristics for the circular nanowire with diameter of 4 nm. The result shows a good agreement between the transfer characteristic for a nanowire MOSFET obtained with mean of the statistical simulations and self-energy simulations. For statistical simulations, an ensemble of 140 instances were used to obtain a correct statistical average. The root mean square of the surface roughness, Δ_{rms}, for statistical simulation was taken to be 0.21 nm which is consistent with the experimental data for bulk Si

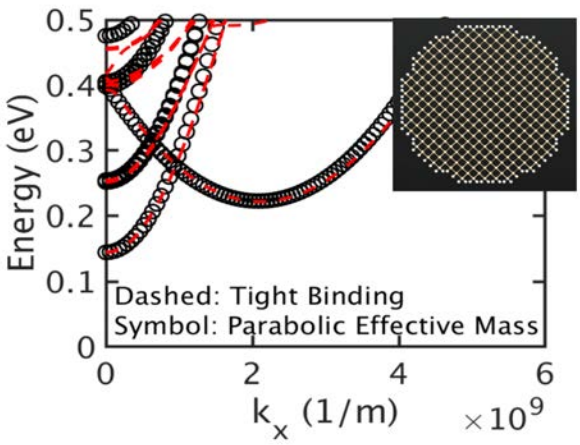

Fig. 2. Comparison between the tight-binding and parabolic effective mass approximation for a circular nanowire with the diameter, D = 4 nm. The inset shows the arrangement of atoms in the cross-section of the nanowire. The bottom of the bulk conduction band edge was taken to be the reference (0 eV).

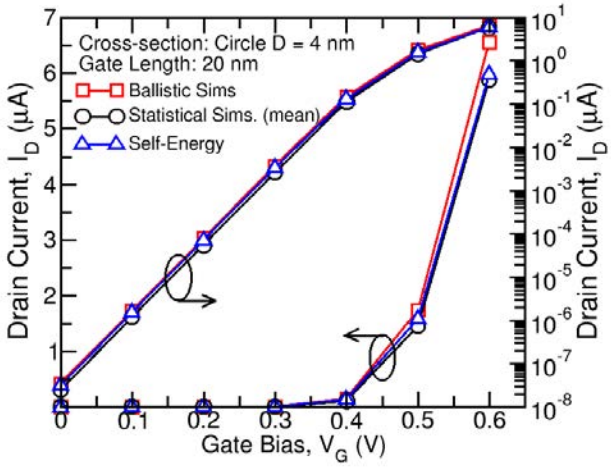

Fig. 3. Comparison of the transfer characteristics calculated with the self-energy formulation and mean of the statistical simulations is reported. The diameter of the device was set to 4 nm. A good comparison between the two methods is obtained.

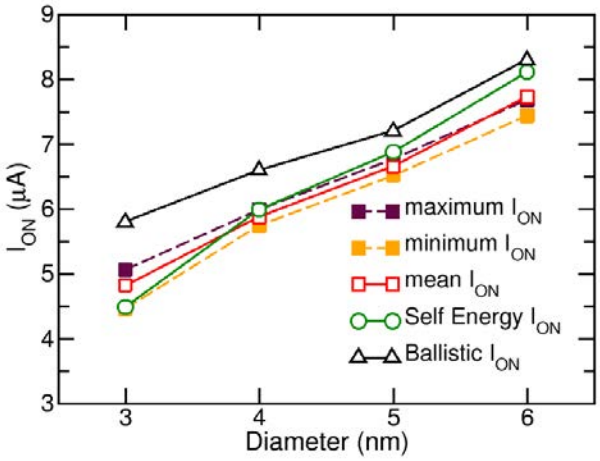

Fig. 4. Comparison of the mean on-current calculated with the statistical simulations and the self-energy method discussed. For comparison, we have also plotted the maximum and minimum on-currents calculated with the statistical simulations. The Δ_{rms} used for the statistical simulation was 0.21 nm while for the self-energy it was taken to be 0.18 nm. The correlation length, L_c, was set to 1.4 nm for all the simulations.

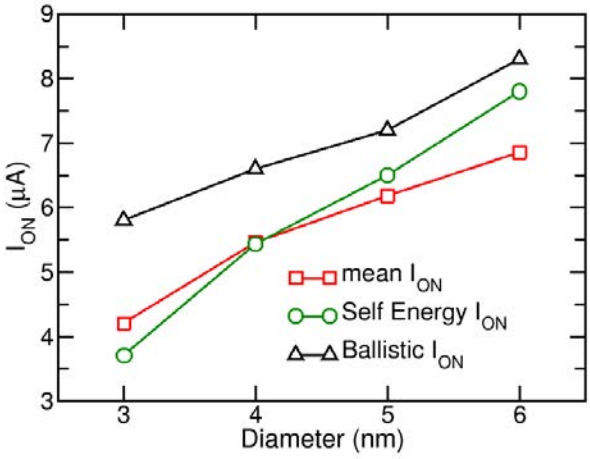

Fig. 5. Comparison of the mean on-current calculated with the statistical simulations and the self-energy method discussed. The Δ_{rms} used for the statistical simulation was 0.31 nm while for the self-energy it was taken to be 0.3 nm. The correlation length, L_c, was set to 1.4 nm.

based transistors [17]. Δ_{rms} for self-energy formulation was calibrated to 0.18 nm to match the statistical simulation. Fig. 4 and Fig. 5 shows the comparison between the mean on-current (I_{on}) calculated with the statistical simulations and with the self-energy for diameters ranging from 3 nm to 6 nm and for different surface roughness values. The I_{on} was defined as the drain current at V_{DS} = V_{GS} = 0.6 V. The results highlight a fair comparison of the I_{on} between the statistical and self-energy based methodologies with some discrepancy at larger diameter (D = 6 nm).

Fig. 6 compares the mobility calculated with NEGF formulation and those reported in the literature [18]. The mobility in this work was calculated using the method discussed Section II-B. For the purpose of the mobility calculations the gate length of 20, 30 and 40 nm were used. The effective electric field (E_{eff}) was calculated at the center of the device and it is given by:

$$E_{eff} = \frac{1}{n_s} \int \int dy\ dz\ n(\mathbf{r}) \left[E_y^2 + E_z^2\right]^{0.5} \qquad (11)$$

where n_s is the total electron density in the cross-section, E_y and E_z are the electric field along the y and z directions and $n(\mathbf{r})$ is the electron density in the cross-section. In order

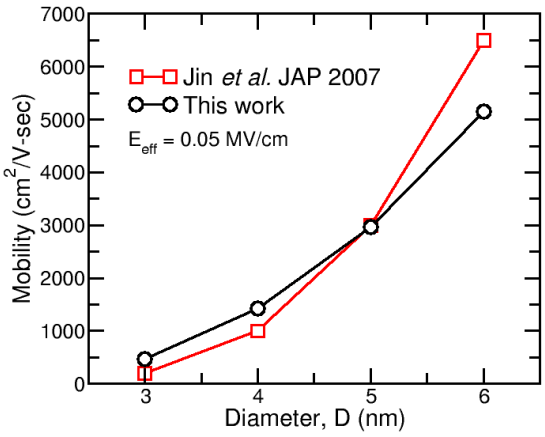

Fig. 6. Comparison between the mobilities calculated from NEGF and ones reported in [18] for circular nanowires with different diameters and for an effective field, E_{eff} = 0.05 MV/cm. The effective mass, oxide-semiconductor barrier are consistent with those used in the Ref. [18].

to match the mobility, $\Delta_{rms} = 0.21$ nm and $L_c = 1.4$ nm were used. A fair agreement is observed between the mobility calculated with NESS-NEGF simulations and the results reported in the literature obtained using the Kubo-Greenwood formulation.

IV. Conclusion

In this paper, we propose a self-energy correction, Σ_{SR}, that allows a perturbative treatment of the surface roughness scattering in 3D NEGF simulations, which greatly reduces the computational burden compared to statistical simulations. The locality of Σ_{SR} in real space makes it easy to implement. The ON-current obtained by the perturbative treatment showed a fair agreement with statistical simulations for different cross-section areas for circular nanowire transistors. The mobility values that we extracted using self-energy formulation in NESS-NEGF follow the same trend as the ones available in the literature.

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