A NEGF Study of the Effect of Surface Roughness on CMOS Nanotransistors

A. Martinez¹, A. Svizhenko², M. P. Anantram¹, J. R. Barker¹ and A. Asenov¹

¹Device Modelling Group, Dept of Electronics & Electrical Engineering, University of Glasgow, Glasgow G12 8LT, United Kingdom
²NASA Ames Research Center, MS:229-1, Moffet Field, California 94035-1000, USA

antonio@elec.gla.ac.uk

Abstract. Start The effect of surface roughness on the electron transport of a double gate nanotransistor has been studied. The study has been carried out using a two-dimensional non-equilibrium Green’s function formalism coupled self-consistently with Poisson’s equation. A novel discretisation scheme for Poisson and the Green’s function equations has been implemented in order to describe properly the surface roughness. The two-dimensional electron and current density landscape for the device with surface roughness exhibit strong inhomogeneity as compare with the smooth case (non-surface roughness). The effects of the specific profile of the surface roughness do not self-average. The total macroscopic current pattern follows the microscopic detail of the roughness.

1. Introduction
The continuing need for device miniaturisation brings the scale of transistors down to dimension of tens of nanometres. At these dimensions the influence of interface roughness between the gate oxide and the channel on carrier transport increases, particularly in thin body double gate devices where the roughness is correlated to body thickness fluctuations. Therefore a perturbative treatment of the surface roughness is no longer valid. A solution to this problem is to treat the interface as a function in a real space. In the past the study of quantum transport through narrow channels in nano-CMOS transistors has been mainly limited to the so called mode space approach applying the 1D NEGF formalism in the transport direction even when 2D and 3D device structures were considered. The realistic treatment of the interface roughness in thin body DG MOSFETs requires a full 3D quantum transport simulation. However, the 2D simulations presented highlight the important effects. When the body thickness of double gate transistors is on the order of a few nanometres the current flow has a two-dimensional character due to the irregular nature of both interfaces. In this work, a new discretisation scheme has been implemented in a quantum device simulator based on a 2D self-consistent non-equilibrium Green’s function (NEGF) formalism [1]. The quantum transport and
surface roughness models used in the simulation are explained in section 2. The device used in the simulation is also described in this section. Section 3 presents the results. Finally, the last section embodies the main conclusions of this work.

2. Device structure
The device used in the simulation is a double gate (Silicon) MOSFET with metal gate contacts and a 1.6 nm oxide (SiO$_2$) thickness. Fig. 2 shows the device structure and dimensions. This device presents electrostatic advantages when compared with the conventional bulk MOSFET devices.

The channel length of the transistor is 10 nm and the body thickness is 2 nm. The doping in the source and drain regions, $N_{d}$, is $10^{20}$ cm$^{-3}$, and the channel doping, $N_{a}$, is $10^{14}$ cm$^{-3}$.

![Fig. 1. Structure of the double gate MOSFET. The channel thickness is 3 nm, the doping in the source and drain regions is $10^{20}$ cm$^{-3}$ and the background channel doping is $10^{14}$ cm$^{-3}$.](image)

3. Model
The channel length of the transistor is on the same length as the mean free distance between external collisions for the electrons, allowing us to employ a ballistic approach for the electron transport. We calculated the diagonal and off diagonal elements of the less than Green function, $G^{<}$, using a recursive technique [1]. The electron density and current are calculated from, $G^{<}$. The electron density has to satisfy Poisson’s equation therefore a self-consistent cycle for calculating the electron density and potential through the device is carried out. The discretisation is based on an integral (control volume) formulation of the NEGF equations and Poisson’s equation around every mesh point. The corresponding discretisation for the Green’s function is shown in Fig. 2.

An impression of a realistic device drawn using TEM pictures is shown in Fig. 3. The picture shows one atomic layer stepping at the middle of the top oxide interface. This feature is represented in our model for one inter-atomic layer spacing. The interfaces are randomly generated assuming an exponential autocorrelation function with correlation length, $\lambda=1.8$ nm and digitised inter-atomic layer step height of 0.3 nm [2]. The grid at the interface is designed to match the one inter-atomic layer interface steps.

In our simulations, the electron density can penetrate into the oxide in order to describe properly the quantum mechanical boundary conditions when small interface irregularities occur. An isotropic effective mass model is adopted, which is chosen to reproduce the density of states for Silicon.
Fig. 2. Discretisation scheme for the Green function operator showing the average on the node (i,k) of the gradient of G.

Fig. 3. Photoshop™ impression of a 10 nm DG MOSFET constructed from TEM images of real interfaces.

4. Results

Devices with different randomly generated interfaces have been simulated and a detailed study of the 2D current densities has been carried out. Figure 4 shows the interfaces of one of the simulated devices.

Fig. 4. Channel discretisation of one of the simulated cases showing various effects created by the interface thickness.
The interaction between the random steps at the interfaces and the body thickness variations results in confinement variations, which produce a meandering flux of the current (see Fig. 5). The current is flowing through an effective body thickness, which is wider than the vertical cross section. This effect modifies the current as compared with a purely horizontal current flow. The 2D profile of the horizontal current (y-direction) is plotted in Fig. 6 (from now on the dark red colour will represent high values of the value of the magnitude while dark blue will stand for low ones). It shows the squeeze of the current (y-direction) when passing the narrower regions with stronger confinement. Because of current conservation, high current density appears in the regions of strong transversal confinement.

**Fig. 5** The 2D current density vector field and the effective cross-section created as a result of the interface roughness.

**Fig. 6** 2D profile of the current in the transport direction showing the non homogeneity along the channel.

**Fig. 7** 2D electron density profile showing the inhomogeneity along the channel.

**Fig. 8** Electron concentration on a vertical cross-section at different positions from the middle of the channel ($y=0.15$) to the source ($y=-5.0$).
The effect of confinement variations on the electron concentration in the channel is shown in Fig. 7. The maximum of the 2D concentration profile is localised at the narrow cross section. In Fig. 8 the electron concentration normal to the channel is plotted at different cross-sections along the channel. There is significant carrier penetration at the interface as consequence of the surface roughness and tunnelling ($y = -5.51$ nm is in the source region and $y = 0.15$ nm is at the middle of the channel). The fluctuation of the electron concentration along the channel ($x = 0.0$ denotes the centre of the channel) at different distance from the upper oxide interface is presented in Fig. 9. It shows that the variation in the electron density near to the interface may be one order of magnitude.

![Graph showing electron concentration](image)

**Fig. 9.** Electron concentration along the channel at different distances from the upper oxide interface (see Fig. 4).

Figs. 10 and 11 illustrate two random generated interfaces which we denote *case 1* and *case 2*, respectively. The confinement for the *case 1* is located at the beginning of the channel whereas in *case 2* the confinement is located at the middle of the channel. Figs. 15 and 16 represent the 2D electron density for the two cases. The electron injection in the channel is greater in *case 2* producing a slightly higher current than in the case of *case 1* as has been show in [3] where a more extensive study has been presented. In [3] we have found a 10 % current fluctuation between devices with different interface roughness profile. This shows the important point that the surface roughness plays a macroscopic role for devices which body thickness is as small as 2 nm.

![Interface roughness](image)

**Fig. 10.** The interface roughness corresponding to *case 1* (see the Fig. 9). The bottleneck is located at the beginning of the channel.

**Fig. 11.** The interface roughness corresponding to *case 2* (see Fig. 9). The bottleneck is located at the middle of the channel.
5. Conclusions
The self-consistent non-equilibrium Green function formalism has been used to simulate the effect of the surface roughness on a nanoscale MOSFET. We presented a non perturbative treatment of the interface roughness which has been validated on experimental grounds. The detailed pattern of the interface profile it is not averaged out and is reflected in the current and density profile of the electron in the channel. The 2D current meanders through the channel due to the confining effects and body thickness fluctuations induced by the roughness. The injection of electron in the channel is affected by the surface roughness. The density exhibits a inhomogeneous pattern in the channel and strong fluctuations close to the interface. In general the particular features of the interfaces affect the behaviour of the devices as the current injection.

References
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