

DFT-NEGF Modeling of Surface Roughness Scattering in Ultra-Thin-Body Si Nanosheets

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Abstract— We present an implementation for the ab-initio NEGF treatment of surface roughness scattering in ultra-thin Si Nanosheets. The method is based on an explicit geometrical description and on a suitable passivation of the Si atoms that are in the roughness region(s). The method is then used to extract both the average effect of SR and its statistical variability on the transport properties of ultra-thin Si nanosheets.

Keywords—Surface roughness, DFT, NEGF, ultra-thin Si, nanosheet

I. INTRODUCTION

There is a regain of interest for ultra-thin-body (UTB) Si nanosheets (NS) with body thicknesses $t_{\text{Si}} \leq 3$ nm for CMOS scaling [1], [2], [3], [4]. In such extremely scaled devices, fully ab-initio atomistic simulation methods provide the most accurate description of the electronic and transport properties. Also, surface roughness (SR) scattering is expected to be strong due to the large quantum confinement (QC) [2], [5], and an efficient first-principles treatment of SR is needed. Using density functional theory (DFT), coupled with the non-equilibrium-Green's functions (NEGF) formalism, we describe here a practical ab-initio treatment of the impact of SR on the transport properties of ultra-thin Si NS.

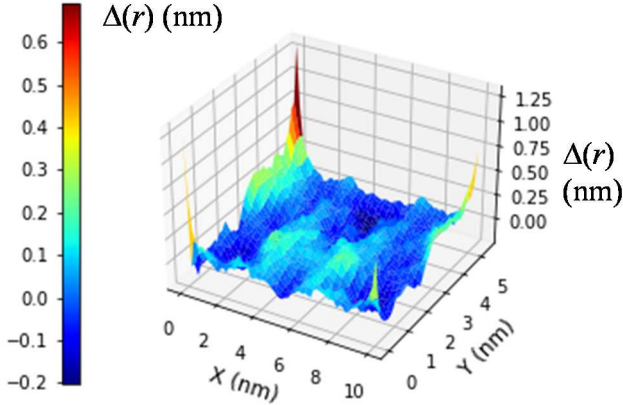


Fig. 1. Randomly-generated sample of local height variations, $\Delta(r)$, obtained from our SR model (eq. (3)) for a surface of $S = L_x \times L_y = 10 \times 5.4$ nm². $\Delta_{\text{SR}} = 0.5$ nm and $L_c = 1.4$ nm.

II. METHODS AND SR MODEL

To compute the DFT-based Hamiltonian (H) and relaxed supercell geometries of the Si NS with t_{Si} ranging from 0.5 to 6 nm, we employed the DFT Package CP2K [6]. We used a double Zeta (DZVP) atomic-orbital basis, meta generalized gradient approximation and the PBE0-TC-LRC Hybrid Functionals [7] to get an accurate E_g (more details on the methodology can be found in [8]). The resulting supercell information are then used in our quantum transport solver,

ATOMOS [4], [8], [9] to perform the self-consistent NEGF calculations, using a mode-space H [10], [11]. Electron-phonon (e-ph) scattering is included within the self-consistent Born approximation, using deformation potential theory with the parameters described in [12].

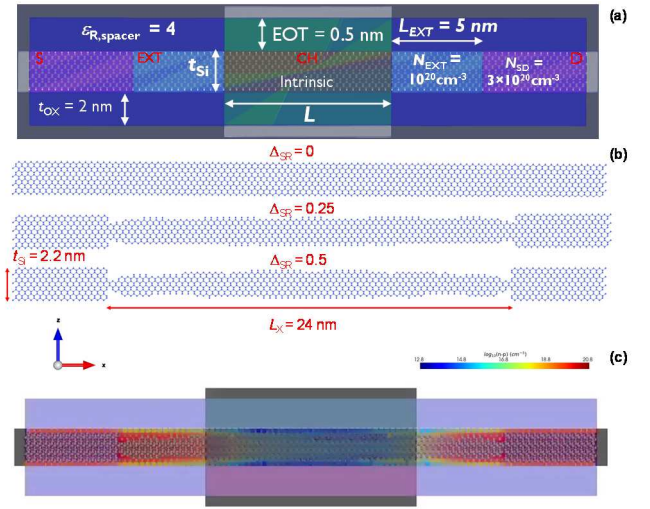


Fig. 2. (a) Atomistic view of a HF-DFT-NEGF simulated Si NS-FET with gate length L , source (S) and drain (D) highly-doped epi regions with n-type doping $N_{\text{SD}} = 3 \times 10^{20}$ cm⁻³, extension regions (EXT) of length $L_{\text{EXT}} = 5$ nm and n-type doping $N_{\text{EXT}} = 10^{20}$ cm⁻³. The channel is intrinsic with nominal thickness t_{Si} . The top and bottom gates with an HfO₂ gate oxide of thickness $t_{\text{OX}} = 2$ nm and relative permittivity $\epsilon_r = 15.6$, as well as spacer oxide ($\epsilon_r = 4$) are also shown. (b) ATOMOS-generated smooth ($\Delta_{\text{SR}} = 0$) and rough ($\Delta_{\text{SR}} = 0.25$ and $\Delta_{\text{SR}} = 0.5$ nm) Si-NS atomistic structures with both front and back Si surfaces with uncorrelated roughness Δ_{SR} over the channel and extension (EXT) regions (so that the total front + back roughness $\Delta_{\text{SR,T}} = 2 \times \Delta_{\text{SR}}$), while the highly-doped S and D epi-regions are kept smooth in all cases. (c) DFT-NEGF-simulated electron concentration superimposed over the device structure of the rough Si n-type NS for the case with $\Delta_{\text{SR}} = 0.5$ nm ($\Delta_{\text{SR,T}} = 1$ nm). $V_G - V_{\text{th}} = -0.15$ V. $V_D = 0.6$ V. $t_{\text{Si}} = 2.2$ nm. $L = 14$ nm.

To model SR, an explicit geometrical description is used here, similarly to previous NEGF studies based on effective masses and $k \cdot p$ H [5], [13]. We start from a typical exponential autocorrelation function [5], [13], [14]:

$$C(r) = \Delta(r')\Delta(r' - r) = \Delta_{\text{SR}}^2 e^{-\sqrt{2}r/L_c} \quad (1)$$

where Δ_{SR} is the rms of the surface height fluctuation and L_c is the correlation length. Each specific realization of SR is generated by first applying a Fourier transformation (denoted by F in eq. (2)) to $C(r)$ to obtain the power density spectrum, PSD :

$$\text{PSD} = |\Delta(q)|^2 = F(C(r)) \quad (2)$$

The randomness is then introduced to the square root of the PSD itself, following the so-called Monte Carlo spectral method [15], [16]. The local height variation, $\Delta(r)$, at a position r on the surface of area S , is finally obtained by performing the inverse Fourier transform (F^{-1}):

$$\Delta(r) = \frac{1}{S} F^{-1}(\sqrt{S}|\Delta(q)| \times \gamma) \quad (3)$$

where, $\gamma(q)$ is a complex random number (both real and imaginary part being independent random numbers with an exponential distribution) with mean of 0 and variance 1. To keep $\Delta(r)$ real, however, the function of q in the inverse Fourier transform of eq. (3) must be Hermitian, which constrains $\gamma(q)$ and $\gamma(-q)$ to be complex conjugates. For the same reason, we must use a real γ to any non-paired frequencies of $|\Delta(q)|$ (e.g., $q = 0$) [15], [16].

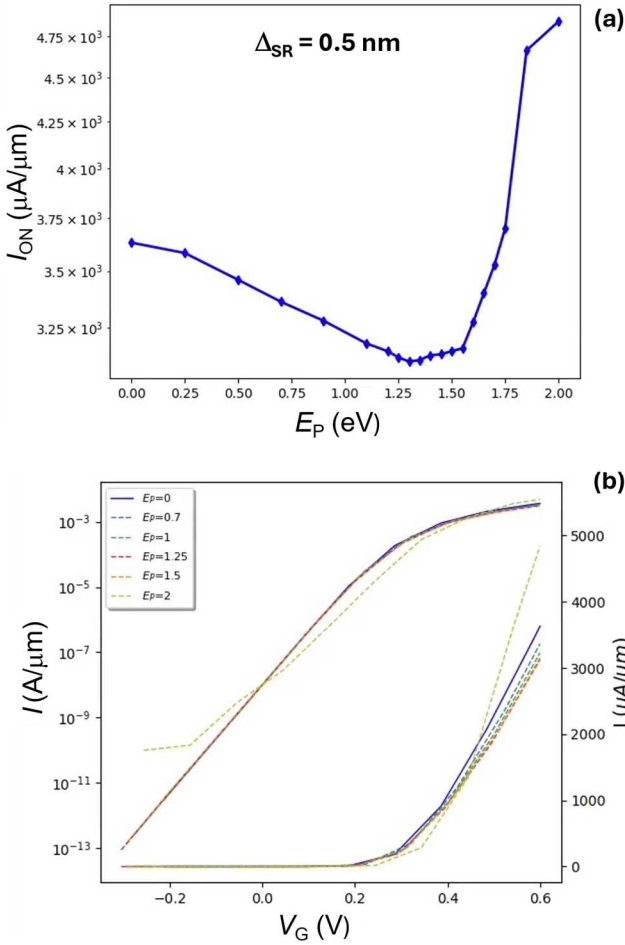


Fig. 3. DFT-NEGF-simulated impact of E_P on (a) I_{ON} at fixed I_{OFF} and V_{DD} and (b) on the full $I_D(V_G)$ characteristics of a Si NS with a given top surface SR profile, $\Delta(r)$, obtained from our SR model (eq. (3)). $\Delta_{SR} = 0.5$ nm and $L_C = 1.4$ nm. $L = 14$ nm. $t_{Si} = 2.2$ nm. $V_{DD} = 0.6$ V. The gate work-function was set so that $I_{OFF} = 10$ nA/ μm at $V_G = 0$ V. The current was normalized by the device width.

An example of generated SR with $\Delta_{SR} = 0.5$ nm is shown on Fig. 1, using $L_C = 1.4$ nm which is typical for Si [5], [13], [14]. The generated SR profile is then translated by ATOMOS into a rough atomic structure (Fig. 2). Rather than fully removing the atoms in the roughness region(s), we passivate them using a passivation potential, E_P , of approximately +1 eV for a n-type (respectively -1 eV for a p-type) NS, in order to create a band-offset aligning the “oxidized” atom

conduction band, E_C , (respectively valence band, E_V) with an energy level inside the bandgap of the un-passivated atoms. This avoids creating dangling bonds and the subsequent need for passivation. It also enables mimicking wave function penetration (WFP), as in a real Si-SiO₂ interface for instance, but at a much reduced computational cost, allowing for an efficient and convenient ab-initio treatment of SR, as we shall show.

Our choice of $E_P = 1$ eV is justified in Fig. 3, where the impact of E_P on the drain-current – gate-voltage characteristics, $I_D(V_G)$, and on-current, I_{ON} , of a rough Si NS is investigated using the same top surface SR profile for all the simulations. Compared to the smooth case ($E_P = 0$), the current (at fixed off-state current, I_{OFF}) first decreases as E_P is increased, as a larger SR scattering is observed due to the larger band offset that induces a stronger confinement and less wave function penetration in the “oxidized” Si atoms. For $1 \text{ eV} \leq E_P \leq 1.5$ eV, however, the current does not vary much anymore, showing that we have reached a saturation (Fig. 3a). For a too large E_P ($E_P > 1.5$ eV), however, as we gradually overcome the Si bandgap and induce a p-type occupation in the passivated atoms, the full shape of the $I_D(V_G)$ curve is affected and the subthreshold slope is degraded (Fig. 3b).

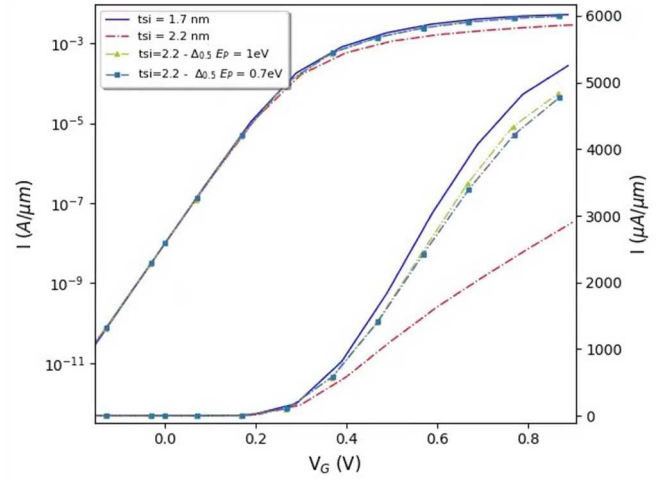


Fig. 4. DFT-NEGF $I_D(V_G)$ characteristics of (a) Si NS with $t_{Si} = 2.2$ nm and the thinner $t_{Si} = 1.7$ nm, as well as with $t_{Si} = 2.2$ nm but with a constant top SR profile, $\Delta(r) = 0.5$ nm ($t_{Si} = 2.2 - \Delta_{0.5}$) using 2 different passivation energies $E_P = 0.7$ and 1 eV. $L = 14$ nm. $V_{DD} = 0.6$ V. $I_{OFF} = 10$ nA/ μm .

As a further test for our passivation potential, in Fig. 4, we compare the $I_D(V_G)$ characteristics of a NS with original thickness $t_{Si} = 2.2$ nm, but where we effectively reduced its thickness to 1.7 nm by passivating its atoms located in its top 0.5 nm region, i.e., using a constant top “roughness” profile, $\Delta(r) = 0.5$ nm ($t_{Si} = 2.2 - \Delta_{0.5}$), to those with the $t_{Si} = 2.2$ nm and the thinner $t_{Si} = 1.7$ nm DFT-supercell original thicknesses. Interestingly, the drive current of a smooth Si NS significantly increases when reducing its cross-section from 2.2. to 1.7 nm. This is linked to favourable electronic property changes (including a lower transport effective mass) induced by the strong QC for $t_{Si} < 2$ nm.

As can be seen, the current increase is also largely observed in the $t_{Si} = 2.2 - \Delta_{0.5}$ case, however to a somewhat smaller extend. The current increase is also slightly reduced, if we use a smaller $E_P = 0.7$ eV instead of our default $E_P = 1$ eV. These current differences are attributed to the WFP in the passivated Si atoms that reduces QC in the $t_{Si} = 2.2 - \Delta_{0.5}$ case, with regards to the $t_{Si} = 1.7$ nm, where no such atoms are

present (in that case the Si surfaces are simply hydrogen-terminated for the dangling bond passivation), in a way similar to what we observe when explicitly including an oxide in our simulations. Hence, our passivation procedure mimics WFP and can, to some extent, be fine-tuned by adjusting E_p .

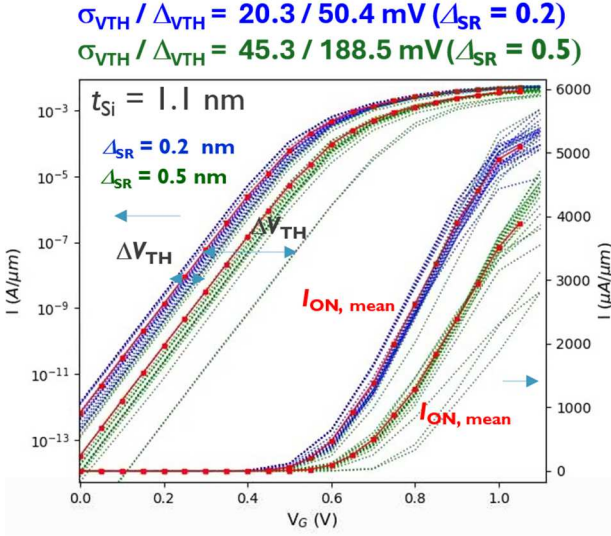


Fig. 5. $I_D(V_G)$ characteristics of $t_{Si} = 1.1 \text{ nm}$ Si NS with randomly-generated top-surface SR with $\Delta_{SR} = 0.2$ (blue lines) and $\Delta_{SR} = 0.5 \text{ nm}$ (green lines). $L_C = 1.4 \text{ nm}$. $E_p = 1 \text{ eV}$. For each population, 30 samples were simulated. Their averaged $I_D(V_G)$ curves are shown in red. $L = 14 \text{ nm}$. $V_{DD} = 0.6 \text{ V}$. The current was normalized by the device width.

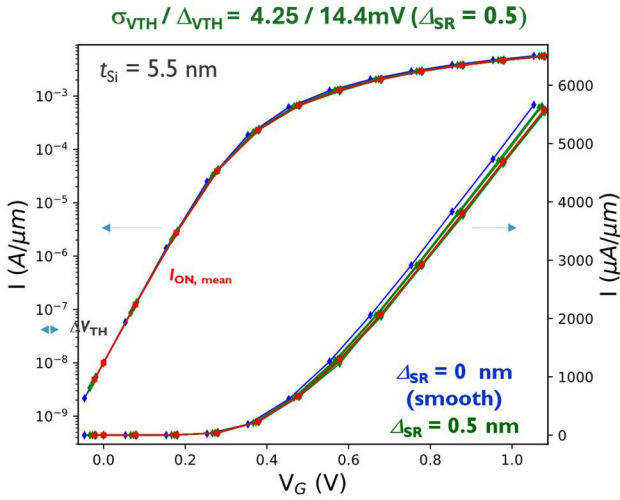


Fig. 6. $I_D(V_G)$ characteristics of $t_{Si} = 5.5 \text{ nm}$ Si NS with randomly-generated top-surface SR with $\Delta_{SR} = 0$ (blue lines, smooth case) and $\Delta_{SR} = 0.5 \text{ nm}$ (green lines). $L_C = 1.4 \text{ nm}$. $E_p = 1 \text{ eV}$. For the rough case population, 30 samples were simulated. The averaged $I_D(V_G)$ curve for the $\Delta_{SR} = 0.5 \text{ nm}$ case is also shown in red. $L = 14 \text{ nm}$. $V_{DD} = 0.6 \text{ V}$. $I_{OFF} = 10 \text{ nA}/\mu\text{m}$. The current was normalized by the device width.

In Fig. 5 and 6, we apply our model and compute $I_D(V_G)$ characteristics of rough $t_{Si} = 1.1$ and 5.5 nm Si NS, respectively. For each different SR population, 30 samples were simulated and their averaged $I_D(V_G)$ characteristics ($I_{ON, mean}$) are also shown in red. In Fig. 5, for $t_{Si} = 1.1 \text{ nm}$, 2 NS populations with randomly-generated SR profiles (one with $\Delta_{SR} = 0.2$ and the second with $\Delta_{SR} = 0.5 \text{ nm}$) are shown, and a relative 98-mV threshold-voltage, V_{TH} , increase for the larger Δ_{SR} case, as well as a $319\text{-}\mu\text{A}/\mu\text{m}$ I_{ON} decrease, ΔI_{ON} , (calculated from the respective $I_{ON, mean}$ characteristics at same $I_{OFF} = 10 \text{ nA}/\mu\text{m}$ and $V_{DD} = 0.6 \text{ V}$) are observed. In addition,

the V_{TH} variations due to SR are also increasing with Δ_{SR} : The rms/maximum V_{TH} spreads ($\sigma_{V_{TH}}/\Delta V_{TH}$) are $20.3/50.4 \text{ mV}$ for $\Delta_{SR} = 0.2 \text{ nm}$, and $45.3/188.5 \text{ mV}$ for $\Delta_{SR} = 0.5 \text{ nm}$.

In Fig. 6, for $t_{Si} = 5.5 \text{ nm}$, a NS population with randomly-generated SR profiles with $\Delta_{SR} = 0.5 \text{ nm}$ is shown and compared to that of a smooth simulation ($\Delta_{SR} = 0 \text{ nm}$) including only e-ph scattering. As can be seen, a smaller impact of SR on I_{ON} ($\Delta I_{ON} = 160\text{-}\mu\text{A}/\mu\text{m}$ when comparing $\Delta_{SR} = 0.5$ and 0 nm) and V_{TH} variations ($\sigma_{V_{TH}}/\Delta V_{TH} = 4.25/14.4 \text{ mV}$ for $\Delta_{SR} = 0.5 \text{ nm}$) is observed.

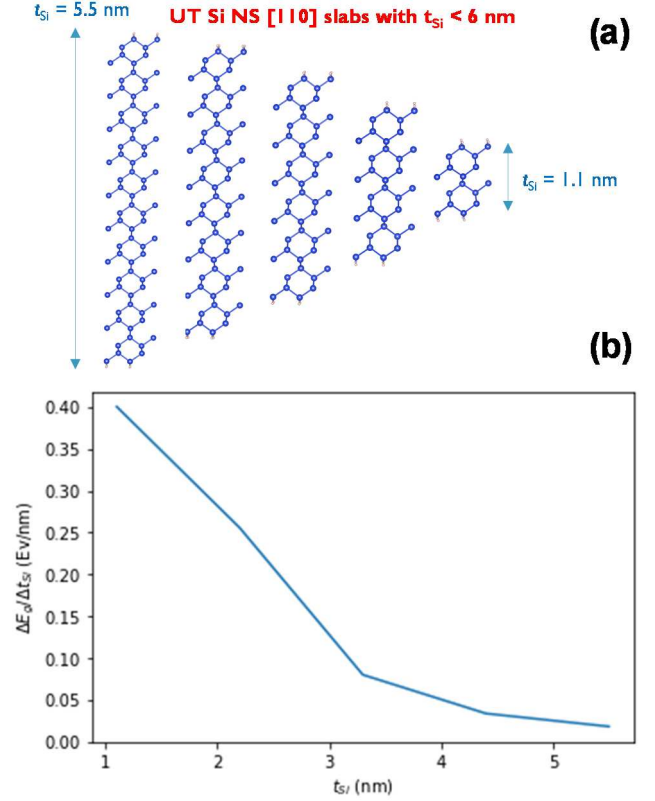


Fig. 7. (a) Atomic structure of several Si DFT-optimized supercells with various t_{Si} used in this study. (b) Bandgap variations with t_{Si} , $\Delta E_G/\Delta t_{Si}$, extracted from the DFT band structure calculations of our Si supercells with t_{Si} ranging from 0.55 to 6 nm .

The SR scattering strength (Σ_{SR}) is theoretically predicted to be proportional to the variation of the surface normal electric field (E_z) and, in confined structure, to a second term related to variation of the conduction band, E_C , with t_{Si} ($\Delta E_C/\Delta t_{Si}$) [17]:

$$\Sigma_{SR} \sim \Delta_{SR}^2 \cdot \left(\int n(z) E_z dz + 1/q \times \Delta E_C/\Delta t_{Si} \right) \quad (4)$$

Also ΔV_{TH} is expected to be proportional to $\sim \Delta E_C/\Delta t_{Si} \times \Delta_{SR}$.

The larger impact of SR on ΔI_{ON} and ΔV_{TH} with smaller t_{Si} is then expected from the larger average QC and related stronger $\Delta E_C/\Delta t_{Si}$ variation as we reduce t_{Si} . $\Delta E_C/\Delta t_{Si}$ is also related at first order to $\sim \Delta E_G/\Delta t_{Si}$, the bandgap variations with t_{Si} . $\Delta E_G/\Delta t_{Si}$ extracted from our DFT band structure is shown in Fig. 7. As expected, $\Delta E_G/\Delta t_{Si}$ is strongly increasing as we reduce t_{Si} .

III. CONCLUSIONS

We reported here a practical implementation for the ab-initio NEGF treatment of surface roughness scattering that we have implemented in our DFT-NEGF solver ATOMOS. The method is based on an explicit geometrical description and on a suitable passivation of the Si atoms that are in the roughness region(s). The method was then used to extract both the average effect of SR and its statistical variability on the transport properties of ultra-thin Si nanosheets.

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