

Quantum Transport Simulation Considering Self-Energy for Surface Roughness in Nanosheet FETs

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Abstract—Roughness at the semiconductor/insulator interfaces is one of the most important factors to determine the inversion layer mobility. In this work, we model the surface roughness scattering in nanosheet transistors by using the Non-Equilibrium Green's Function (NEGF) formalism combined with a local self-energy term. For comparison, a statistical evaluation is performed for various surface roughness profiles which are generated from a Gaussian autocorrelation function. The simulation results reveal that higher roughness levels lead to reduced carrier mobility, exhibiting an electron density dependence that follows a power law with an exponent of -1.5 . Since the NEGF simulation results with the self-energy term do not reproduce the threshold voltage shift observed in the statistical analysis, a more rigorous approach is desirable.

Index Terms—Non-equilibrium Green's function, surface roughness scattering, self-energy

I. INTRODUCTION

Following decades of aggressive device scaling, complementary metal-oxide-semiconductor (CMOS) technology has now reached extremely small dimensions. To accurately describe the underlying physics in these ultra-scaled devices, quantum transport simulation are required. Among various quantum transport simulation methods, the non-equilibrium Green's function (NEGF) formalism [1], [2] has been widely adopted. Over time, NEGF simulation codes have developed to incorporate a wide range of physical effects and computational enhancements [3]–[5]. Its flexibility and applicability enable the NEGF simulation to capture important physical phenomena and assess the potential of novel materials.

A key physical effect is the interaction between electrons and their surrounding environments, commonly referred to as scattering. In the case of the electron-phonon interactions, well-established methods have been developed. In most previous studies, the electron-phonon scattering has been considered using the self-consistent Born approximation (SCBA) and the local scattering approximation [6]. As an efficient alternative to reduce computational costs, the Büttiker probe method has been proposed [7]. In these approaches, the electron-phonon scattering is included by employing scattering self-energies.

In contrast to the electron-phonon scattering described above, another important scattering mechanism to determine the inversion layer mobility – surface roughness scattering – is typically considered using a statistical approach [8], [9]. In this method, several device instances with randomly generated rough interfaces are simulated. The resulting solutions are statistically processed to evaluate the impact of surface roughness. However, the statistical approach requires a large number of samples, leading to high computational costs. To mitigate these limitations, a self-energy approach to model surface roughness scattering in circular nanowire transistors has been recently proposed [10]. It has been reported that the on-current obtained using the self-energy approach agrees well with that from the statistical method. In this work, the self-energy approach in [10] is applied to the nanosheet FET with a rectangular cross-section.

II. METHODOLOGY

The main motivation of the self-energy approach [10] is the similarity between elastic phonon scattering and surface roughness scattering. As a result, surface roughness scattering is implemented by replacing the matrix elements of elastic phonon scattering with those corresponding to surface roughness scattering. The matrix element is given by

$$\begin{aligned} |M_{m,m'}(x_1, x_2)|^2 &= |\langle m, x_2 | H_{\text{pert}} | m', x_1 \rangle|^2 \\ &= \sqrt{\pi} q^2 N_E(m, m')^2 \Delta_m^2 L_C \delta(x_1 - x_2), \end{aligned} \quad (1)$$

where m and m' denote the mode index [10]. It is noted that the one-dimensional real space expression, x_1 and x_2 , is adopted accounting for the mode space approach. The surface roughness is assumed to follow a Gaussian autocorrelation function. It is noted that the surface roughness is commonly modeled using empirically known autocorrelation functions, such as Gaussian or exponential [8], [10]. q is the elementary charge while Δ_m and L_C are the root-mean-square (rms) value of roughness and the correlation length, respectively. Several approximations, including the local scattering approximation, are also adopted in this work. It is noted that x -direction is

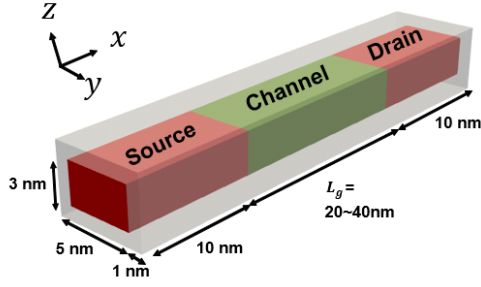


Fig. 1. Structure of the simulated nanosheet FET.

the transport direction. N_E is the effective electric field in the cross-section,

$$N_E(m, m') = \int dA \psi_{m'}(y, z; x) E(y, z) \psi_m(y, z; x), \quad (2)$$

where $E(y, z)$ is the electric field at position x and ψ is the wavefunction of the m -th subband [10]. However, compared with the nanowire device with rotational symmetry, the calculation of the effective electric field in nanosheet devices is not trivial. Therefore, the effective electric field is calculated using the y - and z -directional effective electric fields, $N_{E,y}$ and $N_{E,z}$, [11]

$$N_E(m, m')^2 = N_{E,y}(m, m')^2 + N_{E,z}(m, m')^2. \quad (3)$$

Two directional fields are written as [11]

$$N_{E,y}(m, m') = \int dA \psi_{m'}(y, z; x) E_y(y, z) \psi_m(y, z; x), \quad (4)$$

$$N_{E,z}(m, m') = \int dA \psi_{m'}(y, z; x) E_z(y, z) \psi_m(y, z; x). \quad (5)$$

From the calculated matrix element, lesser and retarded self-energies can be obtained as

$$\Sigma_m^<(x) = \sum_{m'} M_{m,m'}(x) G_{m'}^<(x), \quad (6)$$

$$\Sigma_m^r(x) = \frac{1}{2}(\Sigma_m^>(x) - \Sigma_m^<(x)), \quad (7)$$

where the Hermitian part is not considered in this work [6], [10]. Finally, NEGF relations are written as,

$$[EI - H - \Sigma_{cont}^r(E) - \Sigma_{scat}^r(E)] G^r(E) = I, \quad (8)$$

$$G^<(E) = G^r(E) [\Sigma_{cont}^<(E) + \Sigma_{scat}^<(E)] G^a(E), \quad (9)$$

where the subscript *cont* and *scat* stand for the contact and scattering, respectively. It is noted that all Green functions and self-energies are written with mode space notation.

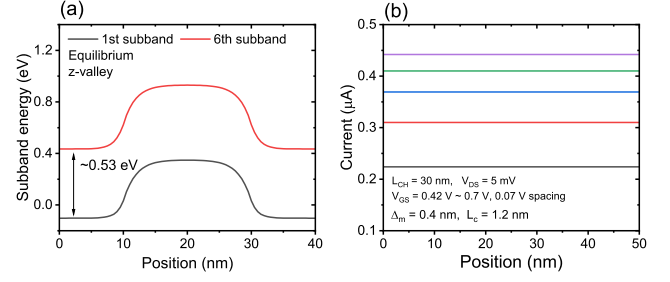


Fig. 2. (a) Subband profile along the channel direction. (b) Current along the channel direction for several drain biases. Δ_m is 0.4 nm and L_C is 1.2 nm.

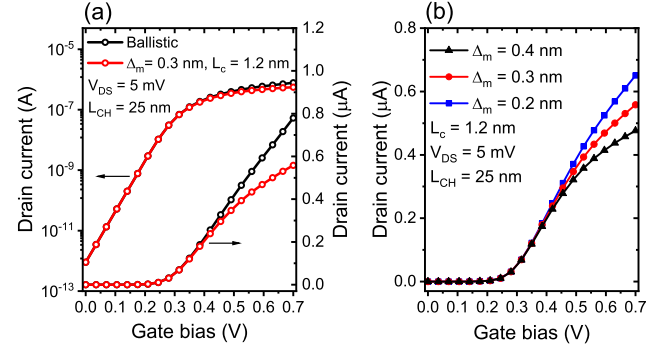


Fig. 3. Input curves are drawn as a function of the gate bias. Drain bias is fixed to 5 mV. Channel length is 25 nm and the correlation length is fixed to 1.2 nm. (a) Ballistic transport result is compared with the inclusion of scattering self-energy case. (b) Input curve is drawn for several Δ_m .

III. SIMULATION RESULTS

The NEGF simulation code is implemented as part of our in-house device simulator, G-Device [12], [13]. Six valleys in the silicon conduction band are considered and the effective mass approximation is assumed. In Fig. 1, the simulated nanosheet FET is illustrated. Source and drain lengths are 10-nm-long equally while the channel varies from 20 nm to 40 nm. The cross-sectional area is set to 3 nm $\times$ 5 nm size with a 1.0-nm-thick oxide layer. Source and drain regions are doped with donors while the channel is intrinsic. Donor concentration is 10^{20} cm $^{-3}$. [100] channel direction and (001) surface are assumed.

To reduce computational cost, the coupled mode-space NEGF approach is adopted, which significantly reduces the burden compared to the real-space NEGF. The subband energy profile of the first and sixth subbands of the z -valley is drawn in Fig. 2 (a). Since the energy separation between them is sufficiently large (about 0.53 eV), six subbands are considered in the simulation for each valley. In Fig. 2 (b), current continuity is observed, indicating that the convergence criterion for scattering is sufficient.

The input characteristics are shown in Fig. 3. The comparison with the ballistic transport is drawn in Fig. 3 (a). Due to the effect of surface roughness scattering at high gate bias, the drain current decreases. Moreover, as the rms value of surface roughness increases, a decreased current is observed as shown

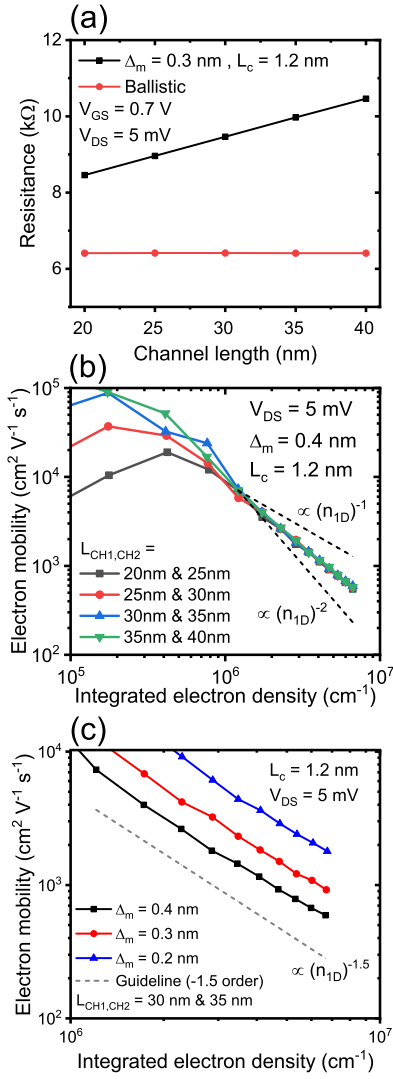


Fig. 4. Resistance and mobility are drawn when the drain bias is fixed to 5 mV. (a) Resistance is drawn as a function of the channel length when the gate bias is 0.7 V. (b) Mobility is drawn as a function of the integrated electron density at the channel. Dashed lines show the trend of mobility to the integrated electron density. Δ_m is fixed to 0.4 nm. (c) Mobility is drawn for several Δ_m .

in Fig. 3 (b).

From the NEGF simulation, the resistance and mobility are extracted at low drain bias conditions [10], [14]. The resistance can be obtained using the drain bias and the drain current, V_{DS}/I_D . Mobility is calculated using the equation,

$$\mu \simeq \frac{L_{CH2} - L_{CH1}}{R_{CH2} - R_{CH1}} \frac{1}{qn_{1D}}, \quad (10)$$

where resistances from two different channels are required. n_{1D} is the integrated electron density in the channel region. Although there are various approaches for determining the appropriate integrated electron density for more precise mobility calculation, the density at the top-of-barrier is selected in this work [14]. The extracted resistance and mobility are

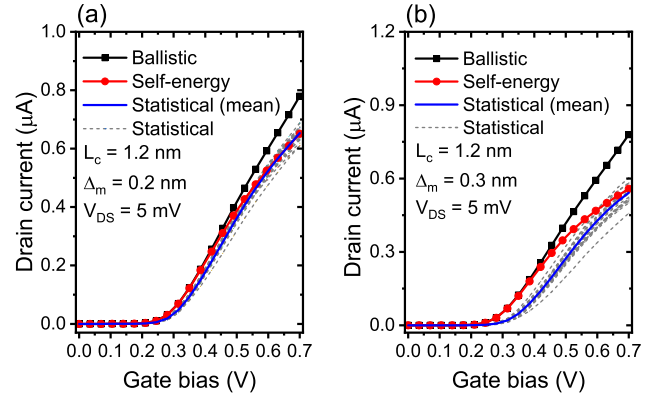


Fig. 5. Input curves are drawn as a function of the gate bias. Drain bias is fixed to 5 mV. Channel length is 25 nm and the correlation length is fixed to 1.2 nm. The self-energy method and the statistical approach are compared. (a) Δ_m is 0.2 nm. (b) Δ_m is 0.3 nm.

drawn in Fig. 4. The resistance from the ballistic transport case is compared to the scattering case in Fig. 4 (a). As the channel length increases, resistance also increases due to the scattering mechanism while electrons are passing the channel. The calculated mobility is shown in Figs. 4 (b) and (c). Mobility degradation appears due to the scattering with increasing integrated electron density. The trend guideline indicates that the mobility decreases approximately as an order of -1.5 to the integrated electron density. Moreover, as the rms of roughness increases, the degradation becomes more pronounced as shown in Fig. 4 (c). However, the dependence of mobility on electron density appears to follow a consistent trend regardless of the rms value.

Finally, the self-energy method is compared with the statistical approach. Random samples are generated using a procedure which has been already well established in previous works [8], [14]. Fig. 5 presents a comparison between the statistical approach and the self-energy method. For the statistical approach, 20 randomly generated device samples are simulated. Due to implementation difficulties, we assumed that corners of each cross-section have no roughness. The self-energy method shows a reasonable on-current level with the statistical approach [10]. However, as Δ_m increases the difference at the subthreshold region becomes large. Especially, the randomly generated devices show a threshold voltage shift relative to the smooth device without roughness, as reported in several previous works [9].

The discrepancy between the self-energy and statistical methods in the subthreshold region shown in Fig. 5 can be understood from the structure of the matrix element. In the present formulation, the scattering strength is proportional to the squared effective electric field, which vanishes in the subthreshold region where the channel field is small. An additional contribution to the matrix element, the Prange-Nee term [15], arises from the kinetic quantization energy shift due to the boundary displacement of the confinement. Its omission is a likely cause of the underestimated scattering

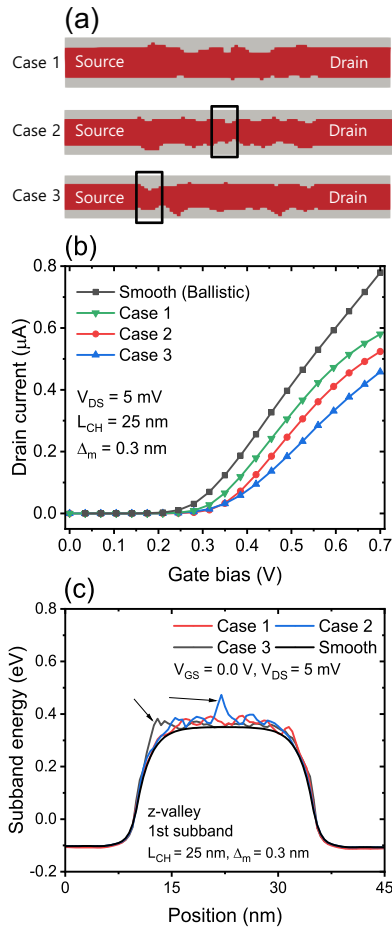


Fig. 6. Results from three samples and smooth device are drawn when channel length is 25 nm and drain bias is fixed to 5 mV. Δ_m is fixed to 0.3 nm and correlation length is set to 1.2 nm. (a) Structure of three samples. (b) Input curves are drawn. (c) First Subband energy profile along the channel when gate bias is 0.0 V. Arrows are pointing black boxes in (a).

in the subthreshold region.

Result for three representative samples are shown in Fig. 6. Although the threshold voltage is higher than that of the smooth device in all three cases, they exhibit significantly difference threshold voltages. Especially, the case 3 – where the locally narrow region appears close to the source region – shows the worst performance. These results highlight that the geometric variation according to surface roughness critically influence the device performance at the subthreshold region. Therefore, a more rigorous model to consider impacts of geometric variations on the device performance is required.

IV. CONCLUSION

In summary, we have implemented the NEGF simulation that accounts for surface roughness scattering via a self-energy term. We have evaluated the mobility and resistance in nanosheet transistors, and it has been found that the implemented self-energy method shows reasonable on-current reduction due to the surface roughness scattering. However,

when compared with the the statistical approach, this method does not accurately predict the subthreshold region. Therefore, to capture the subthreshold behavior more precisely, an improved method of incorporating surface roughness through a self-energy term is highly desirable.

ACKNOWLEDGMENT

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