Surface-Roughness-Limited Mean Free Path in Si Nanowire FETs

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Abstract—The mean free path (MFP) in silicon nanowire field effect transistors limited by surface roughness scattering (SRS) is calculated with the non-perturbative approach utilizing the non-equilibrium Green’s function method. The entrance scattering effect associated with finiteness of the channel length is identified and a method to eliminate it in the calculation of the MFP is developed. The behavior of the MFP with respect to channel length (L), channel width (W), and the root-mean-square (RMS) of the surface roughness is investigated extensively. Our major findings are that the single parameter, RMS/W, can be used as a good measure for the strength of the SRS effects and that the overall characteristics of the MFP are determined by the parameter. In particular, the MFP exponentially decreases with the increase of RMS/W and the MFP versus the gate electric field shows a distinctively different behavior depending on whether the strength of the SRS effects measured by RMS/W is smaller or greater than 0.06.

Index Terms—nanowire, MOSFET, nanowire field effect transistor, quantum transport, mobility, mean free path, surface roughness, non-equilibrium Green’s function.

I. INTRODUCTION

The Si nanowire field effect transistors (SNWFETs) with all around gates have recently emerged as a promising device to replace the conventional planar metal oxide semiconductor field effect transistors (MOSFETs) as the latter face the physical and technological challenges in their scaling-down [1]–[3]. The SNWFETs have the merit of good electrostatic control and hence can deliver high on-state currents. As their overall performance is determined by the aspect ratio of the channel length (L) and channel width (W) [4], it may be desirable to utilize thinner and thinner nanowires. However, rough interfaces between Si and dielectric are unavoidably generated during the fabrication processes, and currents become limited by surface roughness scattering (SRS) as the nanowire cross-sectional size is reduced below 5 nm [5], [6].

The SRS effects in SNWFETs have been a subject of intense theoretical and computational studies. Most of the studies have been performed with the semiclassical approaches such as the Kubo-Greenwood approach [7]–[9], the multi-subband Monte Carlo technique [10], [11], and the direct solution of the one-dimensional Boltzmann transport equation [12], [13]. The Schrodinger-Poisson equations are self-consistently solved in the approaches assuming an infinitely extended homogeneous nanowire, before the nanowire sub-band information is extracted and fed to the semiclassical procedures. There have also been a few studies based the non-equilibrium Green’s function (NEGF) method [10], [14]–[19], where coherent electron transport across the channel region with rough Si/dielectric interfaces is considered fully quantum-mechanically. In the non-perturbative approach, the screening effect, electron phase coherence, and the mode mixing effect, among others, are naturally considered whereas these are hard to be implemented directly or disregarded entirely in the semiclassical approaches.

Most of the NEGF studies have so far focused on the low field electron mobility in nanowires. However, the mobility in the device with a finite channel length is not a proper measure for the device performance, because the mobility increases as the channel length increases whereas there should be more detrimental scattering. As Gnani has pointed out, the mean free path (MFP) should be a better indicator of the device performance [20].

In this work, using the non-perturbative NEGF approach, we have for the first time investigated the SR-limited MFP in SNWFETs. Novelty and contributions of this work are: 1) we have devised a systematic way to calculate the MFP in the device with a finite channel length, 2) we have identified the entrance scattering effect which is unavoidable in the device with a source/channel/drain structure, estimated its
strength, and eliminated it from the MFP calculation, and 3) we have thoroughly investigated the behavior of the MFP with a particular emphasis on its dependence on the strength of the SRS effects. These will be discussed in detail in the following sections.

II. METHODOLOGY

A. Simulated devices and Hamiltonian

The simulated devices in this work are three-dimensional (3D) rectangular silicon nanowire FETs with all-around gates as shown in Fig. 1. The source and drain regions are heavily n-doped with doping concentration of $10^{20}$ cm$^{-3}$ whereas the channel is intrinsic. The SiO$_2$ oxide thickness is assumed to be 1 nm. To describe the electron transport in the conduction band, the effective mass Hamiltonian was used, with the effective masses being scaled according to the tight-binding calculation [21]. All the six equivalent valleys are included in the simulations.

B. Surface roughness generation

The surface roughness (SR) was realized at four Si/SiO$_2$ interfaces in the channel region only. SR was generated according to the exponentially decaying autocorrelation function expressed as

$$ C(\vec{r}) = \Delta_m^2 \exp(-\sqrt{2}r/L_m), \quad (1) $$

where $\Delta_m$ is the root-mean square (RMS) fluctuation of the roughness, $L_m$ is the correlation length, and $r = |\vec{r}|$ is the two-dimensional distance between two points on the interface. By Fourier-transforming the autocorrelation function to obtain the power density spectrum (PDS), multiplying a random phase factor to the square root value of PDS, and inverse Fourier-transforming the randomized PDS, instances of rough Si/SiO$_2$ interfaces were randomly generated [16], [22].

C. NEGF method

We have employed the NEGF method to calculate the charge density and the current in the devices with rough surfaces in the channel region. Self-consistent calculations coupling the charge density from the NEGF equations and the potential from Poisson’s equation were carried out. The methodology is well established in the literature [12], [23].

The NEGF procedure with the rough surfaces is the same as the standard non-diffusive calculation procedure. There is no need to calculate the less-than or greater-than Green’s functions, because the surface roughness scattering (SRS) is not treated by including the self-energy in the Green’s function. Rather, the conduction band edge $E_C(\vec{r})$ at the Si/SiO$_2$ interfaces is spatially varied in accordance with the generated rough surfaces. In other words, in the Hamiltonian

$$ H = H_0 + E_C(\vec{r}) - q_0 \phi(\vec{r}), \quad (2) $$

where $H_0$ is the kinetic part of the Hamiltonian with the inverse effective mass tensor which is not altered by SR,

$$ E_C(\vec{r}) \text{ assumes the value of } 0.56 \text{ eV or } 3.63 \text{ eV, if } \vec{r} \text{ corresponds to silicon or oxide points, respectively. In the Poisson’s equation,}$$

$$ \nabla \cdot (\epsilon(\vec{r}) \nabla \phi(\vec{r})) = q_0 n(\vec{r}) - N_D, \quad (3)$$

$\epsilon(\vec{r})$ is also spatially varying in the same manner as $E_C(\vec{r})$.

In this work, the coupled mode space approach was used [24], [25] with the number of modes ranging from 30 to 50 depending on the cross-sectional width of nanowire. Including higher modes little changed the outcome of the calculations, which validates that the used number of modes is sufficient.

III. ENTRANCE SCATTERING EFFECT

In the nanowire FET in Fig. 1 electrons experience quantum mechanical scattering by the channel potential barrier as they enter the channel region. The channel potential barrier is present due to the fact that the source/drain and channel regions are doped with different doping concentrations. The entrance scattering effect (ESE) takes place even in the ballisticity condition (no rough surfaces in the channel region) and should be separated out from the calculated mean free path. The method to isolate the pure contributions from the channel region is elaborated in section IV.

In the nanowire device under consideration, the ballistic...
The currents are normalized by the current of \( L = 55 \text{ nm} \). Dashed lines are the fit to the function of the form \( A/(B + L) \). The curves for \( V_G - V_T = -0.25 \text{ V} \) and \( 0.15 \text{ V} \) are shifted by -0.2 and 0.1, respectively, for a clearer view. Device width and SR parameters are \( W = 3 \text{ nm} \), \( \Delta_m = 0.3 \text{ nm} \), and \( L_m = 1.0 \text{ nm} \).

\[ \lambda_{SR} = \frac{\lambda_{SR}}{\lambda_{SR} + L}, \]

where \( \lambda_{SR} \) is the mean free path defined in (11) is also displayed. Device width and SR parameters are \( W = 5 \text{ nm} \), \( \Delta_m = 0.2 \text{ nm} \), and \( L_m = 1.0 \text{ nm} \).

Notice that in defining \( \lambda_{SR} \) in (6), \( I_{b\infty} \) is used instead of \( I_b \). If the relationship \( I = \lambda T_{b\infty} \) is used instead of (6), it implies that ESE is disregarded, and we may write

\[ T' = \frac{\lambda_{SR}}{\lambda_{SR} + L}. \]
The MFP $\lambda_{SR}$ of the above equation is related to $\lambda_{SR}$ as:

$$\Lambda_{SR} = \frac{1}{T_{ES}} \lambda_{SR}. \quad (11)$$

That is, the MFP is multiplied by the factor $1/T_{ES}$, which leads to an unphysical peak as demonstrated below.

Before proceeding further, we first show $I$ as a function of $L$ in Fig. 4 which verifies that diffusive transport expressed by Eqs. (8) or (10) actually takes place due to SR. Note that we have deliberately chosen the device width and the SR parameters in the figure so that resultant MFP is as small as about 10 nm (consult Fig. 7a).

Fig. 4 shows thus-calculated $\lambda_{SR}$ for SNWFETs of $W = 5$ nm. For $L$ varying from 60 nm to 250 nm, $\lambda_{SR}$ seems to depend on $L$ weakly. The MFP calculated by using (11) is also displayed in the figure: $\Lambda_{SR}$ shows a pronounced peak around $V_T$ when there is no physical reason for the feature. This supports that $\lambda_{SR}$ is a more natural choice for the MFP than $\Lambda_{SR}$. In the $\lambda_{SR}$ versus $V_G$ curve of Fig. 4, however, there is still some hint of a peak around $V_T$. We believe that this is an artifact which is originated from the imperfect nature in the process of isolating the pure SR contribution in the channel region (7). As a matter of fact, 7 should hold better for greater $L$ because the assumption that the two sources of scattering (ES and SR) are incoherently connected becomes more valid.

Fig. 5 shows the MFP for different $W$’s when $L$ is fixed at 100 nm. The MFP decreases as $W$ becomes smaller, as expected, but the above-mentioned peaky feature near $V_T$ is more pronounced at larger $W$. Hereafter let us set aside the unphysical peaky feature near $V_T$ and concentrate on the MFP in the subthreshold region ($\lambda_{SR}^{sub}$) and the inversion region ($\lambda_{SR}^{inv}$).

Our key findings in this work with regard to the MFP’s are: 1) the dimensionless parameter $\Delta_m/W$ can be used as a good measure of the SRS strength, 2) the MFP’s exponentially decrease with $\Delta_m/W$, and 3) $\lambda_{SR}^{inv}$ becomes greater than $\lambda_{SR}^{sub}$ if $\Delta_m/W \geq 0.06$.

Firstly, both $\lambda_{SR}^{sub}$ and $\lambda_{SR}^{inv}$ exponentially decrease with $\Delta_m/W$ as shown in Fig. 6 where $\lambda_{SR}$’s were calculated for all the possible combinations of $W = 3$, 4, and 5 nm and $\Delta_m$ is 0.1 ~ 0.4 nm. $\lambda_{SR}^{sub}$ and $\lambda_{SR}^{inv}$ were evaluated at $V_G - V_T = -0.3$ V and 0.4 V, respectively. Notice that $W$ is restricted to below 5 nm here. In particular, $\lambda_{SR}^{inv}$ for $W \geq 5$ nm converges to the almost the same value, as shown in Fig. 5.

The fact that the MFP can be described by a single parameter $\Delta_m/W$, even with different $W$’s, is quite interesting. For the size quantization effects associated with channel width, such as the degree of wave-function confinement, the number of subbands, and the degree of the mixing between subbands, are expected to result in the MFP’s dependence on $W$ in a complicate way. Nevertheless, our calculations show the MFP’s exponential dependence on $\Delta_m/W$. This should give a useful guide for the estimation of $\lambda_{SR}$ in Si nanowire devices.

Secondly, we have found that, if the SRS effects become sufficiently strong, $\lambda_{SR}$ increases with the increase of $V_G$ and, as the consequence, $\lambda_{SR}^{inv} > \lambda_{SR}^{sub}$. This is in sharp contrast to the usual case where $\lambda_{SR}$ should decrease with the increase of $V_G$, because more intense scattering is expected to occur at higher gate voltages. In our calculations, the latter is observed for the cases of the SRS effects being relatively weak. See $\lambda_{SR}$ for $W = 5$ nm ($\Delta_m = 0.2$ nm) in Fig. 4 and that for $W = 6$ and 7 nm ($\Delta_m = 0.3$ nm) in Fig. 5 respectively. However, as $W$ becomes smaller in Fig. 5 the usual behavior is not seen.
(b) and (c), the cross-sectional charge densities for the cases effects can be qualitatively explained as follows. In Figs. 8
voltage, the Si/SiO$_2$ interfaces that fluctuate in proportion to nanowires of $W \leq 5$ nm, and consequently, the electrons are concentrated to the center of the nanowire as seen in the figure 4. Hence the 'effective' surface roughness that felt by the electrons is less at high gate voltage than at low gate voltage. This effect intensifies as $\Delta_m$ is increased or $W$ is decreased, resulting in the relationship between $\lambda_{SR}^{init}/\lambda_{SR}^{sub}$ and $\Delta_m/W$ shown in Fig. 7(b). On the other hand, for nanowires of $W > 5$ nm, the confinement effect is weak so the electrons are pushed to the nanowire surfaces at high gate voltage, resulting in the expected behavior that the MFP decreases with the increase of the gate voltage as shown in Fig. 8(a).

V. CONCLUSION

In this work, we have systematically devised the methodology for the calculation of the mean free path in the nanowire field effect transistors with finite channel length. The parasitic entrance scattering effects were identified and carefully eliminated from the MFP calculations. Non-perturbative approach based on the non-equilibrium Green’s function method was used to address the SRS effects in the nanowire transistors. The methodology developed in this work can be applied to any scattering mechanism, although only SRS is considered here.

We have found that the SR-limited MFP can be well described by a function which depends on a single parameter $\Delta_m/W$. In particular, the MFP in the subthreshold regime exponentially decreases with the increase of $\Delta_m/W$. For

![Fig. 7](image1.png)  
![Fig. 8](image2.png)
nanowires of $W \leq 5$ nm, the MFP in the inversion regime also exponentially decreases with $\Delta m/W$.

We have also found that the dimensionless parameter $\Delta m/W$ can be used as a good measure of the SRS strength. If $\Delta m/W < 0.06$, one may expect that the SRS effects should be relatively weak, resulting in the usual behavior that the MFP decreases with the increase of the gate electric field. If $\Delta m/W > 0.06$, on the other hand, the SRS effects can be regarded to be strong, resulting in the extraordinary behavior that the MFP increases with the increase of the gate electric field. Our results should give a useful guide for the estimation of MFP and the strength of the SRS effects in the nanowire devices.

ACKNOWLEDGMENT

This research was supported by the Pioneer Research Center Program and the Basic Science Research Program thorough the National Research Foundation of Korea (NRF) Funded by the Ministry of Education, Science and Technology (Grant No. 2012-0000459 and No. 2012-0002120).

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