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A simple interpolation model for the carrier mobility in Trigate and gate-all-around silicon NWFETs

Zaiping Zeng, François Triozon, Sylvain Barraud and Yann-Michel Niquet

Abstract—We compute the electron and hole mobilities in Trigate and gate-all-around silicon nanowires (SiNWs) within the non-equilibrium Green’s Functions (NEGF) framework. We then derive a simple model for the dependence of the mobility on the SiNW width and height. This model interpolates between the square SiNW and thin film limits. In order to provide a complete description of the mobility in SiNW devices, we calculate the phonon, surface roughness and remote Coulomb limited mobilities of square nanowires and of thin films with side or thickness $t = 5, 7$ and $10 \text{ nm}$. The mobility of arbitrary rectangular SiNWs with width $W = t$ or height $H = t$ can then be reconstructed from these partial mobilities using Matthiessen’s rule. We show that these models successfully reproduce the trends measured on $n$- and $p$-type devices with different widths and orientations.

Index Terms—Green’s functions; Mobility; Nanowire devices

I. INTRODUCTION

F OR the past two decades, metal-oxide-semiconductor field-effect transistors have evolved from planar, single-gate to three-dimensional multi-gate structures such as Trigate and Gate-all-around (GAA) silicon nanowire (SiNW) devices [1]–[4]. The transport properties of SiNWs channels have been extensively studied, both experimentally [5]–[11] and theoretically [12]–[29]. Nonetheless, the transition from rectangular SiNWs to thin films remains unclear. A facet model has been widely used to interpret the size dependence of the carrier mobility in rectangular SiNWs devices [8], [11]. In this model, the SiNW is split into four independent facets, which are assumed to behave as planar channels. However, the facet model does not always reproduce the experimental trends. Sekaric et al. have related these discrepancies to the formation of “corner channels” in SiNWs [8]. The simplest facet model also likely breaks down in ultra-thin SiNWs where the carriers flow closer to the axis of the device.

In this work, we compute the carrier mobility in $n$-type and $p$-type Trigate and GAA silicon nanowire field effect transistors (NWFETs) with [100] and [110] orientations. We use a non-equilibrium Green’s Functions (NEGF) approach [30], which explicitly accounts for quantum confinement and carrier scattering by phonons (PH), surface roughness (SR) and remote Coulomb charges (RCS) (section II). Based on the numerical results, we develop a simple but effective model that describes the size dependence of the carrier mobility in rectangular SiNWs over a wide range of dimensions (section III). This model only takes the mobilities of the thin film devices and of the square NW devices as inputs. These two limits are widely studied experimentally, and are among the easiest to address numerically. In order to provide a complete description of the mobility in these devices, we also compute the partial PH, SR and RCS electron and hole mobilities, for square NW and planar devices with different thicknesses and orientations. We finally show that these models successfully reproduce the experimental trends for different channel orientations (section IV).

II. DEVICES AND METHODOLOGY

The simulated devices are undoped, rectangular GAA and Trigate SiNW channels with width $W$ and height $H$. The Trigate devices are etched in a (001) Silicon-On-Insulator (SOI) layer. They are lying on a 25 nm thick buried oxide (BOX), and either a $n$-doped substrate for $n$-NWFETs (donor concentration $N_d = 10^{18} \text{ cm}^{-3}$) or a $p$-doped substrate for $p$-NWFETs (acceptor concentration $N_a = 10^{18} \text{ cm}^{-3}$). All facets except the bottom one are surrounded by the gate. We consider both [100] [with {001} facets] and [110] [with horizontal (001) and vertical (110) facets] channel orientations. The gate-stack is made of 0.6 nm of SiO$_2$ (dielectric constant $\epsilon = 3.9$) and 2.4 nm of HfO$_2$ ($\epsilon = 20$). Surface roughness (and remote Coulomb charges at the SiO$_2$/HfO$_2$ interface when specified) are explicitly included in the geometries. We use a Gaussian auto-correlation function model for SR with correlation length $\Lambda_{SR} = 1.0 \text{ nm}$ [31]. The current is computed in a self-consistent NEGF framework [30], [32], on top of the effective mass approximation (EMA) or two bands $k \cdot p$ model for electrons, and on top of the three bands $k \cdot p$ model for holes. The NEGF equations are solved in a fully coupled mode space approach (80 modes to 420 modes depending on the device cross section and on the band structure model), on a finite differences grid with step $2 \AA$. Carrier-phonon scattering is described by local, imaginary self-energies and the deformation potential theory. For electron-phonon scattering, we include intra-valley acoustic phonon scattering (with deformation potential $D_{ac} = 14.6 \text{ eV}$) and...
III. RESULTS AND DISCUSSION

A. Size dependence of the carrier mobilities

In this section, we analyze the dependence of the electron and hole mobilities in rectangular GAA and Trigate SiNWs on width $W$, height $H$, and orientation. For that purpose, we have computed the phonon+SR mobility in devices with one fixed dimension $W$ or $H = 7$ nm, and the other dimension ranging from $7$ to $49$ nm. The surface roughness rms is $\Delta_{SR} = 0.45$ nm. We have also computed the mobility for the planar limits: in GAA SiNWs, $W$ or $H \to \infty$ corresponds to a double-gate (DG) device. In Trigate SiNWs, $H \to \infty$ also corresponds to a DG device while $W \to \infty$ corresponds to a planar fully-depleted SOI (FDSOI) device. The electron and hole band structures are described with the EMA and three bands $k \cdot p$ models, respectively, and the wave function can not penetrate into the oxide. The mobility has been extracted from a quasi-Fermi level analysis in 30 nm long channels.

The results are shown in Fig. 1 (symbols). For electrons, we find that (i) [100] $n$-NWFETs perform better than [110] $n$-NWFETs, and (ii) [110] $n$-NWFETs with width $W > H$ show larger mobilities than [110] $n$-NWFETs with height $H > W$. This holds for both GAA and Trigate devices. This can be

the 3 $f$-type and the 3 $g$-type processes of Ref. [33]. We use a diagonal hole-phonon interaction with one single acoustic deformation potential $D_{ac} = 16.5$ eV and one single optical deformation potential $D_{opt} = 1.5$ eV/Å [34]. Details about the NEGF implementation can be found in Ref. [32].

The carrier mobility is calculated with two different methods. First, the quasi-Fermi level profile can be reconstructed from the NEGF data, and the mobility extracted from the slope of the quasi-Fermi level in the channel [35]. Second, the mobility can be computed from the slope of the total resistance $R$ of the device with respect to the channel length $L$ (numerical transmission line method) [32]. This method is more accurate but more demanding than the quasi-Fermi level analysis, since the calculation must be repeated on long devices. The device-to-device variability is small for SR but is significant once RCS is included [32]. We choose the distributions of RCS charges according to Ref. [32] in order to reduce that variability. Moreover, the mobilities are averaged over 5 distributions of RCS charges (but a single SR profile). In the following, the carrier densities per unit area are normalized with respect to the perimeter $W_{eff}$ of the SiNWs ($W_{eff} = 2W + 2H$ for GAA and $W_{eff} = W + 2H$ for Trigate devices).

![Graph](image-url)
explained by band structure effects [21]–[25]. In [100] SiNWs, the Δ valleys split into light ($m^* = 0.19 m_0$) $\Delta_{yz}$ valleys at the Γ point, and much heavier ($m^* = 0.92 m_0$) $\Delta_x$ valleys at $k \neq 0$. In the strong inversion regime, the electron gas is confined at the surface of the SiNW by the electric field, mostly in the light $\Delta_y$ valleys on the lateral (010) facets, and mostly in the light $\Delta_z$ valleys on the top and bottom (001) facets. In [110] SiNWs, the Δ valleys split into light ($m^* = 0.19 m_0$) $\Delta_x$ valleys at Γ and heavier ($m^* = 0.55 m_0$) $\Delta_{xx,yy}$ valley off Γ. Again, in the strong inversion regime the electron gas is mostly confined in the light Δ, valleys on the top and bottom (001) facets, but in the heavier $\Delta_{xy}$ valleys on the lateral (110) facets. Therefore, wide [110] SiNWs with dominant (001) facets ($W > H$) perform better than tall [110] SiNWs with dominant (110) facets ($W < H$). Likewise, [100] NWs with only {001} facets show better mobilities than [110] SiNWs with mixed facets.

The trends are opposite for p-NWFETs. Tall [110] SiNWs ($H > W$) indeed perform better than wide [110] SiNWs ($W > H$), and [110] always outperform [100] p-NWFETs. These trends can again be understood with band structure arguments [23]–[28]. Indeed, holes confined on {110} facets tend to show lighter transport masses than holes confined on {001} facets [36]. In strongly confined square [110] SiNWs, the highest valence subbands have a clear light hole character and are well separated from the others, while in square [100] SiNWs, the topmost valence bands are almost degenerate and heavy, which decreases carrier velocity and enhances inter-subband scattering [24].

We find that the carrier mobility generally increases with increasing NW cross section. The only exception is [110] p-type Trigate NWFETs with $W > H$ [28], since the increase of the (100) facet area with lower hole mobility is detrimental. When increasing $W$ or $H$, the carrier mobility tends to the expected DG or FDSOI limit. However, the convergence can be slow, especially for electrons in [110] SiNWs with $W > H$. $W$ and $H$ play the same role in [100] GAA devices as (010) and (001) facets are equivalent. This is not the case, however, in [100] Trigate devices as the side and top/bottom facets are not equivalent any more; the [100] Trigates with $H \gg W$ actually perform better than the [100] Trigates with $W \gg H$. This is particularly evident for p-NWFETs. As a matter of fact, the limiting (100) DG devices show better mobilities than the limiting (100) FDSOI devices because the carriers are distributed slightly more homogeneously over the thickness of the film [37].

### B. A simple interpolation model

In order to model these trends, we have analyzed the carrier density in the channel. We focus on n-type GAA devices, but the same arguments hold for Trigates. As shown in Fig. 2a, the density in the moderate to strong inversion regime peaks in four “corner channels” that tend to merge in two “side channels” when the size of the small facets is in the sub-10 nm range [8]. The electron and hole mobility can then be written:

$$\mu = \frac{n_{\text{in}}}{n_{\text{in}} + n_{\text{side}}} \mu_{\text{DG}} + \frac{n_{\text{side}}}{n_{\text{in}} + n_{\text{side}}} \mu_{\text{side}},$$

where $n_{\text{in}}$ and $n_{\text{side}}$ are the charge densities per unit length in the inner region and side channels of Fig. 2a, and $\mu_{\text{DG}}$ is the mobility in the limiting DG device. The mobility $\mu_{\text{side}}$ in the side channels can be extracted from the NEGF data at a given size. We set $T = 3.5$ nm for the thickness of the side channels, which gives a reasonable partition of the carrier density in the $n = 2 \times 10^{12} - 10^{13}$ cm$^{-2}$ range. $\mu_{\text{side}}$ is plotted in Fig. 2b.
for [110] GAA SiNW devices. It is, as expected, smaller on (110) than on (001) facets. It is also smaller than in DG (or FDSOI) devices due to lateral quantum confinement in the side channel, which enhances SR and phonon scattering. \( \mu_{\text{side}} \) is, therefore, dependent on the thickness of the Si channel, which is not accounted for in the simplest facet model [8], [11]. Eq. (1) with the data of Fig. 2b provides a fair description of the mobility for all sizes and carrier densities. \( n_{\text{in}} \) increases linearly with \( W \) or \( H \), while \( n_{\text{side}} \) remains nearly constant. However, over 20% of the total charge remains located in the side channels with much lower mobility even when \( W \) or \( H \approx 50 \) nm. This explains the slow convergence of the mobility towards the planar limit.

We can further simplify the model if we assume that the charge in both the inner and side channels is ruled by simple electrostatics and is thus proportional to the inner/side perimeters, e.g. \( n_{\text{in}} \propto \alpha(W - 2T) \) and \( n_{\text{side}} \propto \alpha(H + 2T) \) when \( W > H \). Then Eq. (1) turns into a simple interpolation formula between the mobility \( \mu_{\text{SQ}} \) of the square NW (\( H = W \)) and the mobility of the limiting DG device \( \mu_{\text{DG}} \), namely:

\[
\mu \approx \frac{W - H}{W + H} \mu_{\text{DG}} + \frac{2H}{W + H} \mu_{\text{SQ}} \tag{2a}
\]

when \( W > H \), and:

\[
\mu \approx \frac{H - W}{W + H} \mu_{\text{DG}} + \frac{2W}{W + H} \mu_{\text{SQ}} \tag{2b}
\]

when \( W < H \). For Trigate devices, the interpolation formula is:

\[
\mu \approx \frac{W}{W + 2H} \mu_{\text{FDSOI}} + \frac{3H}{W + 2H} \mu_{\text{SQ}} \tag{3a}
\]

when \( W > H \), and:

\[
\mu \approx \frac{2H}{W + 2H} \mu_{\text{DG}} + \frac{3W}{W + 2H} \mu_{\text{SQ}} \tag{3b}
\]

when \( W < H \). In Eqs. (3), \( \mu_{\text{FDSOI}} \) is the mobility of the limiting FDSOI device, and \( \mu_{\text{SQ}} \) the mobility of the square Trigate device. These equations reproduce the NEGF results very well over a wide range of dimensions and carrier densities, as shown in Figs. 1 and 2c. The discrepancies between this model and the NEGF data are maximal for [110] GAA n-NWFETs with \( W > H \).

### C. Carrier mobilities in square nanowires and thin films

Eqs. (2) and (3) use the carrier mobilities of the square NW devices (\( \mu_{\text{SQ}} \)) and of the limiting thin film devices (\( \mu_{\text{DG}} \) and \( \mu_{\text{FDSOI}} \)) as inputs. These mobilities are limited by phonons, SR and RCS. In order to dembed different contributions in the experimental data, we have computed the PH, SR and RCS mobilities in \( n \)-type and \( p \)-type, square Trigate and GAA SiNW devices with various sizes (\( W = H = 5, 7, 10 \) nm), and in the corresponding DG and FDSOI devices. The SR and RCS mobilities are defined with respect to the phonon-limited mobility \( \mu_{\text{PH}} \) as

\[
\mu_{\text{PH}}^{-1} = \mu_{\text{PH}+M}^{-1} - \mu_{\text{PH}}^{-1}, \tag{4}
\]

where \( M \) is a given elastic mechanism (SR or RCS), and \( \mu_{\text{PH}+M} \) is the NEGF mobility computed with phonons and that scattering mechanism. Including phonons in each calculation limits wave interferences and localization, and the partial mobilities defined above satisfy Matthiessen’s rule for multiple mechanisms better than the usual, direct single mechanism calculations [32]. We report data for a reference SR rms \( \Delta_{\text{SR}}^{\text{ref}} = 0.45 \) nm and correlation length \( \Lambda_{\text{SR}}^{\text{ref}} = 1 \) nm, and for a reference density of RCS charges \( n_{\text{RCS}}^{\text{ref}} = 2 \times 10^{13} \) cm\(^{-2}\). It is well known that the EMA tends to overestimate the electron mobility though it is computationally less demanding. In what follows, we have therefore employed a two bands \( k \cdot p \) model for the electrons in order to provide more accurate results for comparison with experiment. The wave function is also allowed to penetrate into the oxide layer. The carrier mobilities are extracted with the transmission line method.

The phonon mobility \( \mu_{\text{PH}} \) and the SR mobility \( \mu_{\text{SR}} \) decrease, in general, as a function of carrier density. SR scattering is, however, dominant at high inversion density, as the carriers get confined to the Si/SiO\(_2\) interface by the electric field. \( \mu_{\text{PH}} \) and \( \mu_{\text{SR}} \) also tend to decrease when the cross sectional area of the SiNW is reduced (except notably for [110])
Electron mobility [cm$^2$/V/s] in the "side channels" of $W_{[100]}$.

IV. COMPARISON WITH EXPERIMENTAL DATA

As an illustration, we compare the calculated mobilities with experimental data on rectangular Trigate devices with height $H = 11$ nm fabricated at CEA/LETI [42]. The equivalent oxide thickness (EOT) of the high-k/metal gate stack is approximately 1.3 nm. The parameters $\Delta_{SR}$ and $n_{RCS}$ in Eq. (7) have been adjusted in order to reproduce the dependence of the experimental mobility on carrier density for the $n$-type [110] square Trigate device and for the $n$-type, 11 nm thick FDSOI device. In this procedure, we have used the partial mobilities computed for the 10 nm square Trigate and FDSOI thin film. The optimal values are $\Delta_{SR} = 0.43$ nm and $n_{RCS} = 1.42 \times 10^{13}$ cm$^{-2}$.

The mobility can then be computed for arbitrary $n$- and $p$-type devices with Eq. (3a) and Tables I and II. The experimental and calculated mobilities are plotted as a function of $W$ in Fig. 3, at carrier density $n = 10^{13}$ cm$^{-2}$. The agreement is not perfect, but there is some experimental variability for the smallest $W$'s. We point out that we are not only able to reproduce the mobility of the target [110] $n$-type Trigates, but also the mobility of the [100] $n$-type Trigates and, more importantly, of all $p$-type devices (which were not included in the optimization of $\Delta_{SR}$ and $n_{RCS}$). A two parameters model for the mobility, Eq. (7), and the interpolation formula,
Hole mobility \([\text{cm}^2/\text{V}\cdot\text{s}]\)

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\[\Delta V = 0.43 \text{ nm}, n_{\text{RCS}} = 1.42 \times 10^{13} \text{ cm}^{-2}\]

\[
W \text{ [nm]} \quad 10^1 \quad 10^2 \quad 10^3 \quad 10^4
\]

(a) Electron mobility [\(\text{cm}^2/\text{V}\cdot\text{s}\)]

(b) Hole mobility [\(\text{cm}^2/\text{V}\cdot\text{s}\)]

Fig. 3. (a) Electron and (b) hole mobilities as a function of width \(W\) in rectangular Trigate devices (\(H = 11\) nm), at carrier density \(n = 10^{13} \text{ cm}^{-2}\). The symbols are the experimental data, while the solid and dashed lines are the mobilities interpolated from Eqs. (3a), (7) and Table II (\(\Delta V = 0.43\) nm, \(n_{\text{RCS}} = 1.42 \times 10^{13} \text{ cm}^{-2}\)).

Eq. (3a), can hence describe the experimental trends whatever the SiNW orientation and nature of the carriers. The above equations can, therefore, be used to explore the performances of next generation FinFETs or stacked SiNWs devices.

V. CONCLUSIONS

We have performed quantum calculations of the carrier mobilities in \(n\)-type and \(p\)-type, gate-all-around and Trigate SiNW devices using a non equilibrium Green’s Functions approach. The mobility tends to the planar double gate or FDSOI limit when the nanowire width or height is increased. However, the convergence can be rather slow. This results from the formation of “side channels” with low mobility. Their contribution remains significant even in rectangular devices with large width or height up to 50 nm.

We have derived from the numerical results a simple but effective interpolation model for the size dependent carrier mobilities in rectangular SiNW devices. The inputs of this model are the mobilities of the square SiNW devices and of the limiting thin film devices. Theses mobilities can be reconstructed from the contributions of the main scattering mechanisms using Matthiessen’s rule. We have therefore computed the phonons, SR and RCS mobilities of square SiNW devices and thin films with various sizes in the sub-10 nm range, and have given simple analytical expressions for practical usage. Finally, we have successfully validated these models against experimental data on Trigate devices. The results shall be useful for compact modeling and optimization of SiNW devices such as FinFETs and stacked nanowire transistors.

REFERENCES


[38] Strong confinement indeed promotes light hole bands in [110] p-NWFETs. The increase of hole velocities can overcome the enhancement of scattering. Therefore, the mobility might be non monotonous with carrier density and/or NW size depending on the strength of SR and RCS.


