Electron Dynamics in Silicon Nanowire using a Monte-Carlo Method

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Abstract. We present a theoretical study of electron transport in silicon nanowire (SNW). A self-consistent 2D-Poisson-Schrödinger solver provides the band structure. Then, both electron velocity and low-field electron mobility along the SNW axis are computed with an ensemble Monte-Carlo method. Scattering mechanisms due to phonons (acoustic phonons, zero-order and first-order intervalley phonons) and surface roughness are taken into account. We investigate the effect of cross section size and transverse electric field on electron mobility in SNW.

1. Introduction
Semiconductor nanowires represent an important and broad class of one-dimensional nanostructures at the forefront of nanoscience and nanotechnology. Recent advances in growth, characterization, assembly and integration of nanowires have enabled the emergence of a large number of applications in nanoelectronics, nano-optoelectronics, nanosensors, nanobiotechnology and energy harvesting [1]. Most of these applications, like transistors, sensors and thermoelectric devices are based on charge transport. Consequently, the knowledge of low-field electron mobility is essential to determine the performance of such devices. In this work, we computed electron velocity and low-field electron mobility at room temperature for a [100]-oriented silicon nanowire (SNW) with a square cross section surrounded by oxide materials (SiO₂/HfO₂) and metal gate.

This paper is organized as follows: sec. 2 explains the self-consistent calculation of the band structure. Sec. 3 contains a description of scattering mechanisms. Sec. 4 presents both electron velocity and low-field electron mobility in SNW obtained by Monte-Carlo simulation.

2. Band structure
The band structure of the SNW is computed with a 2D-Poisson-Schrödinger solver using the effective mass approximation (EMA) model. We obtain electronic states and corresponding wavefunctions as well as the potential distribution along the cross section. These results constitute the basis of our transport simulation. Comparisons with tight-binding simulations have shown that simulations with EMA are valid for large SNWs (over 5 nm in width) [2].

Because of 2D quantum confinement, the reciprocal space is restricted to 1D and the first Brillouin zone extends over [−π/a₀; π/a₀], where a₀ is the silicon lattice parameter. The six Δ conduction valleys in the bulk split into two groups: one group of four valleys ([100], [100], [010], [010]...).
and $[0\bar{T}0]$ is projected at $k = 0$ and the other group ($[001]$, $[00\bar{T}]$) is projected at $k \simeq 0.33\pi/a_0$ (for narrow nanowires, subband minima shift towards $k = 0$) [3].

3. Scattering mechanisms
Using first-order perturbation theory, the scattering rates of electrons with phonons and surface roughness are computed.

3.1. Electron-phonon
In this study, acoustic phonon, zero-order and first-order intervalley phonon scattering rates are computed using the deformation potential approximation.

For acoustic phonons, we analyze phonon quantum confinement due to the reduction of nanowire width and we compare elastic bulk phonon scattering with inelastic confined phonon scattering. In order to compute the scattering rates, the phonon dispersion is required. For bulk phonons, the phonon dispersion is approximated with a linear relation. Considering the dimensions of the SNWs in this study, confined phonon modes are obtained by solving elastic continuum equation thanks to the $xyz$ algorithm with free-standing boundary conditions [4, 5]. The figure 1 shows the lowest subbands of confined acoustic phonon dispersion for a SNW of 6 nm in width. The figure 2 shows the acoustic phonon scattering rates for the first subband of a SNW of 6 nm in width. Elastic bulk acoustic phonon scattering rates are proportional to the electron density of states. An electron is able to scatter into a subband, if its energy reaches the subband energy minimum. For inelastic confined acoustic phonon scattering, scattering rates is composed of two groups of peaks, which are localized on both sides of elastic bulk acoustic phonon scattering peaks. The group below the subband energy levels corresponds to phonon absorption and the group above the subband energy levels corresponds to phonon emission. Inelastic confined acoustic phonons scattering rate is higher than the acoustic scattering rate calculated using bulk phonons, because confined phonon group velocity is smaller than bulk phonon group velocity and scattering rates are inversely proportional to group velocity [6].

Zero-order and first-order intervalley are composed of long wavevector acoustic or nonpolar optical phonons. Intervalley phonons are considered as bulk phonons and the phonon dispersion is assumed to be constant. Zero-order intervalley scattering is modeled using the nonpolar optical model and first-order intervalley phonon following the approach developed by Monsef et al. [7].

3.2. Surface roughness
The imperfections of Si/SiO$_2$ interface induce fluctuations of electrostatic potential, energy levels, wavefunctions and also a redistribution of electron density within the cross section. Our model, based on Jin’s model, will be restricted only to the fluctuations of potential, energy levels and wavefunctions [6, 8].

4. Transport
The electron transport along the SNW axis is simulated with an ensemble Monte-Carlo method. Both electron velocity and mobility are extracted at room temperature under a constant electric field applied along the transport direction.

The deformation potential values of electron-phonon scattering have been calibrated in order to recover bulk mobility for a large cross section size (typically 30 nm) in the flat band regime, because it is assumed that the electronic properties of a large SNW are quasi-identical to those of bulk silicon and consequently, mobility too. The parameters for surface roughness (rms height $\Delta = 0.35$ nm and correlation length $\Lambda = 1.3$ nm) are adjusted in the high inversion density $N_{inv}$ range in order to reproduce experimental mobility variations measured in large SNWs [10].
Figure 1. Confined acoustic phonon dispersion calculated using the $xyz$ algorithm for a SNW of 6 nm in width. Only the lowest phononic subbands are shown.

Figure 2. Acoustic phonon scattering rate in relation with electron energy for a SNW of 6 nm in width. Only the first subband is shown.

Figure 3. Electron mean velocity limited by bulk phonon as a function of the longitudinal electric field for different SNW widths. The bulk values are provided by ref. [9].

Figure 4. Phonon limited low-field mobility for a SNW of 6 nm in width assuming bulk and confined acoustic phonons.

Figure 5. Low-field mobility as a function of SNW width at weak ($N_{inv} = 10^8$ m$^{-1}$) and high ($N_{inv} = 10^9$ m$^{-1}$) inversion densities.

Figure 6. Low-field mobility as a function of inversion density for two SNW widths (6 nm and 10 nm).
First, the velocity-field characteristics in undoped SNW are calculated for various cross-section sizes (cf. figure 3). Only the electron-bulk phonon scattering rates are taken into account. The behavior in presence of longitudinal electric field is different for large and thin SNWs due to the modification of valley populating between large and thin SNWs.

The figure 4 shows the impact of phonon confinement. In this figure, low-field phonon limited mobility is calculated using both bulk and confined acoustic phonon scattering rates for a SNW of 6 nm in width. Low-field phonon limited mobility is smaller with inelastic confined acoustic phonon scattering than with elastic bulk acoustic phonon scattering. The next calculations are done using only bulk phonons.

In figure 5, low-field mobility is plotted as a function of the SNW width for various inversion densities. Regardless the scattering mechanisms considered, the mobility is degraded with the reduction of SNW width. With the decrease of SNW width, subband modulation tends to suppress intersubband and intervalley transitions. This should induce an increase of mobility. Unfortunately, the scattering rates increase with decreasing the SNW width. Indeed, the electron-phonon scattering depends both on electron density of states and overlap between wavefunctions of initial and final states. When SNW width is reduced, electron density of states decreases, whereas the overlap of wavefunctions increases. So, the reduction of low-field phonon limited mobility is mainly due to the increase of wavefunction overlap. The decrease of mobility observed when the surface roughness scattering is taken into account is mainly due to the wavefunction fluctuations, which becomes the dominant term.

The figure 6 presents the low-field mobility as a function of inversion density for a large SNW (10 nm in width) and a small SNW (6 nm in width). We can notice that the mobility is reduced as the inversion density increases. Phonon scattering rates increase with increasing N_{inv} because of the wavefunction overlap which is enhanced by the confinement induced by the transverse field. The contribution of potential fluctuations, strongly dependent on N_{inv}, become more important for large SNWs than for small SNWs. This is due to the localization of electrons close to the Si/SiO_{2} interface for large SNWs, when N_{inv} is high. This explains why mobility for large SNWs is more impacted by a transverse field. This figure also shows that surface roughness scattering has a strong impact on low-field electron mobility and appears as the major scattering mechanism.

5. Conclusion
We have performed a complete study of low-field electron mobility in SNW using an ensemble Monte-Carlo method. To do that, the band structure with the effective mass approximation and scattering rates have been calculated. From these simulations, we can conclude that: (i) low-field mobility decreases both with the reduction of SNW width and with the increase of inversion density, and (ii) surface roughness appears to be the major scattering mechanism.

References
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