One-Dimensional Multi-Subband Monte Carlo Simulation of Charge Transport in Si Nanowire Transistors

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***Abstract*— In this paper, we employ a newly-developed one-dimensional multi-subband Monte Carlo (1DMSMC) simulation module to study electron transport in nanowire structures. The 1DMSMC simulation module is integrated into the GSS TCAD simulator GARAND coupling a MC electron trajectory simulation with a 3D Poisson–2D Schrödinger solver, and accounting for the modified acoustic phonon, optical phonon, and surface roughness scattering mechanisms. We apply the simulator to investigate the effect of the overlap factor, scattering mechanisms, material and geometrical properties on the mobility in silicon nanowire field-effect transistors (NWTs). This paper emphasizes the importance of using 1D models that include correctly quantum confinement and allow for a reliable prediction of the performance of NWTs at the scaling limits. Our simulator is a valuable tool for providing optimal designs for ultra-scaled NWTs, in terms of performance and reliability.**

Keywords*— *One-Dimensional Multi-Subband Monte Carlo (1DMSMC); Nanowire FETs; Charge Transport;

I. Introduction

Nanowire transistors (NWTs) are attracting significant interest as an extension of the FinFET CMOS technology to the ultimate scaling limits. The benefits of NWT technology have been discussed in many publications (see for example [1]). Advantages of the gate-all-around (GAA) NWTs are numerous and include better charge transport control in the channel reducing the short channel effects, and the possibility of strain and material engineering to improve device performance.

Considerable work has been carried out to evaluate the mobility of Si nanowires, relying mainly on the Kubo-Greenwood formalism [2]–[4], and to a lesser extent on Monte Carlo and other 1D Boltzmann equation solvers [5], and atomistic simulation methods [6]. However, more work is needed to evaluate the performance potential of NWTs with silicon and alternative material channels at the scaling limit. In this work, we utilize a newly-developed one-dimensional multi-subband Monte Carlo (1DMSMC) module, which is integrated into the Gold Standard Simulation (GSS) TCAD simulator GARAND [7] to investigate the effect of the overlap factor, scattering mechanisms, material and geometrical properties on mobility in silicon NWTs.

II. Simulation Method

The functionality of the GSS 'atomistic' simulator GARAND has been extended to include a 1DMSMC module currently in the final stages of development. The simulator is well-suited for the study of a variety of NWTs and FinFETs, based on Si, Ge, SiGe, III-V and other materials. The 1DMSMC simulator couples a MC transport simulation with a 3D Poisson – two-dimensional (2D) Schrödinger equation solver, as illustrated in Fig. 1, which accurately captures the effect of confinement on charge dynamics.

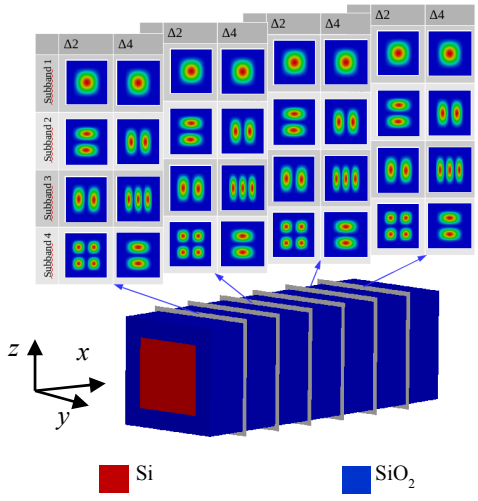

Fig. 1. Coupling the 2D solution of Schrödinger equation in multiple slices, to a 3D Poisson solution and charge dynamics in the structure, which is based on a Si gate-all-around nanowire channel FET.

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Considering the importance of spatial confinement in advanced More Moore devices, such as NWTs or indeed FinFETs, the basic properties of electron transport derived under the assumption of a bulk crystal must be revised. Since charge carriers are confined in a given direction, the Bloch theorem is no longer valid. Electrons are not point-like particles anymore, and cannot move freely in each direction. In this case, the momentum of a localized electron is not well defined due to the position-momentum uncertainty relations. Instead, the energy is quantized into subbands, momentum conservation is only valid in the transport direction, while scattering rates are modified by the overlap factor of the eigenfuctions of the subbands involved in the transition.

Currently, the simulator includes modified acoustic phonon, optical phonon, and surface roughness scattering mechanisms. Acoustic phonon scattering is considered within the elastic equipartition approximation, in the short wavevector limit. Also, the energies of the different branches of the deformation potential optical phonons are approximated with constants, following most of the standard approaches. Surface roughness scattering is most pronounced in nanostructures where confinement keeps electrons close to non-ideal interfaces, as is the case for quantum wires. The extent of the interaction with surface imperfections is dependent on the force normal to the interface, and the statistics given by the height and correlation length of the roughness model [4]. In this work, the calculations are performed within the ellipsoidal non-parabolic bandstructure valley approximation.

III. Device Structure and Simulation Experiments

The simulated device is a GAA NWT, as shown in Fig. 1. We focus on the calculation of the electron mobility for nanowire widths within the range 3–8nm. The gate oxide thickness is 0.8 nm. The channel is undoped and assumed to be infinitely long. Unless specified otherwise, the presented results are for a square nanowire. The gate bias is adjusted to obtain the 1D charge sheet density at which the mobility is reported. In the long-channel simulation framework used here, the electric field in the transport direction (along the nanowire) is fixed to a low value (1kV/cm in this work). The potential profiles in the nanowire cross section and the corresponding eigenfuctions of the subbands are pre-calculated using a drift-diffusion simulator coupling the current continuity equation to a 2D solution of the Schrödinger equation in multiple slices and a 3D Poisson solution.

IV. Results and Discussions

Figure 2 shows the calculated phonon scattering-limited low-field mobility, as a function of nanowire width for three different crystal orientations: [100], [110] and [111]. The results are consistent with established mobility trends [2]–[6]. To understand the effect of the overlap factor, we compare conventional 3D MC with 1DMSMC simulations. In the latter, we consider two types of simulations: the first type uses the typical overlap factor that is computed self-consistently, while the second type uses a constant overlap factor that is chosen conveniently to highlight its impact. It should be noted that the use of a constant overlap factor here is solely for demonstrative purposes, and it is not a recommended practice. Figure 3 shows a typical variation of the overlap factor with nanowire diameter. Figure 4 shows the variation of mobility with the diameter for both types of simulations. Indeed, Fig. 4 highlights the significant effect of the overlap factor on mobility, especially at small widths.

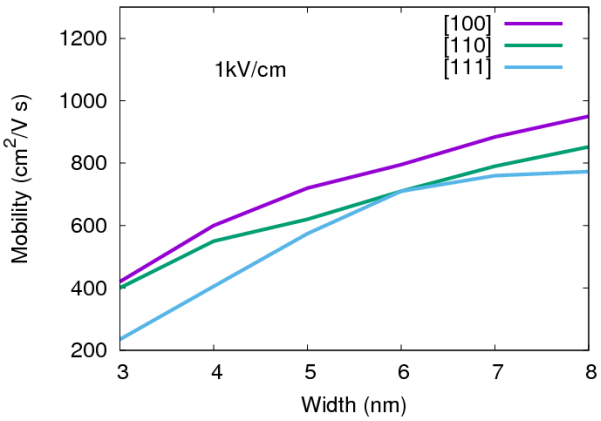

Fig. 2. The calculated low-field electron mobility for a square nanowire, as a function of nanowire width and material orientation, for a nanowire density of ~5x10^6 cm^{-1}.

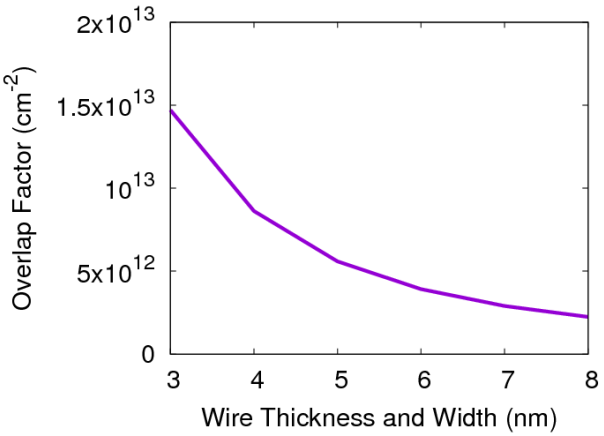

Fig. 3. Typical overlap factor values as a function of diameter.

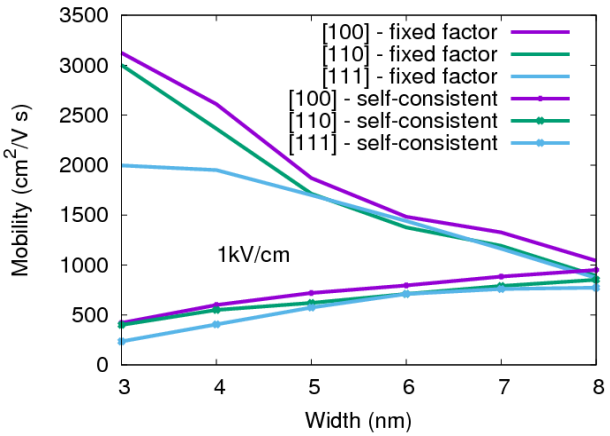

Fig. 4. Electron mobilities using the self-consistent and the fixed overlap factors.

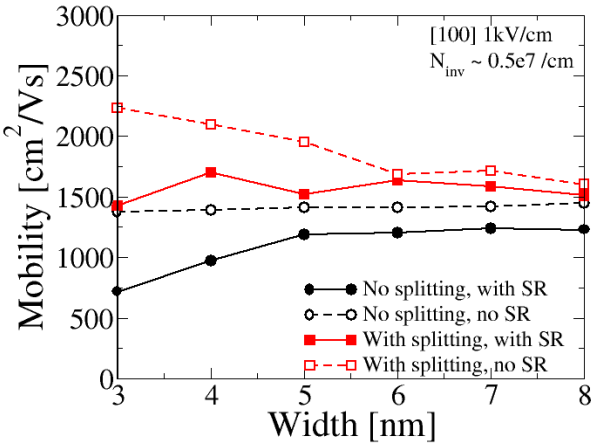

Fig. 5. Low-field electron mobility as a function of nanowire width from the 3D Monte Carlo simulator, with and without considering valley splitting and surface roughness scattering. The results are for a nanowire density of ~5x10^6 cm^{-1}.

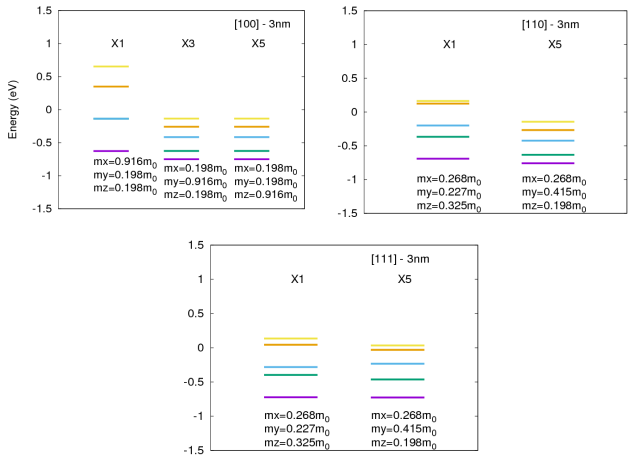

Fig. 6. Energy levels for a 3nm width and different orientations, showing band splitting and the effective masses in different directions for each set of valleys (x being the direction of transport). For the [100] orientation, the set of valleys X1, X3 and X5 are all characterized by two-fold degeneracies. For the [110] and [111] orientations, the X1 valleys set has a four-fold degeneracy while the X5 valleys set has a two-fold degeneracy.

Figure 5 shows the variation of low-field mobility with diameter, as calculated using the 3D MC simulator, by including and disabling band splitting. The results highlight how band splitting enhances the mobility at smaller nanowire widths, as lower valleys are characterized by a smaller effective mass along the transport direction. The trend in Fig. 5 is similar to the 1DMSMC trend shown in Fig. 4, when fixing the overlap factor. Figure 6 shows the energy levels for different NWT diameters and orientations obtained from 1DMSMC simulations, and the effective masses in different directions for each set of valleys. It is clear that, for the [100] orientation, the set of valleys X1, X3 and X5 are all characterized by two-fold degeneracies. With the [110] and [111] orientations, the X1 valleys set has a four-fold degeneracy while the X5 valleys set has a two-fold degeneracy. By observing both Figs. 2 and 6, mobility is generally highest in [100] devices because, among other reasons, the transport-direction effective masses are lower at the lowest valleys. On top of this, the energy offset between the lower and upper valleys is higher minimizing possible electron transitions to the upper valleys. Mobility is generally lowest in [111] devices, due to the lower valley splitting energy and higher transport masses.

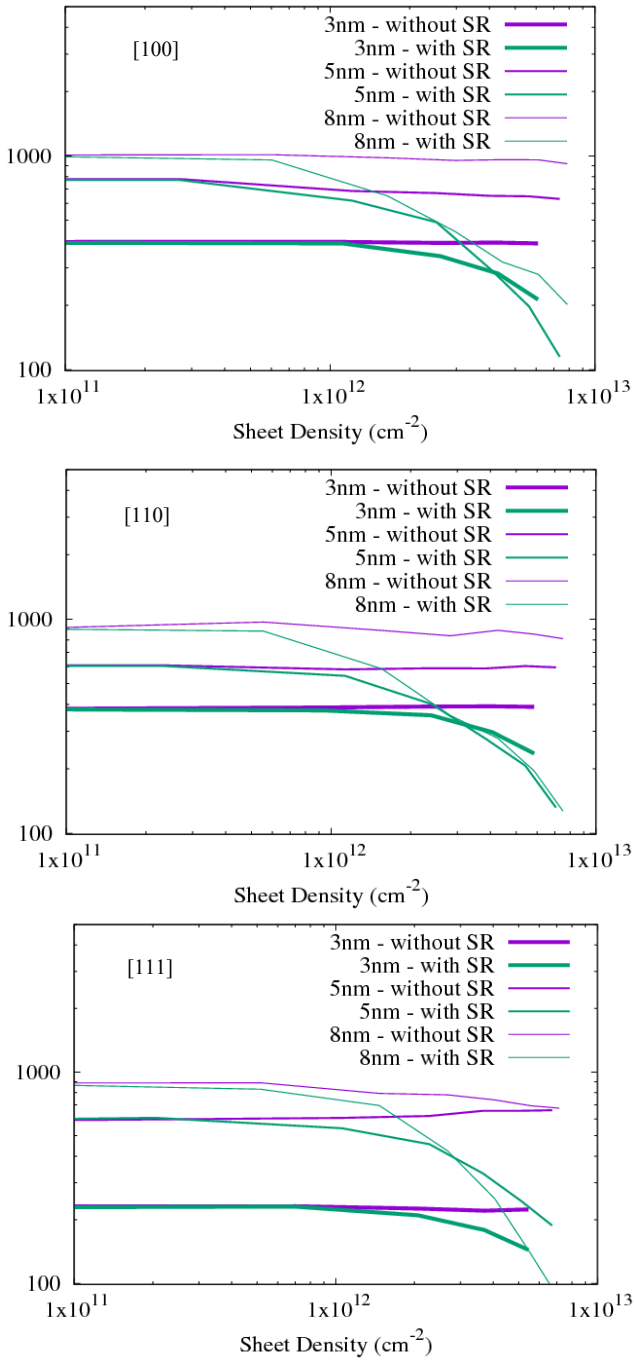

Fig. 7. The electron mobility, with and without surface roughness scattering, as a function of nanowire sheet density, widths and channel orientation, from the 1DMSMC Model.

Figure 7 shows the electron mobility as a function of the nanowire sheet density, widths and orientation, obtained from the 1DMSMC Model, with and without including surface

roughness scattering. Figure 7 illustrates how the impact of surface roughness scattering is more pronounced at higher sheet densities, and varies from one width to another, in agreement with published data [2]–[6]. Figure 8 shows the phonon-scattering limited mobility of square, circular, and elliptical nanowires, for different orientations, as a function of the cross section area. The cross section shape affects directly the subband energy levels and eigenfunctions, as illustrated in Figs. 9 and 10 showing eigenfunctions for different nanowire shapes for a 5nm diameter and a [100] orientation. The direct impact on the valley splitting energy and the overlap factor (and other important parameters) may enhance or degrade the mobility, as demonstrated in Fig. 8. The presented results in this study highlight usefulness of 1DMSMC simulations that include correctly quantum confinement, via the solution of the Schrödinger equation, allowing for the accurate evaluation of mobility in NWTs at the scaling limits, with different materials and geometries, and under strain.

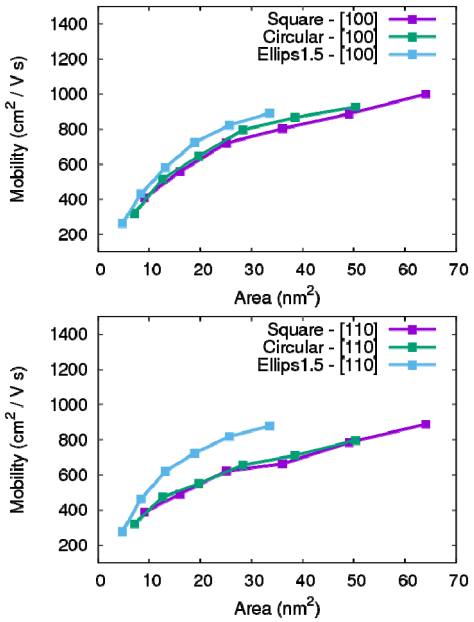

Fig. 8. Phonon-scattering limited mobility as a function of the cross section area, for square, circular, elliptical [major diameter (*y*-axis) / minor diameter (*z*-axis) = 1.5] nanowires, for [100] and [110] orientations.

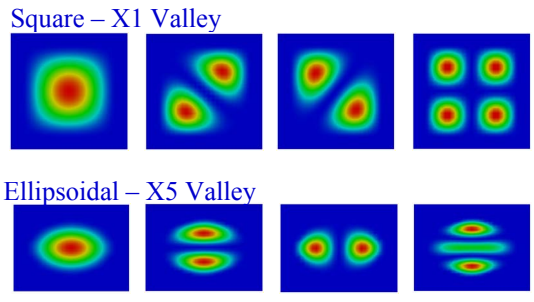

Fig. 9. The eigenfunctions of the first four subbands, for square and ellipsoidal nanowires, for a diameter of 5nm and a [100] orientation.

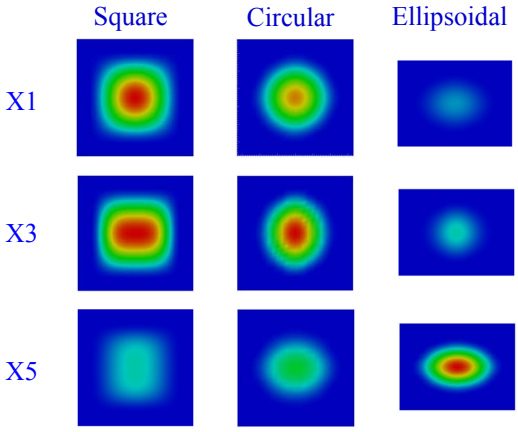

Fig. 10. The eigenfunctions of the lowest subbands for each valley, for square, circular and ellipsoidal nanowires, for a diameter of 5nm and a [100] orientation.

V. Conculsions

In this work, we introduce a newly-developed one-dimensional multi-subband Monte Carlo simulation module, which is suitable for the study of electron transport in nanowire transistors. We employ the simulation module to explore the effect of the overlap factor, scattering mechanisms, nanowire shape and channel orientation on the mobility of Si nanowire devices. In this paper, we emphasize (i) the importance of using multi-subband models accounting correctly for quantum confinement to provide a reliable prediction of device performance, and (ii) the qualitatively different predicted trends compared to the traditional 3D ensemble MC simulations. The simulation framework is a valuable tool for technology option screening for ultra-scaled NWTs, in terms of performance.

Acknowledgment

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