Study of the 1D Scattering Mechanisms' Impact on the Mobility in Si Nanowire Transistors

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***Abstract*— The most extensive research of aggressively scaled nanoelectronic devices involves the inclusion of quantum confinement effects and their impact on the performance of new architectures. This work implements a set of multisubband phonon and impurity scattering mechanisms and the Kubo-Greenwood theory in order to study the mobility in Si nanowire structures.**

Keywords-Phonon Scattering; Impurity Scattering; Kubo-Greenwood Formalism; Matthiessen rule; Nanowire FETs

I. INTRODUCTION

Nanowire transistors (NWTs) are being considered as an alternative to replace standard CMOS technology due to their better charge transport control in the channel. In the simulation framework, it has been mandatory to develop different schemes in order to reduce the computational effort of the quantum transport theories. One of the most popular trends is to incorporate into semi-classical simulators models with refined macroscopic quantities and physical analysis accounting for important quantum effects. The approach considered herein combines quantum effects with the semi-classical Boltzmann transport equation (BTE) using the relaxation time approximation and the Kubo-Greenwood formalism [1]-[3]. This strategy provides reliable mobility values at low-field near-equilibrium conditions, based on the rates of the relevant scattering mechanisms governing multisubband transistors in quantum wires [4]. In this work, we study the effect of quantum confinement on the electron mobility in NWTs including phonon and impurity scattering. In addition, we analyze the impact of the nanowire size and geometry on the transport properties.

II. METHODOLOGY

Long-channel simulation is a convenient framework for assessing low-field electron mobilities in devices which incorporate a confining structure, such as gate-all-around. It directly studies the effect of charge confinement on transport as a function of out-of-plane (lateral) applied electric field. The channel is assumed to be infinitely long and the electric field in the transport direction is fixed to a low value. First, multiple cross sections of the device are simulated using the coupled 3D Poisson and 2D Schrödinger solver (Fig. 1) integrated in the TCAD simulator GARAND from Synopsys. Second, the potential and the corresponding eigenfunctions of the subbands are included in the particular scattering rates, whose expressions have been directly developed from Fermi's Golden Rule accounting for the multi-subband quantization in the normal to the wire plane of confinement. In this work, we have included: *(i)* acoustic phonons which are considered within the elastic equipartition approximation in the short wave vector limit; *(ii)* optical phonons including fixed parameters for the different branches; and *(iii)* ionized impurity scattering which is relevant for all types of doped nanostructures due to the short range Coulomb interaction with the carriers. The mobilities are calculated by applying the Kubo-Greenwood formula to the relaxation times corresponding to the linearized BTE. Finally, Matthiessen's rule [5] is used to combine the scattering probabilities, and so both the individual and the total mobilities of the simulated device are analyzed separately.

III. RESULTS

Fig.1 shows the device parameters for the NWTs herein analyzed. Both square and circular shapes are studied. Despite NWTs start to have a bulk-like behavior only at diameters higher than 8nm, we use bulk effective mass values. Fig.2 presents the scattering rates as a function of the total energy for electrons calculated for impurity, acoustic phonon, and optical phonon (including f-, g-type and total) scatterings for a square NWT with 3nm (top) and 8nm (bottom) widths for a [100] orientation and 20 subbands. The multisubband effects in the scattering rates are generally more pronounced for smaller wire width. This is associated with the higher energy difference between the lower and upper subbands (Fig.3), which minimizes the possible electron transitions between subbands. This fact results in the reduction of the mobility (both the individual and the total) for higher confined devices (Fig.4). Moreover, for these particular devices, the mobility is limited by acoustic phonon scattering due to its high scattering rates, especially at low energy (Fig.4). Finally, Fig.5 shows the total mobility of square and circular NWTs as a function of the cross section area: the latter affects directly the subband energy levels and eigenfunctions. Consequently, the change in these parameters may enhance or degrade the mobility substantially. The results presented in Fig. 5 are in good agreement with our previous work [6] where we observed higher mobile charge in circular NW in comparison to the square device.

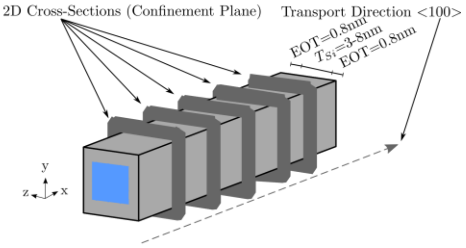

Figure 1. NWT structures analyzed in this work with widths ranging from 3nm to 8nm. The coupled 2D Schrödinger and 3D Poisson equation are solved for each cross-section (confinament plane) and then the scattering rates are calculated accounting for the potential and the eigenfunctions for each subband.

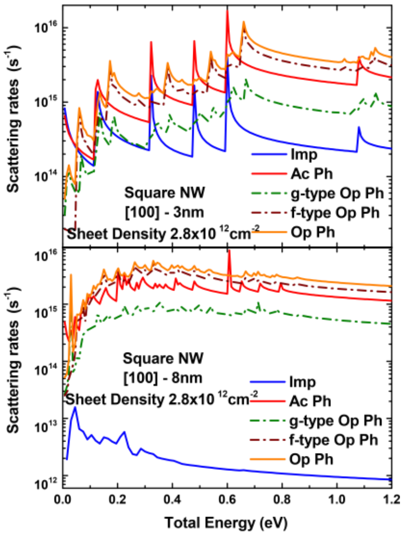

Figure 2. Impurity scattering rate (Imp) as well as acoustic (Ac Ph), optical (including g-type, f-type and total (Op Ph)) phonon scattering rates as a function of the total energy for a square NW with 3nm (top) and 8nm (bottom) width for [100] orientation and sheet density of 2.8x10^{12}cm^{-2}.

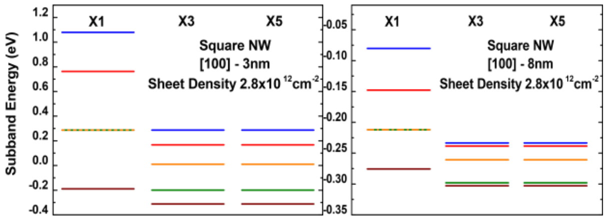

Figure 3. Energy levels for a square NW with 3nm (top) and 8nm (bottom) width for [100] orientation and sheet density of 2.8x10^{12}cm^{-2}, showing band splitting for the set of valleys X1, X3 and X5.

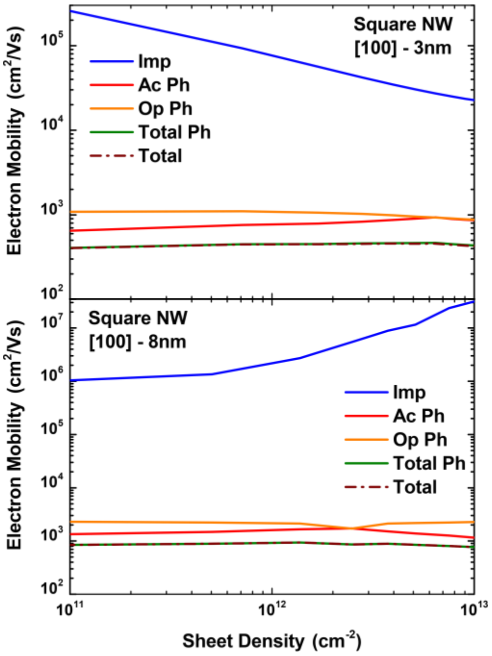

Figure 4. Electron mobility as a function of the sheet density considering the impurity (Imp) as well as the acoustic (Ac Ph), optical (Op Ph), and total (Total Ph) phonon scattering separately as well as combined for a square NW with 3nm (top) and 8nm (bottom) width for [100] orientation.

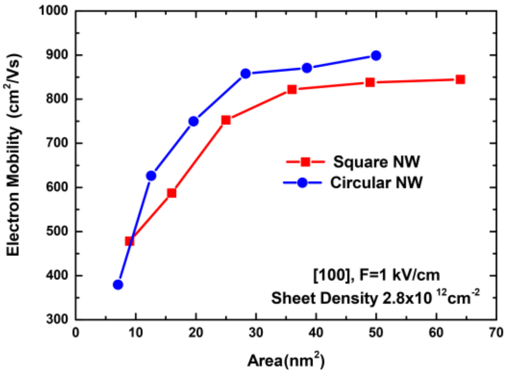

Figure 5. Electron Mobility as a function of the area for a square and circular NW with sheet density of 2.8x10^{12}cm^{-2}.

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