Electronic Properties of Silicon Nanowires: Confined Phonons and Surface Roughness

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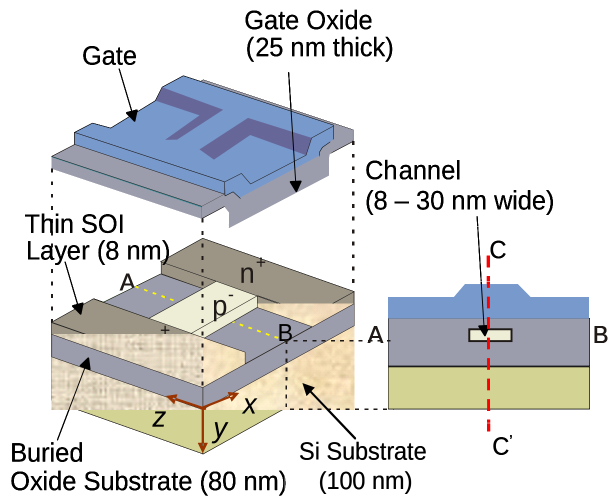
***Abstract*—Electron mobility in narrow, rectangular silicon nanowires is calculated using a Schrödinger-Monte-Carlo-Poisson transport simulator. Mobility lowering due to the carrier scattering with confined phonons in narrow wires and the influence of surface roughness within Ando's model are investigated.**

Keywords - silicon nanowire, surface roughness, confined phonons

Nanostructures with spatial confinement along two directions are termed nanowires. It has been experimentally shown [1] that, besides the channel thickness, the channel width can also be reduced down to nanometer scale. The resulting quasi-one-dimensional nanostructures are expected to play a key role in future nanotechnology, as well as to provide model systems to demonstrate quantum size effects. Silicon nanowires (SiNWs) in particular are potentially very attractive, given the central role of silicon in the semiconductor industry and the existing set of known fabrication technologies.

In our recent work [2], we investigated the mobility of electrons in a rectangular SiNW, by taking into account the major scattering mechanisms, namely acoustic phonon scattering, non-polar optical phonon scattering and surface roughness scattering. Surface roughness scattering was modeled using Ando's model [3], and the phonons were treated in the bulk mode approximation. The effect of impurity scattering was not included, since the channel was very lightly doped. Fig. 1 shows the schematic of the ultrathin-body SOI (UTBSOI) device considered in the work, and the potential profile along the cutline CC', which was obtained by solving 3D Poisson and 2D Schrödinger equations self-consistently.

The device of width 30 nm [at this width electrons in the channel feel very weak spatial confinement along the width and hence behave like a two-dimensional electron gas (2DEG)] was used to compare the mobility results obtained from our simulator with the experimental data of Koga et al. [4] for a 2DEG of the same thickness. Fig. 2 shows the calculated low-field electron mobility. Although there is a good agreement with the experimental data, we find that the simulator overestimates the mobility in moderate effective field region, where phonon scattering dominates. This discrepancy is due to assuming bulk phonons in the calculation of the phonon



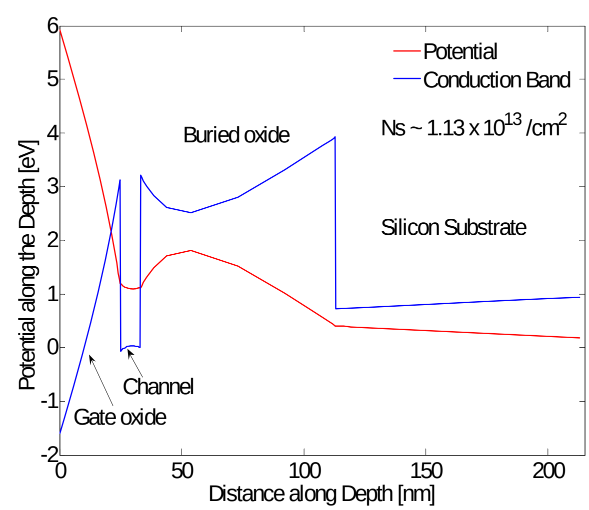


Figure 1. Top panel: Schematic of the simulated SiNW on ultrathin SOI. The conduction band profile depicted in the bottom panel is taken along the red cutline CC' from the top panel.

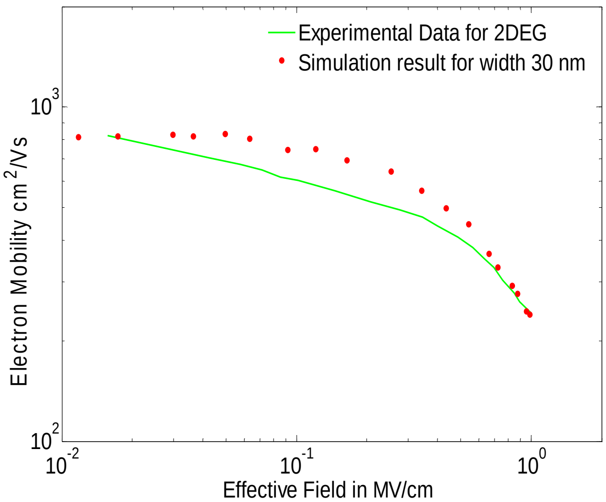


Fig. 2. Low-field mobility of 30 nm wide SiNWs as a function of the effective transverse field, as obtained from the calculation (circles) and the experiment by Koga *et al.* [4] (solid line). Overestimation of the mobility at moderate fields is due to the assumed bulk phonon scattering, and should be remedied by the incorporation of confined phonons.

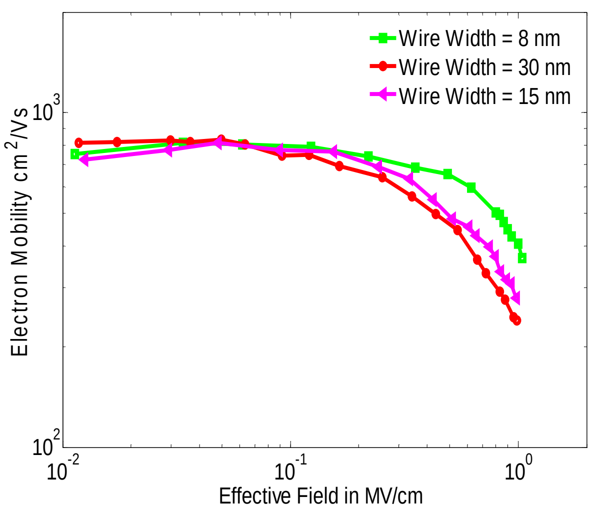


Figure. 3. Variation of the field-dependent mobility with varying SiNW width [2].

scattering rates. Fig. 3 shows the field-dependent mobility for different SiNW thicknesses. Phonon-limited mobility is found to decrease with decreasing width, because the overlap between the phonon and electron wavefunctions is larger in narrower wires. In contrast, surface-roughness scattering mobility increases with decreasing wire width, because electrons in narrow (1D) wires are located near the wire center, as opposed to near the side interfaces in wide (2D) wires.

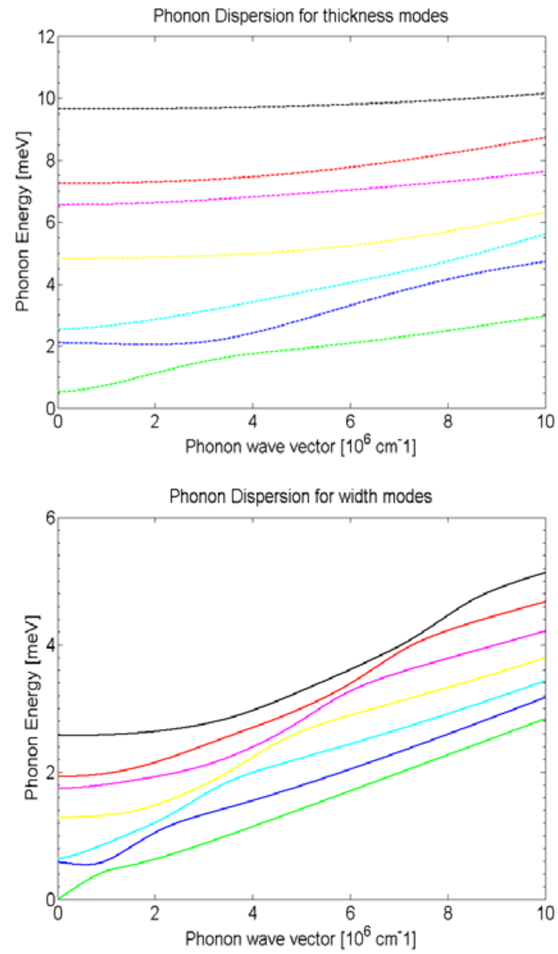


Figure. 4. Confined phonon dispersion modes. Top panel: thickness modes, bottom panel: width modes.

Presently, we are investigating the effect of confined phonons on the phonon scattering, and the variation of mobility for SOI thickness and width below 8 nm, and the results of these computations will be presented at the conference. Modification of the phonon spectrum due to the spatial confinement is expected to enhance the overlap of the electron and confined phonon wave function [5], thereby increasing the electron-phonon scattering rates. Fig. 4 shows the calculated phonon dispersion for the thickness and width modes (top and bottom panels, respectively). For SiNWs narrower than 5 nm, we expect the effect of surface roughness to be more detrimental to the mobility, because the average distance of the carriers from the interfaces would be less than 2.5 nm, even though they are located near the wire center.

ACKNOWLEDGMENT

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