Low-Field Mobility of Ultra-Narrow Si Nanowire MOSFETs Using Self-Consistent Full-Band Simulations

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Silicon nanowires (NWs) have attracted significant attention as candidates for high performance transistor channels. In this work, we calculate the low-field mobility in n-type and p-type NWs of diameters up to D=12nm (up to ~5500 atoms in the unit cell) in the [100], [110] and [111] transport orientations. We use the $sp^3d^5s^*$ atomistic tight-binding model for the electronic structure, self-consistently coupled to the 2D Poisson equation [1], as shown in Fig. 1. Upon convergence, the mobility is extracted using linearized Boltzmann transport theory, considering acoustic phonons, optical phonons, and surface roughness scattering (SRS) [2].

We show that under strong inversion conditions, strong variations appear in the dispersion relations, especially for p-type NWs. The dispersions acquire lighter subbands for the [110] and [111] NWs, similar to what is observed under structural cross section confinement [2]. This has consequences in the NWs' mobility as shown in Fig. 2. The formation of the lighter subbands, causes the mobility to increase by almost ~50% with increasing V_G in the cases of the [111] and [110] NWs (solid lines). Such behavior is in contrast to the usual trend, which dictates that the mobility drops monotonically with V_G. The observed increase is large enough to even compensate for the detrimental effect of SRS (dashed lines). We also note that a strong mobility anisotropy is also observed in the entire V_G range, with the [111] NW having ~2x and ~3x higher performance compared to the [110] and [100] NWs, respectively. For n-type NWs, other than the usual prime-unprimed valley shifts, the bandstructure is not altered significantly. We validate our results using k·p calculations as well. Finally, we discuss the meaning of mobility for quasi-ballistic transistors, and show that the "apparent" mobility (measured in experiments) is influenced by the "ballistic" mobility and is lower that the macroscopic "diffusive" mobility.

[1] N. Neophytou et al., IEEE TED, 55, 1286, 2008. [2] N. Neophytou and H. Kosina, PRB, 84, 085313, 2011.

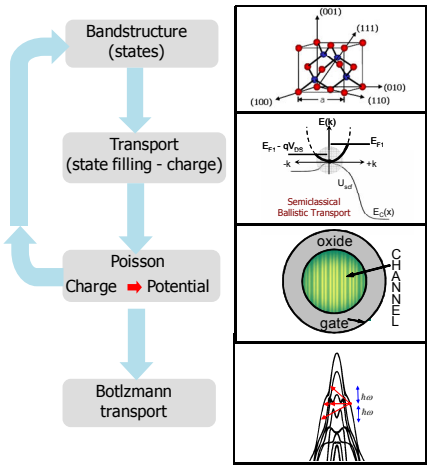

Fig. 1: Simulation procedure. (a) The NW bandstructure is calculated using the $sp^3d^5s^*$ TB model. (b) A semiclassical ballistic model is used to calculate the charge distribution. (c) The charge is self-consistently coupled to a 2D Poisson equation for the electrostatic potential in the cross section. The oxide is SiO_2 of thickness t_{ox}=1.1nm (d) Upon convergence, Boltzmann transport theory, including all relevant scattering mechanisms, is used for mobility calculations.

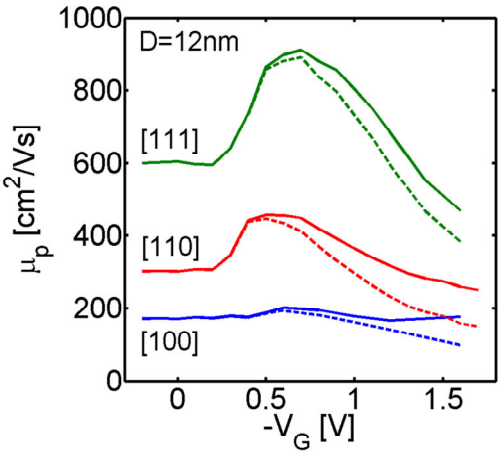

Fig. 3: Low-field hole mobility for NWs of diameter D=12nm in the [100], [110], and [111] transport orientations versus gate bias ($-V_G$). Solid lines: Phonon-limited mobility. Dashed lines: Phonon plus surface roughness scattering (SRS) limited mobility. A large anisotropy is observed. The mobility unexpectedly increases by ~50%, before following the usual decreasing trend as the channel is driven into inversion.