Thermoelectric properties of gated Si nanowires

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This work introduces a self-consistent atomistic $sp^3d^5s^*$ tight-binding bandstrusture simulator that computes the electronic structure of ultra-narrow semiconductor nanowires in the presence of a gating electrostatic potential. The $sp^3d^5s^*$ tight-binding model is coupled iteratively to the 2D Poisson equation, as shown in Fig. 1 [1]. Upon convergence, the mobility is extracted using the full band information and linearized Boltzmann transport theory, considering all relevant scattering mechanisms, i.e. acoustic phonons, optical phonons, surface roughness scattering, and ionized impurity scattering [2]. The model is computationally robust to allow atomistic description of the electronic properties for NWs with diameters even up to 25nm, consisting of several thousands of atoms in the computational domain. Using the simulator we compute the electronic and thermoelectric properties of p-type NWs of D=12nm in the [110] transport orientation. Figure 1b shows the carrier mobility versus density for two different device cases: i) the gated channel, considering phonon (red-solid-dot line) and surface roughness (red-dashed-dot line) scattering, and ii) the doped channel, considering phonons, surface roughness, and ionized impurity scattering (black-solid line). It can be observed that the mobility of the gated channel is largely increased compared to the mobility of the doped channel because of the absence of ionized impurity scattering, but also because electrostatic confinement (at concentrations $p \sim 10^{19}/cm^3$) causes a severe valence bandstructure modification, increasing the band curvature, increasing carrier velocities, and thus mobility, even in the presence of surface roughness scattering. Figure 1c shows the thermoelectric power factor of the NW under direct doping and under gating. A large improvement in the power factor is observed as a result of the improved conductivity of the NW upon absence of ionized impurity scattering and bandstructure modifications under electrostatic confinement [3].

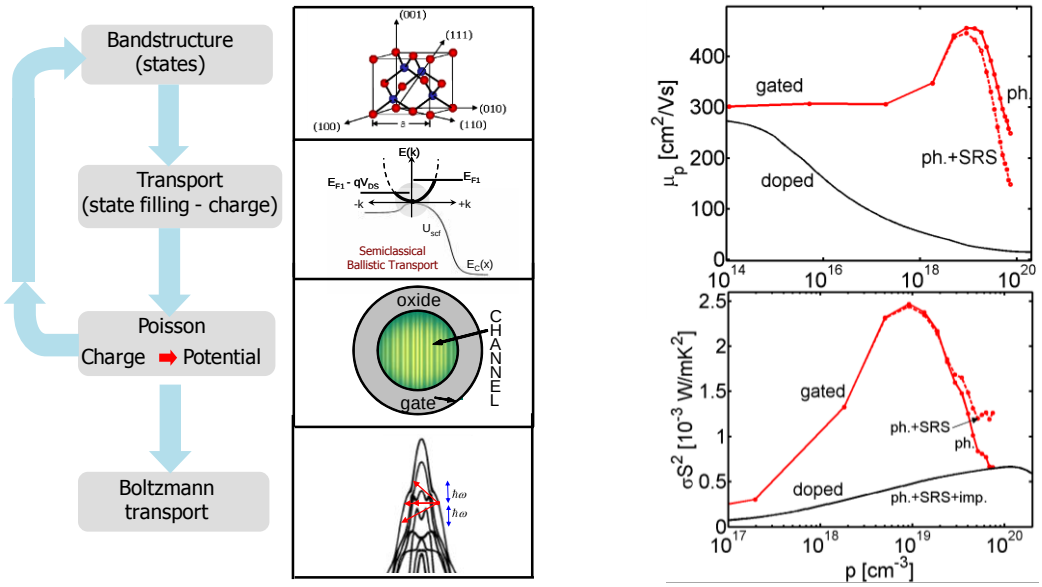

Figure 1: (a) The self-consistent atomistic bandstructure model for examining the transport properties of NWs. (b) The [110] D=12nm Si NW mobility under doped and gated conditions. (c) The thermoelectric power factor for the same NW and conditions.

References

[1]N. Neophytou et al, *Solid State Electronics*, 90, 44, 2013. [2]N. Neophytou and H. Kosina, *PRB*, 84, 085313, 2011. [3]N. Neophytou and H. Kosina, *Appl. Phys. Lett.*, 105, 073119, 2014.