Atomistic simulations of electronic and thermoelectric transport in Si nanowires: Influence of confinement and orientation

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Using the $sp^3d^5s^*$-spin-orbit-coupled atomistic tight-binging model and Boltzmann transport we theoretically investigate the effect of bandstructure on the electronic properties of ultra scaled Si nanowires (NWs). We present a comprehensive analysis of NW transport properties considering: i) n- and p-type NWs, ii) [100], [110], and [111] transport orientations, and iii) diameters from D=12nm (electronically almost bulk like) down to D=3nm (ultra scaled). We compute quantities relevant to electronic and thermoelectric transport i.e. the electrical conductivity, low-field mobility, the Seebeck coefficient, and the thermoelectric power factor.

We show that the electronic structure of ultra narrow NWs is sensitive to confinement and orientation. Geometrical factors such as: i) the length scale of the cross section, ii) the transport orientation, and iii) the orientation of the confining surfaces, can act as degrees of freedom in engineering/optimizing the NW properties. For example, we find that in the cases of p-type [111] and [110] oriented NWs, large phonon-limited mobility enhancements (of the order of ~8X) can be achieved as the diameter scales down to D=3nm.