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Atomistic Design of Ultra-Narrow Silicon Nanowires for Improved Electronic and Thermoelectric Applications

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Abstract: Ultra-narrow silicon nanowires (NWs) with diameters from a few to several nanometers have recently attracted significant attention for electronic, optoelectronic, biosensing, thermoelectric devices, and so forth. At these dimensions, the length scale can provide an additional degree of freedom in engineering material properties. The electronic structure becomes geometry dependent, and the confinement length scale, and the transport and confinement orientations can be used to design optimized electronic properties. In this work, we employ atomistic tight-binding bandstructure calculations to calculate the electronic structure of Si NWs from 3nm up to 12nm in diameter. For a comprehensive study, we investigate n-type and p-type NWs, in various transport and confinement crystallographic orientations. We extract the relevant transport quantities such as the effective mass of the bands, the carrier velocity, conductivity, and carrier mobility. We show that these quantities are strongly anisotropic and diameter dependent. Diameter scaling provides larger carrier velocities of the order of ~30% for the n-type [110] NW. More importantly, in the case of p-type [110] and [111] NWs, diameter scaling can provide up to 2X higher carrier velocities, and up to 4X higher mobilities compared to bulk. We provide explanations for this behaviour through features of the bulk bandstructure. Although we consider Si NWs, we believe our results would be broadly applicable for other common semiconductor NWs as well. We further exploit the use of such bandstructure engineering techniques in the design of NWs with improved thermoelectric (TE) performance. This is a topic of high interest, after it was demonstrated that TE performance enhancement up to 100X can be achieved in Si NWs compared to bulk Si. We show that proper electronic structure optimization can also provide an additional factor of 2-3X to the TE performance.