Atomistic Analysis of Thermoelectric Properties of Ultra Narrow Nanowires

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The progress in nanomaterials' synthesis allows the realization of thermoelectric devices based on low dimensional nanostructures. In these confined systems the electrical and thermal conductivity, and the Seebeck coefficient can be designed to some degree independently, providing enhanced ZT values compared to their bulk material's value. We calculate the electrical conductivity, the Seebeck coefficient, and the electronic thermal conductivity of scaled silicon and germanium nanowires using an atomistic $sp^3d^5s^*$-spin-orbit-coupled tight-binding model. This atomistic model accurately captures the electronic structure of the nanowires while being computationally affordable. We examine n-type and p-type nanowires of diameters/thicknesses from D=3nm to 12nm with various aspect ratios, in [100], [110] and [111] transport orientations, at different doping levels and temperatures. Using experimentally measured values for the lattice thermal conductivity, the expected ZT values of the nanowires are calculated.