Low Dimensional Semiconductor Thermoelectric Materials: Design Approaches from Atomistic Calculations for Electrons and Phonons

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Low-dimensional materials such as ultra-narrow nanowires (NWs) and ultra-thin layers (UTLs) have attracted significant attention as efficient thermoelectric materials because of their low thermal conductivity [1, 2]. Such benefits, however, although large, are reaching their limits, since thermal conductivities are already close to the amorphous limit. Further *ZT* improvements could come from the power factor. The initial suggestions, however, that low dimensionality can improve the Seebeck coefficient [3], are not experimentally verified to date. For this, proper modeling tools that account for all important features of the electronic structure of low-dimensional systems are necessary in order to guide designs.

In this work, we employ atomistic calculations using the $sp^3d^5s^*$ tight-binding model and Boltzmann transport theory to investigate the thermoelectric properties of low-dimensional semiconductor materials (1D NWs and 2D UTLs) [4]. For thermal conductivity calculations we employ the atomistic valence-force-field method together with the phonon Boltzmann equation. In this way we calculate the power factor and *ZT* figure of merit from fully atomistic considerations. We address channels of several nanometers in thickness, containing thousands of atoms in the simulation domain. This allows the investigation of the influence of length scale on the thermoelectric coefficients, and provides design strategies for improved performance. We find that: i) Most of the improvement at low dimensionality originates from conductivity improvements, rather than the improvement of the Seebeck coefficient; ii) The sharp features in the density-of-states function, DOS(E), do not necessarily offer an advantage in the Seebeck coefficient; iii) The specific geometry of the confined structure (transport orientation, confinement orientation, confinement length scale) can provide large variations in the power factor and thermal conductivity, which can lead to significant ZT enhancements; iv) The effects of strain and electrostatic gating can alter the bandstructure and scattering mechanisms and provide additional advantages. We finally note that although our investigations consider semiconductor materials such as Si, Ge and SiGe, our main conclusions are generally applicable to other materials as well.

[1] Boukai *et* al., Nature, 451, 168, 2008.
[2] Hochbaum *et* al., Nature, 451, 163, 2008.
[3] Hicks *et* al., PRB, 47, 16631, 1993.
[4] Neophytou et al, PRB, 83, 245305, 2011.