Thermoelectric Properties of Scaled Silicon Nanostructures Using the $sp^3d^5s^*$-SO Atomistic Tight-Binding Model

Neophytos Neophytou and Hans Kosina

Institute for Microelectronics, TU Wien, Gußhausstraße 27-29/E360, A-1040 Wien, Austria

e-mail: {neophytou|kosina}@iue.tuwien.ac.at

The progress in the synthesis of nanomaterials allows the realization of low-dimensional thermoelectric devices based on 1D nanowires (NWs) and 2D superlattices. These confined systems offer the possibility of partially engineering the electronic and phononic dispersions and scattering mechanisms. Thus, 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 [1]. Enhanced performance was recently demonstrated for silicon NWs [2,3], a more common and economically feasible material. Although bulk silicon has a ZT~0.01, the ZT of silicon NWs was experimentally demonstrated to be ZT~1. Understanding the properties of NW demands proper modeling tools supporting material properties and structure parameter optimization in order to achieve the highest possible ZT values.

In this work, we calculate the electrical conductivity, the Seebeck coefficient, and the electronic part of thermal conductivity of scaled silicon NWs using an atomistic $sp^3d^5s^*$-spin-orbit-coupled tight-binding model. This atomistic model provides an accurate estimate of the electronic structure, while being computationally affordable. For a comprehensive study, we examine: i) n-type and p-type NWs, ii) diameters (cylindrical shape) / thicknesses (rectangular shape) from D=3nm to 12nm, iii) various width/height aspect ratios, iv) in [100], [110] and [111] transport orientations, v) different doping levels. The thermoelectric parameters of interest (electrical conductivity, Seebeck coefficient and the electronic part of the thermal conductivity), are calculated within the framework of the linearized Boltzmann transport equation including all relevant scattering mechanisms. A theoretical upper limit is also provided assuming ballistic transport. Finally, using experimentally measured lattice thermal conductivity values, the ZT of the NWs are calculated, and compared to experiments.

[1] Hicks *et* al., PRB, vol. 47, p. 16631, 1993.

[2] Hochbaum *et* al., Nature, vol. 451, p. 163, 2008.

[3] Boukai *et* al., Nature, vol. 451, p.168, 2008.