Thermoelectric Power Factor of Narrow Silicon Nanowires from Atomistic Considerations

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

Silicon nanowires (NWs) of small diameters have attracted significant attention as efficient thermoelectric materials since the work of Hicks and Dresselhaus [1], who pointed out that low dimensionality can be beneficial to the Seebeck coefficient. The recent results of Boukai *et* al. [2], and Hochbaum *et* al. [3] showed that it is indeed possible to achieve ZT~0.5 at room temperature in Si NWs of diameters less than 50nm (compared to bulk Si ZT_{bulk}~0.01). This, however, is mostly a result of significant reduction in the thermal conductivity. To fully understand the properties of NWs and exploit the potential benefits for the power factor as well, proper modeling tools that account for all important low dimensional electronic structure features are necessary.

We calculate the electrical conductivity and Seebeck coefficient of silicon NWs using an atomistic $sp^3d^5s^*$-spin-orbit-coupled tight-binding model coupled to linearized Boltzmann transport. All relevant scattering mechanisms are considered. For a comprehensive study, we examine: i) n-type and p-type NWs, ii) diameters from D=3nm up to 12nm (~5500 atoms in the simulation domain), iii) [100], [110] and [111] transport orientations, iv) different doping levels. We show that improvements to the Seebeck coefficient due to lower dimensionality appear for diameter scales below ~7nm and can reach up to ~70% as the diameter is reduced to 3nm. The influence of feature size reduction, however, appears to affect the conductivity more, which finally determines the power factor. In most cases, enhanced phonon and predominantly surface roughness scattering strongly degrade the conductivity resulting in power factor reduction. We identify subband engineering techniques, however, that improve the conductivity with feature scaling. For some cases this improvement is large enough to over-compensate the detrimental effect of enhanced scattering, and improved power factors with diameter scaling can be achieved.

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

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

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