Thermal Conductivity of Si Nanowires and Ultra Thin-Layers Using Atomistic Phonon Dispersions

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Low dimensional materials allow for a drastic reduction in thermal conductivity due to enhanced phonon-boundary scattering, such that high ZT values are achieved. This was also experimentally demonstrated for traditionally poor thermoelectric materials such as silicon [1,2]. The structure of phonon modes in low dimensional channels and their influence on thermal conductivity, however, is still not well understood. Theoretical investigations on this topic require the consideration of atomistic phonon dispersions (beyond the traditionally employed bulk dispersions). These can provide insight into the nature of low-dimensional thermal transport and guidance for improved thermoelectric efficiency.

We investigate thermal conductivity in low dimensional Si channels (1D nanowires and 2D ultra-thin-layers) of thicknesses from 20nm down to 1nm using the atomistic valence force field model and Boltzmann transport theory [3, 4]. The phonon dispersion in ultra-narrow 1D and 2D structures is significantly different from the bulk dispersion, which leads to different thermal properties. We show that the 1D phonon dispersion yields a finite density-of-states (DOS) value as the frequency goes to zero, instead of zero DOS as in the 3D case. Because of this, traditional bulk-based phonon-phonon scattering models cause divergence in the thermal conductivity and lose their validity. This singularity can be removed by introducing an additional 3-phonon scattering rate [5]. We show that although the thermal conductivity follows the usual decreasing trend with material thickness, once a purely 1D channel (diameter < 5nm) is formed it surprisingly starts to increase [6]. We also show that in the presence of boundary scattering: i) Almost 50% of the heat is carried by phonons with mean-free-paths less than 50nm. ii) Interestingly, the effective specularity parameter is large, p~0.8, indicating that the overall scattering is almost specular in such narrow nanowires. Although our simulations are for Si, we expect that our findings are generally applicable in low-dimensional materials.

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