Calculations of confined phonon spectrum in narrow Si nanowires using the valence force field method

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Low dimensional silicon nanowires (NWs), and silicon based ultra-thin layers have attracted significant attention as efficient thermoelectric materials after it was demonstrated that the thermal conductivity in such materials can be drastically reduced compared to bulk. Values as low as k=2W/mK (compared to k=140W/mK for bulk Si) were achieved [1, 2]. This resulted in ZT values close to ZT~0.5, a large improvement compared to the ZT of bulk Si, ZT_{bulk}~0.01 [1, 2]. The large reduction in the thermal conductivity was attributed to enhanced phonon surface scattering. On the other hand, the role of low dimensionality on the phonon mode structure, and whether phonon confinement could also be responsible for thermal conductivity reduction, has not yet been clarified.

In this work we address the effect of structural confinement on the phonon spectrum of narrow Si NWs using an atomistic valence force field model. The model accurately captures the bulk Si phonon spectrum as well as the effects of confinement [3]. We consider NWs up to 10nm in diameter, and investigate the effects of transport orientation, confinement orientation and confinement length scale on the phonon spectrum. Relevant quantities such as the longitudinal and transverse sound velocities as well as the specific heat are calculated, and compared to the corresponding bulk values. In general, we observe a ~2X reduction in the sound velocities as the NW diameter is reduced, which could partially justify the reduction in the thermal conductivity of confined Si materials. In addition, the density of phonon states at low frequencies increases with reducing diameter, which results in a higher value of specific heat in low dimensional NWs. Our results could provide insight into the nature of phonons at low dimensionality, as well as opportunities to design thermoelectric materials with lower thermal conductivity.

[1] Boukai *et* al., Nature, vol. 451, p.168, 2008.
[2] Hochbaum *et* al., Nature, vol. 451, p. 163, 2008.
[3] A. Paul et al., J. Comput. Elect., vol. 9, p. 160, 2010.