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Atomistic Modeling of the Thermoelectric Properties in Silicon Nanowires ABHIJEET PAUL, GERHARD KLIMECK, Purdue University — The thermoelectric properties of Silicon can be improved due to nano-sized structuring and modulation. The effect of crystal orientation, cross-sectional dimension and source-drain doping on Seebeck coefficient (S) and electronic conductance (σ) in silicon nanowires is studied theoretically in this work. From the electronic structure obtained using an atomistic 10 band $sp^3d^5s^*$ Tight-Binding model with spin orbit coupling, we calculate these parameters using the Landauer formula. Conductivity increases with increasing cross-section size since the number of modes per energy increases. Different orientations show different conductivity. However, Seebeck coefficient is quite independant of the orientation and cross-section size. But, the power factor ($S^2\sigma$), can be improved with size and orientation mainly due to the improvement in conductivity. In these nanowires, phonon scattering at the wire boundary further reduces the lattice thermal conductivity (κ_l) which plays a positive role in improving the thermoelectric figure of merit (ZT) bringing it close to 1 at 300K.

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