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Silicon Nanowire Thermoelectrics: Surface Roughness and Quantum Confinement[1] EDWIN RAMAYYA, JIE CHEN, IRENA KNEZEVIC, Electrical Engineering Dept., University of Wisconsin-Madison — The thermoelectric figure of merit (ZT) of silicon nanowires (SiNWs) can be almost two orders of magnitude higher than that in bulk silicon, holding promise for all-silicon on-chip cooling. However, the physics behind the increase in ZT is not clear. We calculate the ZT using a detailed Monte Carlo technique that accounts for the localization of phonons at the rough boundaries and the 2D confinement of carriers. We show that the ZT enhancement in SiNWs is primarily because of strong phonon-boundary scattering that degrades the lattice thermal conductivity. In extremely small wires, contrary to the conventional belief, decreasing the cross section does not necessarily result in an increase in ZT because of the rapid decrease in electrical conductivity owing to strong electron-surface roughness scattering. Roughness also smears the high peaks in the 1D density of states, negating potential benefits that quantum confinement could have on the Seebeck coefficient. We also calculate the optimal roughness for maximal ZT in wires of different cross sections.

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