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Thermal conductivity of Si nanowires: the impact of the surface BYUNGKYUN KANG, Texas Tech University, STEFAN ESTREICHER TEAM — The thermal conductivity of Si nanowires is calculated from first principles at T=125K using the theoretical "laser-flash" method. The nanowires are represented by the 1-D periodic supercells $Si_{200}X_{32}$ and $si_{296}X_{112}$, where X is H or D or an OH group. The present focus is on the impact of the surface of the nanowire on the thermal conductivity. The bulk phonons cannot "scatter" off the surface of the nanowire as this would require exciting modes with frequencies higher than bulk-mode frequencies, a low probability event. Instead, the high-frequency wag modes of the H surface atoms couple resonantly to each faster than they decay into linear combinations of bulk modes. Thus, the surface reduces the thermal conductivity of the nanowire because heat propagates at the surface much slower than in the bulk.

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