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Anderson Localization of Phonons in Random Multilayer Thin Film Thermoelectrics ANTHONY FRACHIONI, BRUCE WHITE, Binghamton University — Anderson localization of phonons in random multilayer thin films has been explored as a means for reducing latttice thermal conductivity in thermoelectric materials. Silicon based systems have been explored due to silicon's high crust abundance and Seebeck coefficient. Reverse non-equilibrium molecular dynamics simulations have been used to determine the thermal conductivity of silicon in which randomly selected atomic planes (20% of lattice planes) are subject to mass increase. The simulation results indicate that the lattice thermal conductivity of silicon can be decreased by a factor of over ten thousand (to 15 $\mathrm{mW/m \cdot K}$). Based on models in which the charge carrier mean free path is limited by scattering from the planes with mass disorder, the mobility of silicon is expected to reach values of 10 $\mathrm{cm^2/V \cdot s}$. At this mobility the thermoelectric figure of merit, ZT, is found to be greater than ten when the mass ratio of the disordered planes to that of silicon approaches 10. These results indicate that the pursuit of nanostructured silicon thermoelectric materials in the form of random multilayers may provide a path to efficient and sustainable thermoelectric materials.

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