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Lattice thermal conductivity of porous silicon : Molecular dynamics study JOO-HYOUNG LEE, University of California, Berkeley, JEFFREY GROSSMAN, Unversity of California, Berkeley, JOHN REED, ANDREW WILLIAMSON, Lawrence Livermore National Laboratory, GIULIA GALLI, University of California, Davis — Thermoelectric (TE) materials, which are important for power-generation and solid-state refrigeration devices, have received revived interest due to the discovery of a high figure of merit, ZT, in materials with reduced dimensions such as BiTe/SbTe superlattices or BiTe nanocomposites. Recently, nanowires and nano-porous materials have also been considered experimentally as good candidates for increasing ZT beyond 3, considered a minimum for practical applications of TE materials. Although such materials are very promising, it is important to understand the underlying principles of how charge and heat transport occur at the nanoscale in order to predict the dependence of ZT on, e.g., structure, surface chemistry, and defects. In this work, we perform theoretical studies of lattice thermal conductivities, κ_L, of nano-porous silicon with a range of configurations. Specifically, κ_L is calculated using classical molecular dynamics with varying hole diameter, hole-hole distance, and hole passivation chemistry. These results are compared both with bulk calculations as well as the inverted case of nanowires, and κ_L is discussed in terms of specific phonon scattering at surface boundaries.

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