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Minimum thermal conductivity in superlattices: A first-principles formalism[1] JIVTESH GARG, GANG CHEN, Massachusetts Institute of Technology — In certain superlattice systems such as silicon-germanium superlattices a minimum in thermal conductivity with increase in period thickness has been observed. This minimum has been reported at a relatively short superlattice period of a few nanometers and cannot be explained by existing formalisms. An accurate prediction of this minimum thermal conductivity holds importance for thermoelectrics where low thermal conductivity is desired. We develop a first-principles formalism based on use of harmonic and anharmonic force-constants derived from density-functional perturbation theory and single-mode relaxation time approximation to predict the thermal conductivity of superlattices. The phonon relaxation times are computed based on scattering due to both anharmonicity and interface roughness. We show that the formalism leads to an excellent agreement between predicted and measured values and also explains the observed minimum in thermal conductivity.

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