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Prediction of phonon transport properties and thermal conductivities in superlattices by anharmonic lattice dynamics calculations JOSEPH TURNEY, ALAN MCGAUGHEY, Carnegie Mellon University, CRISTINA AMON, University of Toronto — Phonon transport in superlattices is investigated using anharmonic and quasi-harmonic lattice dynamics calculations. Within the lattice dynamics framework, we develop a method for predicting the properties of both coherent and incoherent phonons. The method is implemented for test systems consisting of Stillinger-Weber silicon-germanium superlattices. In these systems the mode dependent frequencies, heat capacities, group velocities, transmission coefficients, and relaxation times of the phonons are computed and used to predict the thermal conductivity. We relate changes in the superlattice structure (e.g., period length and interface roughness) to the predicted phonon properties and, for each structure, identify the phonon modes that dominate thermal transport.

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