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Phonon Scattering by Molecular Dynamics: Temperature Dependence and Effect of Structural Disorder CHRISTOPHER KIMMER, EDMUND WEBB III, Sandia National Laboratories — We use molecular dynamics to simulate individual phonon-grain boundary scattering events in Silicon as a function of temperature and grain-boundary disorder. The temperature dependence of the scattering is investigated by varying the lattice parameter and incident phonon's properties to match the equilibrium bulk crystal's lattice spacing and dispersion relation at the prescribed temperature. For a given twist angle, different grain boundary structures are formed by a simulated growth process wherein cooling from the melt permits different grains to grow towards one another and eventually impinge, resulting in a boundary. The effect of boundary disorder on the reflected and transmitted phonons is then characterized. The temperature dependence incorporated in this manner may be compared with existing scattering models in the continuum limit while the effects of disorder can be used to estimate uncertainties in scattering models for larger–scale methods such as direct-simulation Monte Carlo.

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