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**Molecular Dynamics Study of Heat Transport in Silicon–Germanium Nanoscale Metamaterials** WEINAN CHEN, Materials Science Department, Pennsylvania State University, GERALD MAHAN, VINCENT CRESPI, Department of Physics,Pennsylvania State University, ISMAILA DABO, Materials Science Department, Pennsylvania State University — We have studied the thermal properties of Si–Ge metamaterials with lattice constants of up to tens of nanometers using molecular dynamics simulations and the Green–Kubo method. Validation of this approach is provided by comparing computed thermal conductivities to experimental data for bulk Si–Ge alloy systems. Close agreement with experiment in a large temperature range is found when isotopic effects are taken into account and interatomic potentials are directly parameterized against higher-level semilocal density-functional theory calculations. These simulations highlight the importance of surface morphology, isotopic substitution, alloy fraction, and superlattice periodicity in determining the thermal properties of these metamaterials, suggesting design strategies to control heat transport in nanostructures.

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