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Thermal conductivity of "nanoparticle in alloy" materials from a first principles approach[1] DAVID BROIDO, Boston College, NATALIO MINGO, CEA Grenoble and UC Santa Cruz, DEREK STEWART, Cornell Nanoscale Facility, Cornell University — It has been demonstrated that nanoparticles embedded in alloys can produce large reductions in lattice thermal conductivity with corresponding increases in the thermoelectric figure of merit [1,2]. Here we present an *ab initio* approach to calculate the lattice thermal conductivity of an SiGe alloy host containing embedded nanoparticles. This approach is based on density functional perturbation theory and employs a virtual crystal approximation for the alloy and a relaxation time approximation for anharmonic, alloy disorder, and nanoparticle scattering. We apply the method to nanoparticles with a range of different chemical compositions, concentrations and sizes embedded in the SiGe alloy. We compare our first principles based results to those from previous calculations [2] based on the debye approximation.

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