Abstract Submitted
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Thermal conductivity of nano-structured materials CHANDAN BERA, Department of Atomistic Modelling and Simulation, ICAMS, Ruhr-Universität Bochum, Germany, LASSE BJERG, Center for Materials Crystallography, Department of Chemistry & iNANO, Aarhus University, Denmark, ANKITA KATRE, GEORG K.H. MADSEN, Department of Atomistic Modelling and Simulation, ICAMS, Ruhr-Universität Bochum, Germany — Manipulating the thermal properties of materials by nano-structuring is new successful route to improve the performance of thermoelectric materials. We present a new parameter free model to predict anharmonic scattering in bulk and nanoscale materials. Velocities and anharmonic scattering rates are calculated from the Grüneisen parameter of the full phonon dispersions and used to calculate the lattice thermal conductivity using the phonon Boltzmann transport equation in the relaxation time approximation. We find good agreement with experiments for a range of materials. Furthermore, we show that our model, as opposed to simple models based on only the acoustic bands, finds the correct trend in the thermal conductivity of Mg2Si, Mg2Ge and Mg2Sn. We also examine thermal transport in more complex materials like Type-I Si clathrates and zinc-antimonides. Finally, discuss how nano-structure and disorder effect the thermal conductivity.

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