Analyzing the Effect of Nanoparticles on Lattice Thermal Transport for Improved Thermoelectric Performance

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Effectiveness of radioisotope thermoelectric generators (RTGs), devices which use thermoelectric (TE) materials to convert heat from a decaying radioactive isotope into electrical power, is challenged by poor energy conversion efficiencies of current TE materials. TE performance is directly proportional to electrical conductivity (σ) and inversely proportional to thermal conductivity (κ). Heat conduction in a material is due to electron transport and lattice vibrations (collective motions of the atoms in a crystal). Since electron transport is vital to a high σ, researchers focus on reducing the contribution of the lattice vibrations also known as phonons to thermal transport (κ_L). We present our current work on κ_L reduction via nanoparticles (NPs) embedded in a host crystal. Our specific objective is to determine an optimal size distribution of NPs that best minimizes κ_L. This research is motivated by complexity of phonon transport as there is great variance in mean free path, frequency, and lifetime among phonons; suggesting there is no single NP size that would best attenuate all phonon contributions of which lattice dynamics calculations demonstrate is non-uniform. We conduct three different types of molecular dynamics simulations: phonon wave-packet, single-NP thermal conductance (G), and multiple-NP κ_L calculations to obtain a holistic view of how NPs affect lattice thermal transport. Wave-packet and single-NP G simulations analyze how a single phonon mode and collective phonon transport is affected by a single NP, respectively. Multiple-NP κ_L simulations mimic thermal transport in a realistic device where effects such as phonon localization and dependent scattering take place due to many NPs. We detail our preliminary results from these simulations and describe how our results guide us to design an optimally efficient TE material that may enhance performance of RTGs in future NASA applications.