Atomistic Investigation of Phonon Wave Transport Through Embedded Nanoparticles

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Many NASA applications, such as space probes and rovers, use radioactive thermo-electric generators (RTG) as a power-source. RTGs work by implementing a thermo-electric material (TEM) to convert heat from a decaying radioactive isotope into electrical power. As current TEMs are challenged by poor energy conversion efficiencies, it is of increasing interest to discover material design structures that are more performant. Such efforts require an improved understanding of the thermal physics in solids so that optimal material designs may be identified. Crystals containing embedded nanoparticles (NP), nanometer sized dopant particulates embedded within the host lattice, are promising low cost, but high efficiency TEMs. There is currently a minimal understanding of how phonons, the primary heat carriers in non-metallic materials, interact with NPs. A better understanding of phonon-NP scattering may lead to design of improved NP-laden TEMs, which when integrated into RTGs, could expand the operational capabilities of NASA missions. We present our current work on understanding the fundamental physics of phonon wave scattering by spherical NPs. The molecular dynamics-based wave-packet method is rigorously applied to study mode-resolved phonon-NP interactions. We also conduct comparative analyses of phonon scattering by a thin slab (TS) (a junction of two planar heterogeneous interfaces whereas the NP is non-planar) with the same size as the NP in order to investigate the effect of interfacial geometry on phonon scattering. The phonon-NP scattering behavior expectedly varies with NP size. However, scattering by the TS and NP is observed to deviate as the scatterer size is increased, contradicting existing continuum theories. The characteristics of phonon-NP scattering are taken to be the result of an unreported phonon lensing effect, where refraction of the phonon wave at the non-planar interfaces of the NP induces non-trivial wave dynamics inside the NP. We quantify and discuss these novel phonon wave behaviors.