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

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Introduction

- Radioisotope thermoelectric generators (RTGs), devices that use thermoelectric (TE) materials to convert heat from a decaying radioactive isotope into electricity, are effective power sources for space probes and rovers.
- However, RTG capabilities are challenged by poor energy conversion efficiencies of current TE materials, motivating a great research effort to improve TE performance.

TE Figure-of-merit

$$zT = \frac{S^2\sigma}{\kappa_e + \kappa_L}T$$

- σ = electrical conductivity
- κ = thermal conductivity contributed to by electron & lattice vibrations

Figure 1: *Diagram of Multi-Mission RTG*

- Due to direct proportionality to σ, thus electron transport, researchers desire reducing the contribution of the collective lattice vibrations termed “phonons” to the thermal conductivity κ_L as an approach to raise zT.
- We present our current research on κ_L reduction by embedded nanoparticles in a host crystal, evaluated by several molecular dynamics (MD) simulations.

Research Objectives

- NPs have been shown to reduce κ_L in materials, however, minimal research has been made to determine the optimal size distribution of NPs to best minimize κ_L.
- This problem is motivated by the complexity of phonon heat conduction as there is great variance in mean free path, frequency, and lifetime among phonons, suggesting no single NP size would best attenuate all phonon contributions.
- Our objective is to analyze how NPs affect phonon thermal transport so that we may determine an optimal size distribution and understand why such distribution best minimizes κ_L.

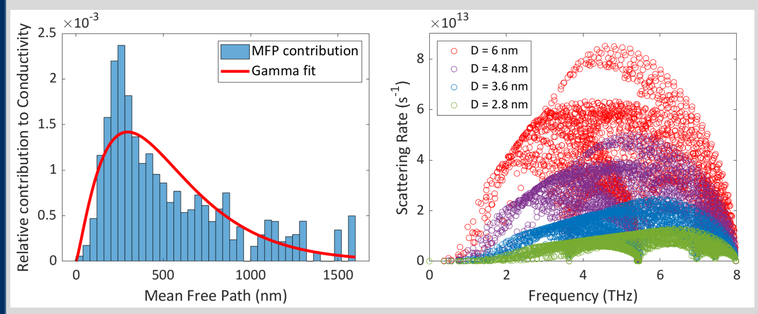

Figure 2: *Distribution of the relative contributions to κ_L per phonon mean free path in Lennard-Jones Argon.*

Figure 3: *Computed scattering rate from widely-used literature model for each phonon mode at different NP sizes in 1% doped Lennard-Jones Argon.*

Molecular Dynamics Simulations

- MD simulations simulate atomic motion according to classical mechanics equations. In this research, we conduct 3 different types of MD simulations of varying orders of complexity for our analyses.

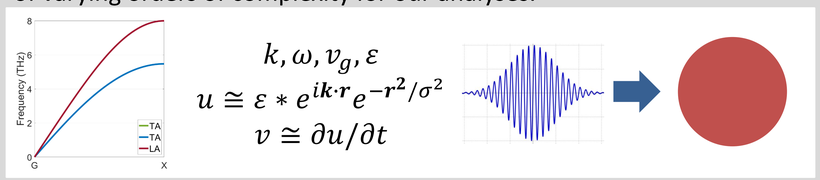

Figure 4: *Single-NP Phonon Wave-Packet Simulation.*

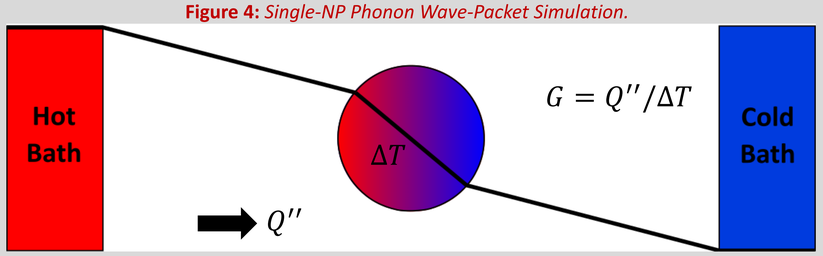

Figure 5: *Single-NP Thermal Conductance G Simulation.*

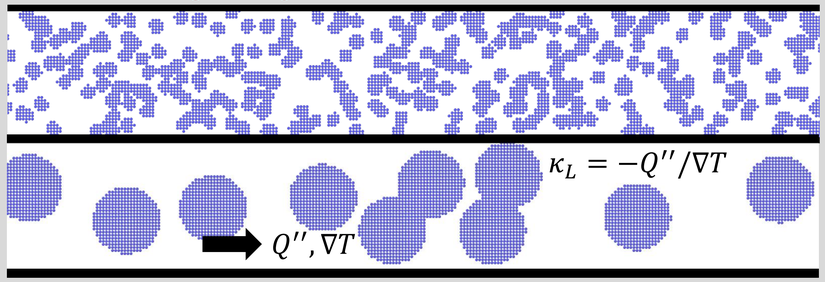

Figure 6: *Multiple-NP κ_L Simulation Structures (NP spheres do not overlap).*

- Phonon wave-packet simulation is used to analyze how a single phonon mode is reflected and transmitted through a NP.
- Single-NP G and multiple-NP κ_L simulations study how a single vs. many NPs influences thermal transport; essentially analyzing the effect of NPs on collective phonon propagation.

Preliminary Results

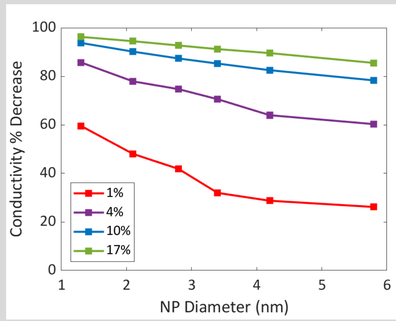

Figure 7: *Percent Decrease in κ_L from pure material by fixed concentration of nanoparticles of a single size.*

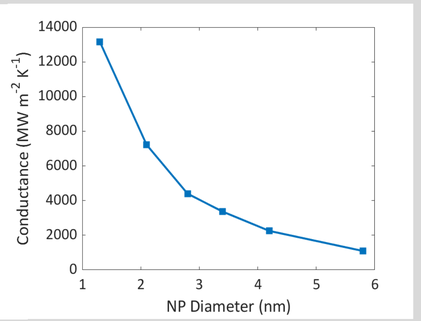

Figure 8: *G values from Single NP Thermal Conductance Simulations.*

Conclusions

- Phonon wave-packet, single-NP thermal conductance G, and multiple-NP thermal conductivity κ_L molecular dynamics simulations together provide a holistic understanding of how nanoparticles affect phonon heat conduction.
- We found in multiple-NP simulations with fixed dopant concentration, structures with smaller NP sizes (thus larger count) exhibit lower κ_L than larger sizes. Probable reasons are phonon localization and strong dependent phonon scattering between NPs which suppresses incoherent phonon transport.
- Lowest κ_L was achieved at the random alloy limit. Further research will be done to investigate whether an optimized NP size distribution can break this limit as superlattices have.
- These preliminary κ_L results and observed power-law decrease in G with increasing NP size suggest a size distribution to best minimize κ_L may skew significantly to smaller sizes while containing several large NPs for maximal phonon impedance.
- A TE material with such NP size distribution may yield improved energy conversion efficiency and enhance the performance of RTGs, providing new capabilities for future NASA space applications.

Acknowledgements

- This material is based upon work supported in part by the National Aeronautics and Space Administration under Cooperative Agreement No. NNX15AK48A. We also acknowledge the financial support of the U.S. Nuclear Regulatory Commission.

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