Simulations and Machine Learning of Energy Transport

OBJECTIVES

Achieving high ZT by reduced thermal conductivity

- Dimensionality and surface conditions of nanostructures are expected to have impact on the thermal transport

Synthesis of nanocrystals

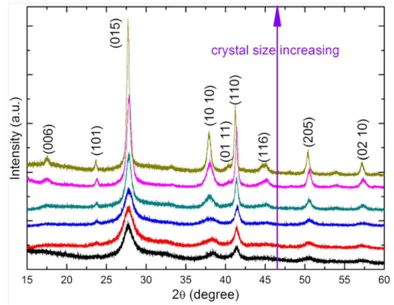
- Synthesize nanocrystals that can be hot-pressed into nanocomposites with good thermoelectric performance.

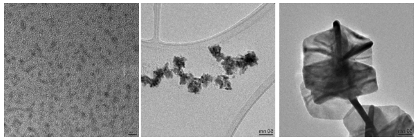
METHODS

Reduction of lattice thermal conductivity by nanostructuring

- Classical potential development and atomistic simulation of thermal transport in various nanostructures with representative structural features.
- Synthesize nanocrystals from various precursors. Use either Spark Plasma Sintering (SPS) or mechanical hot-pressing to achieve dense nanocomposites.

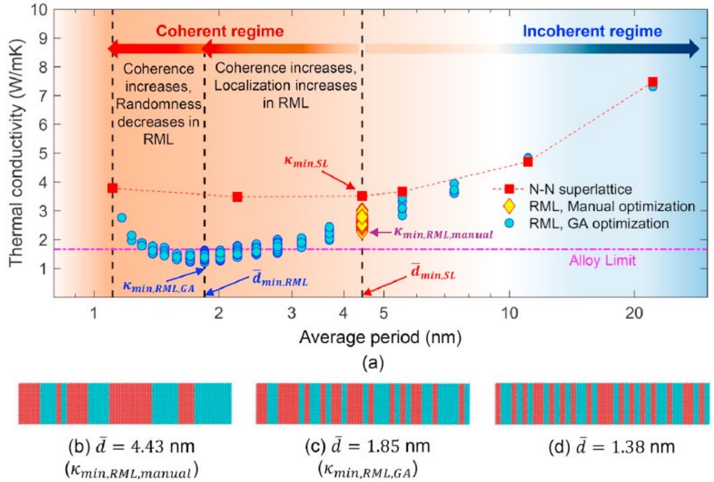
KEY RESULTS AND FINDINGS:





Left: XRD spectra showing phase identification and size evolution. Top: synthesized Bi_2Te_3-based nanocrystals showing various shapes and sizes.

- Solution-based growth of Bi_2Te_3 nanocrystals • Control of synthesis conditions to yield Bi_2Te_3 nanocrystals of desired types • Development of classical interatomic potentials for Bi_2Te_3 • Atomistic simulations of Bi_2Te_3 bulk, nanowires, stacked thin-films and nanoporous films, revealing the capability of thermal conductivity reduction due to different nanogeometrical factors.



Machine leanring-enabled design and optimization of superlattices. We show that manual search only optimizes to a local minimum of the thermal conductivity, while machine learning can accomplish the global minimum of the thermal conductivity.

QUANTITATIVE IMPACT

Impact

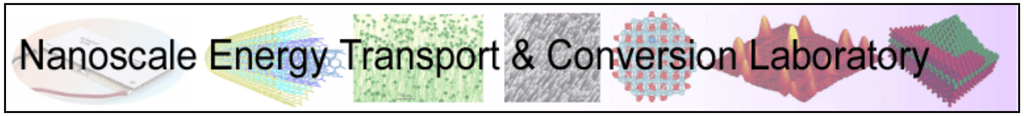
- The first two-body classical potential for Bi_2Te_3, enabling efficient atomistic simulations
- The first systematic study of thermal transport in Bi_2Te_3-based bulk and nanostructures.
- Synthesis of extremely small Bi_2Te_3 nanocrystals with sizes down to 4 nm.

Applications

- Shape and quality control of the growth of bismuth telluride nanocrystals
- Machine learning-enabled design and optimization of nanomaterials.
- Thermal barrier coatings for turbomachinary

Selected Publications:

- Luo, Yang, Feng, Wang, and Ruan, *Nat. Commun.* (2020).
- Chowdhury, Reynolds, Garrett, Feng, Adiga, and Ruan, *Nano Energy* 69, 104428 (2020).
- Feng, Yao, Wang, Shi, Li, Cao, and Ruan, *Phys. Rev. B* **95**, 195202 (2017).



PURDUE ENGINEERING Think impact.