# Reduction of Thermal Conductivity and Enhancement of Efficiency in Nanostructured Thermoelectric Materials

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## OBJECTIVES

### Nanostructural Effects on Thermal Conductivity

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

### Synthesis of Bismuth Telluride Nanocrystals

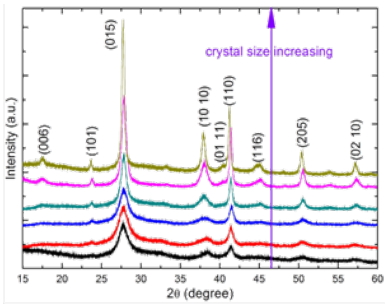
- Synthesize $Bi_2Te_3$-based nanocrystals that can be hot-pressed into nanocomposites with good thermoelectric performance.

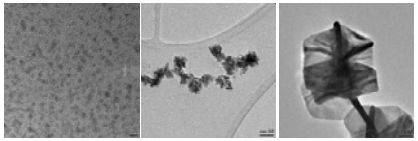
## METHODS

### Reduction of Lattice Thermal Conductivity by Nanostructuring

- Classical potential development and atomistic simulation of thermal transport in various $Bi_2Te_3$-based nanostructures with representative structural features.
- Synthesize $Bi_2Te_3$-based nanocrystals from various precursors. Use either Spark Plasma Sintering (SPS) or mechanical hot-pressing to achieve dense nanocomposites.

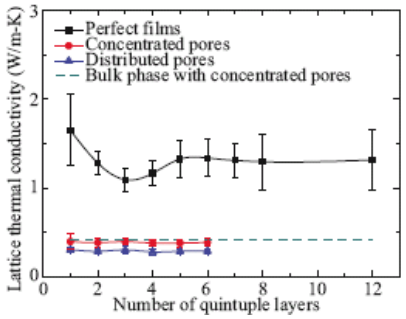
## KEY RESULTS AND FINDINGS:



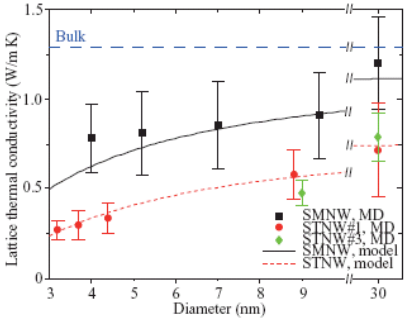



Left: XRD spectra showing phase identification and size evolution. Top: synthesized $Bi_2Te_3$-based nanocrystals showing various shapes and sizes.

• 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.




Molecular dynamics (MD) simulations of stacked and nanoporous $Bi_2Te_3$ thin-films. Novel dimensional crossover depending on number of layers was found.




MD simulations of $Bi_2Te_3$ nanowires with different diameters and surface conditions. Rough and thin nanowires were found to effectively reduce 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
- Suggested possible design of nanostructured bismuth telluride with low thermal conductivity

### Selected Publications:


- Bo Qiu , Lin Sun and Xiulin Ruan, *Phys. Rev. B* **83**, 035312 (2011).
- Bo Qiu and Xiulin Ruan, *Appl. Phys. Lett.* **97**, 183107 (2010).
- Bo Qiu and Xiulin Ruan, *Phys. Rev. B* **80**, 165203 (2009)