# Enhancing Thermoelectric Performance of Half-Heusler Compounds via Nanostructuring Approaches

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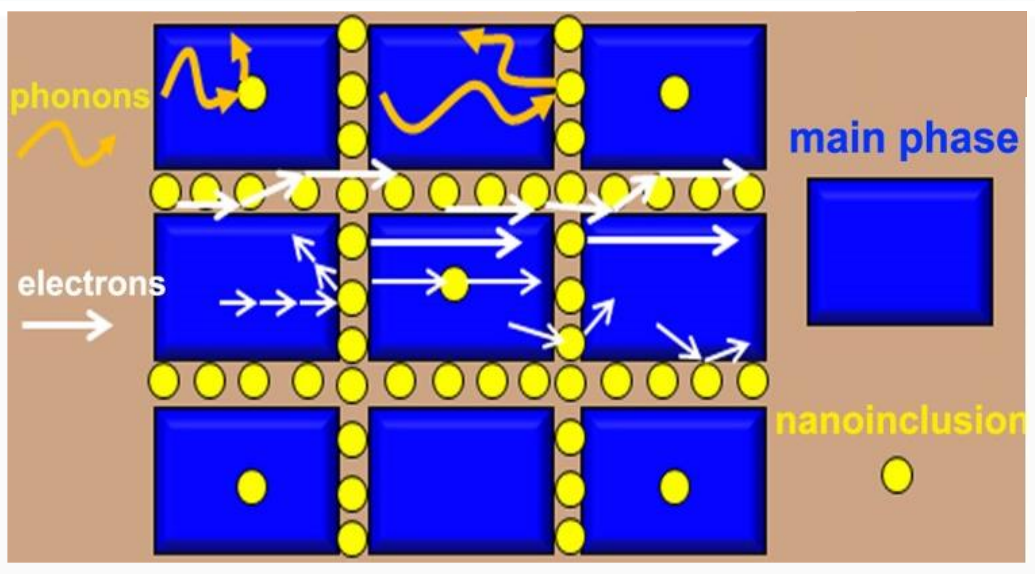
## Introduction

Half-Heusler compounds have attracted considerable interest as promising thermoelectric (TE) materials in the temperature range around 700 K and above, which is close to the temperature range of most industrial waste heat sources. In this poster, we summarize our recent progress in improving the thermoelectric performance of half-Heusler compounds via nanostructuring approaches. We successfully utilized nanostructuring approaches to decouple thermal and electrical transport properties in half-Heusler compounds. By controlling the *in-situ* formation of InSb [1-2], MnSb [3] and full-Heusler nanoinclusions [4] in the half-Heusler matrix, it was shown experimentally that the Seebeck coefficient ($\alpha$), electrical conductivity ($\sigma$) and thermal conductivity ($\kappa$) can be independently manipulated in a manner that significantly enhances the figure of merit ($ZT$) of these materials.

## Graphical Abstract

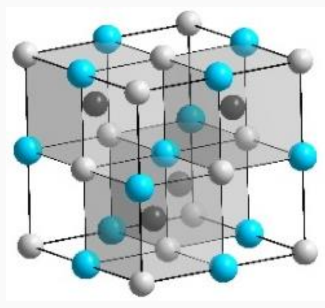



**The roles of nanoinclusions (NI)**

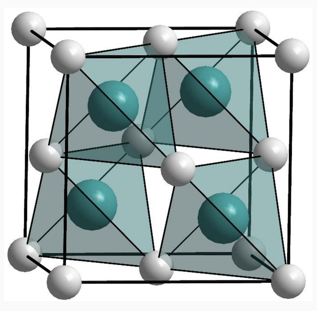
1) **Electron filtering effect** → $\alpha\uparrow$
2) **Electron injection effect** → $\sigma\uparrow$
3) **Boundary scattering of phonons** → $\kappa\downarrow$

The *in-situ* formed nanoinclusions in half-Heusler compounds can induce combined *high mobility electron injection* (thick long arrow), *low energy electron filtering* (narrow short arrow), *and boundary scattering* (wavy arrow) effects, and lead to a simultaneous improvement of all three individual thermoelectric properties of half-Heusler nanocomposites.

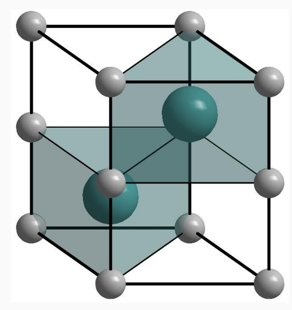
## Building Blocks



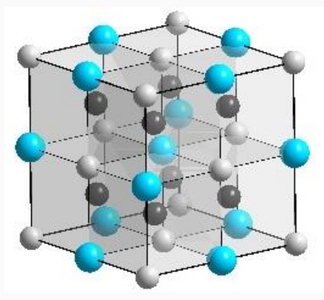
**half-Heusler**



**InSb (NI)**

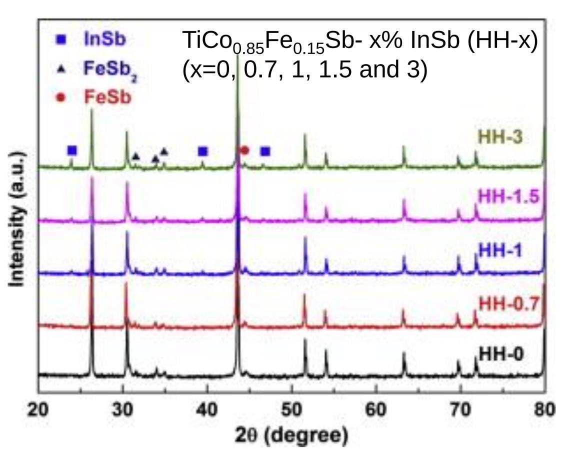


**MnSb (NI)**

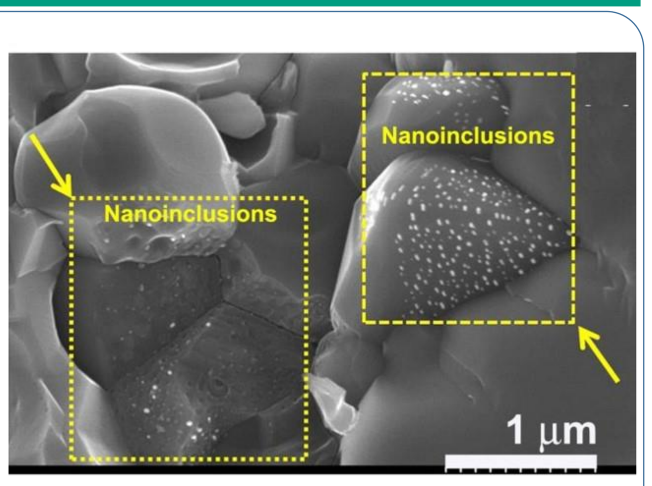


**full-Heusler (NI)**

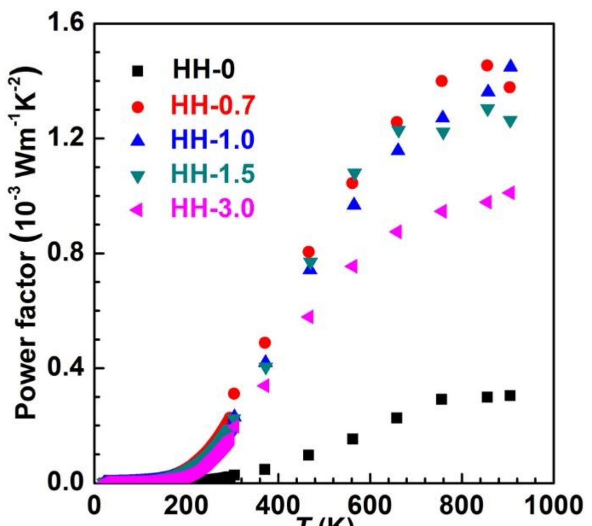
## $TiCo_{0.85}Fe_{0.15}Sb$-InSb



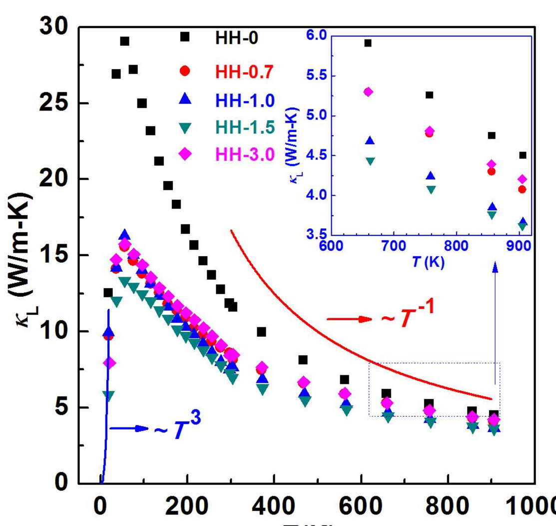

XRD of TiCoSb-x%InSb



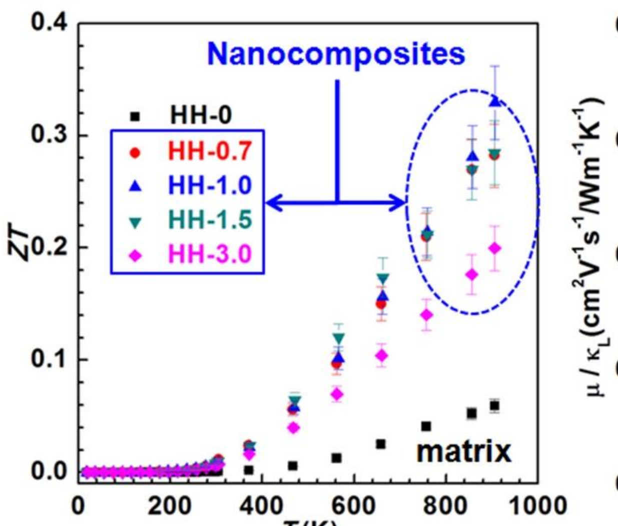

SEM of TiCoSb-3%InSb



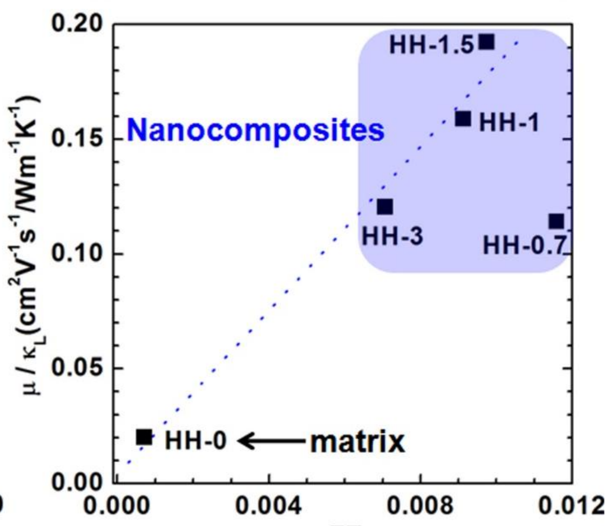

Power factor (*PF*)




Lattice thermal conductivity




*ZT* values

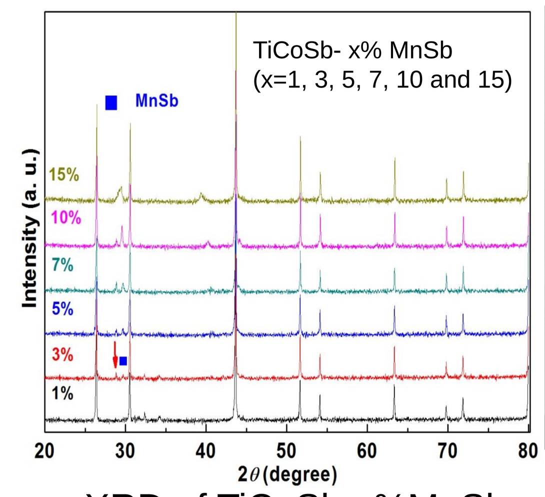



*ZT* dependence of $\mu/\kappa_L$

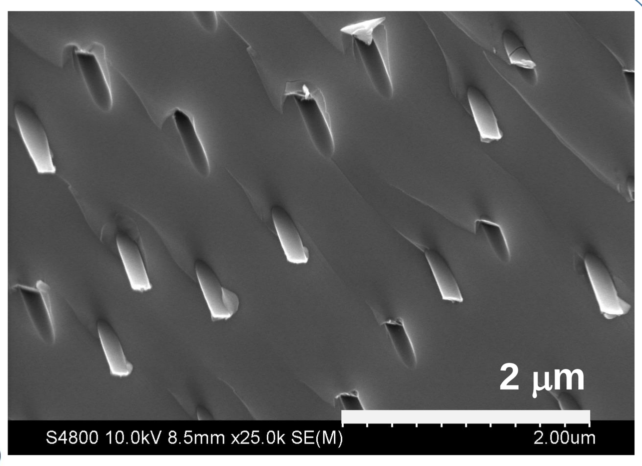
**Checklist:**

1) **Electron filtering effect** → $\alpha\uparrow$ ✓
2) **Electron injection effect** → $\sigma\uparrow$ ✓
3) **Boundary scattering of phonons** → $\kappa\downarrow$ ✓

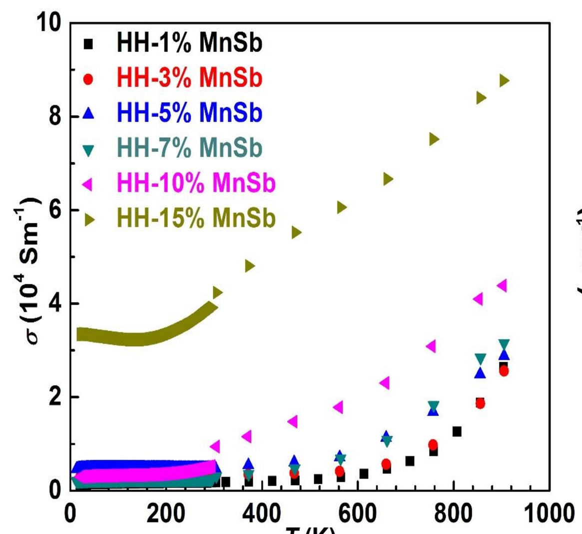
## TiCoSb-MnSb



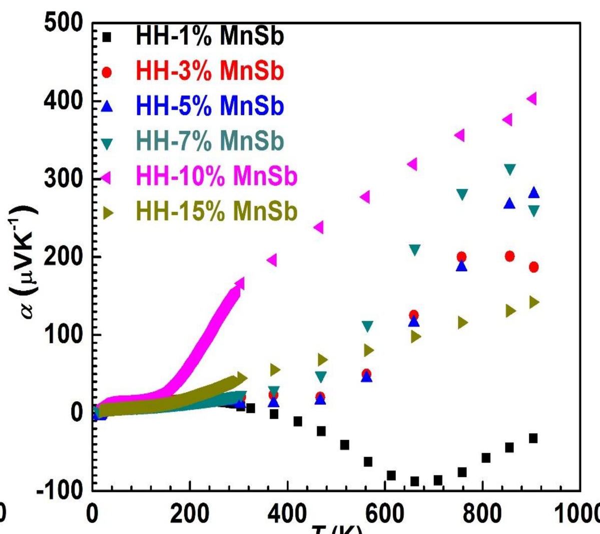

XRD of TiCoSb-x%MnSb



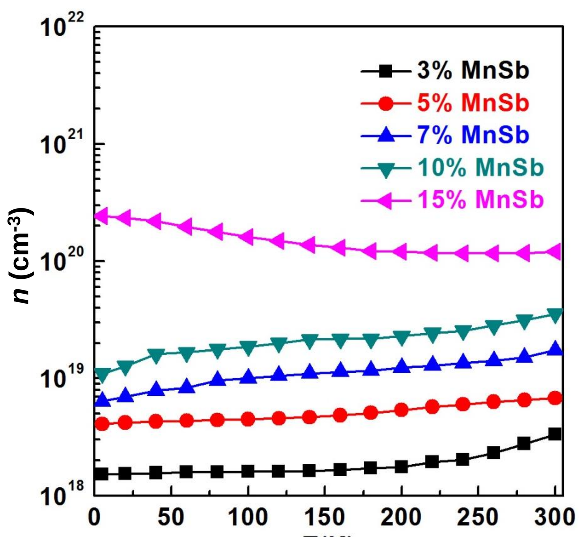

SEM of TiCoSb-7%MnSb



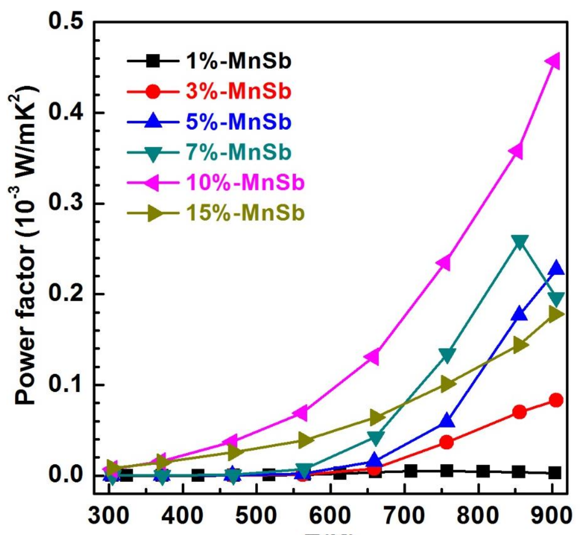

Electrical conductivity




Seebeck coefficient




Carrier concentration

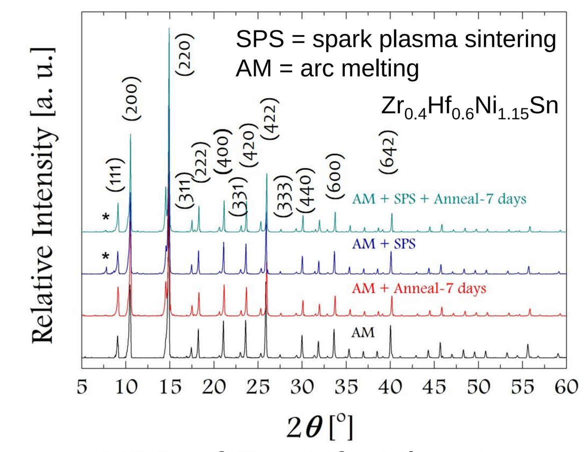



Power factor (*PF*)

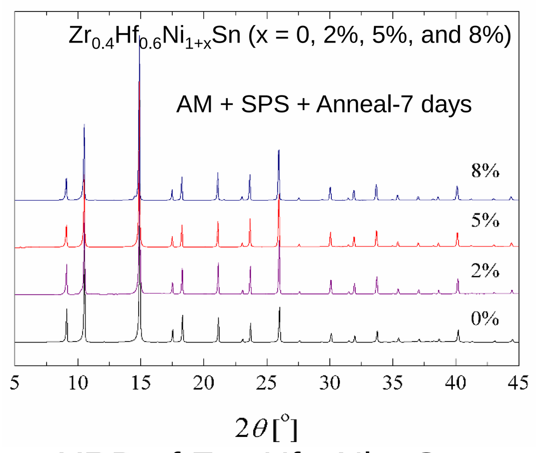
**Checklist:**

1) **Electron filtering effect** → $\alpha\uparrow$ ✓
2) **Electron injection effect** → $\sigma\uparrow$ ✓
3) **Boundary scattering of phonons** → $\kappa\downarrow$ ✓

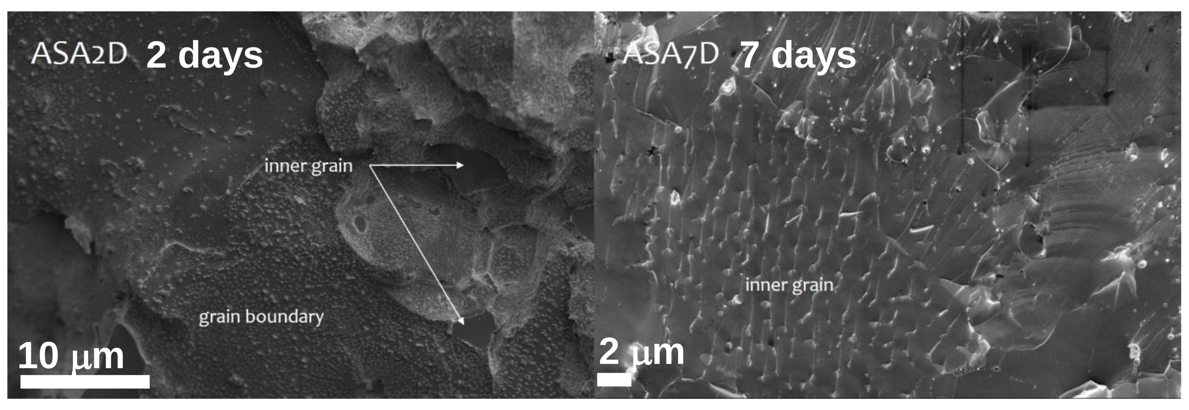
## $Zr_{0.4}Hf_{0.6}Ni_{1+x}Sn$



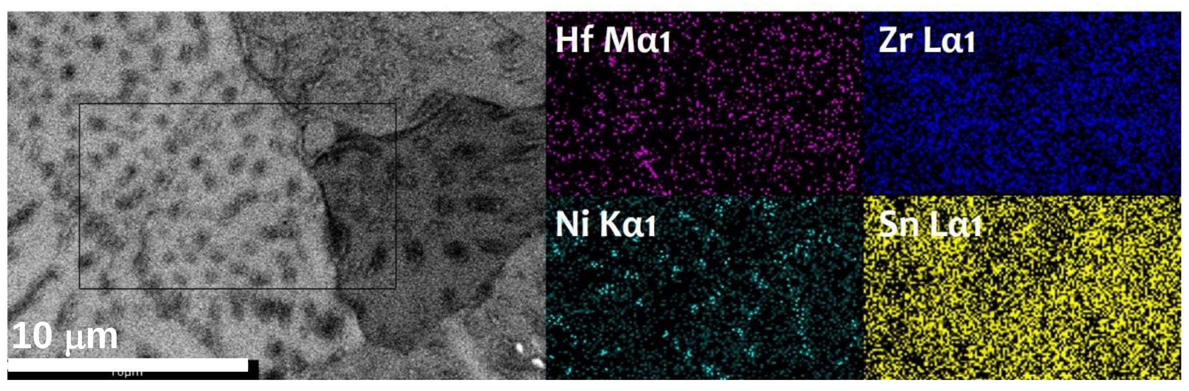

XRD of $Zr_{0.4}Hf_{0.6}Ni_{1.15}Sn$



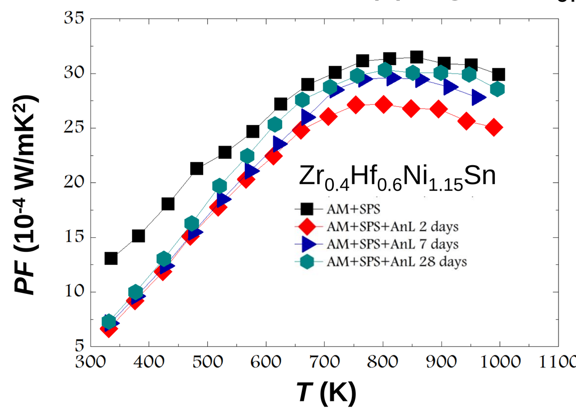

XRD of $Zr_{0.4}Hf_{0.6}Ni_{1+x}Sn$



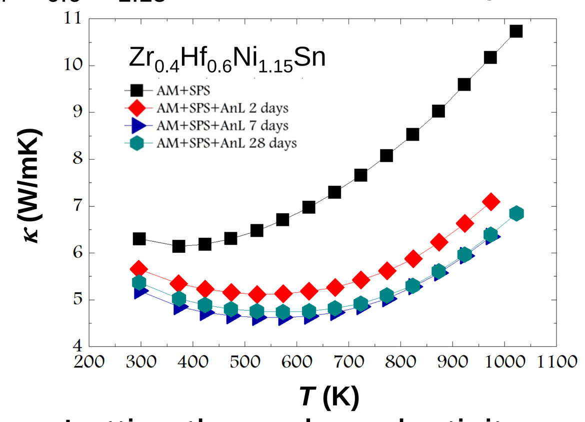

SEM images of $Zr_{0.4}Hf_{0.6}Ni_{1.15}Sn$ annealed 2 days and 7 days




SEM and EDS mapping of $Zr_{0.4}Hf_{0.6}Ni_{1.15}Sn$ annealed 28 days




Power factor (*PF*)




Lattice thermal conductivity

**Checklist:**

1) **Electron filtering effect** → $\alpha\uparrow$ ✗
2) **Electron injection effect** → $\sigma\uparrow$ ✗
3) **Boundary scattering of phonons** → $\kappa\downarrow$ ✓

## References

1. W. J. Xie, Y. G. Yan, S. Zhu, M. H. Zhou, S. Populoh, K. Gałązka, S. J. Poon, A. Weidenkaff, J. He, X. F. Tang, T. M. Tritt, Acta Materialia **61**, 2087–2094 (2013).
2. W. J. Xie, J. He, S. Zhu, X. L. Su, S. Y. Wang, T. Holgate, J. W. Hubbard, V. Ponnambalam, S. J. Poon, X. F. Tang, Q. J. Zhang, T. M. Tritt, Acta Materialia, **58**, 4705–4713 (2010).
3. W. J. Xie, T. M. Tritt, A. Weidenkaff, in preparation.
4. W. J. Xie, J. Feng, T. H. Zou, X. X. Xiao, M. Widenmeyer, A. Weidenkaff, in preparation.

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MARIE CURIE ACTIONS