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Northwestern University Materials Research Center

mrc@northwestern.edu

847-491-3606

Effect of Grain Boundary Phases in the Thermoelectric Properties of Half Heusler Materials

Many thermoelectric materials benefit from complex microstructures. Grain boundaries cause desirable reduction in the thermal conductivity by scattering phonons, but often lead to unwanted loss in the electrical conductivity by scattering charge carriers. In this talk, grain boundary engineering is explored to suppress the grain boundary electrical resistivity^[1] or to increase the overall conductivity^[2]. The characteristics of grain boundary segregations and grain boundary phases are revealed in Fe-doped TiCoSb and Ti-doped NbFeSb half-Heusler materials respectively using a combination of scanning transmission electron microscopy and atom probe tomography. On one hand, chemical segregation in TiCoSb is correlated with electrically conductive grain boundaries. On the other hand, hexagonal close-packed grain boundary phases are found in NbFeSb and correlated to their electrical behaviour transitioning from resistive to non-resistive by increasing the doping content. Such grain boundary segregations and grain boundary phase transitions open a new design space to decouple the intertwined electronic and phononic transport in thermoelectric materials and thus improve efficiency.

[1] R. Bueno Villoro, D. Zavanelli, C. Jung, D. A. Mattlat, R. Hatami Naderloo, N. Pérez Rodríguez, K. Nielsch, G. J. Snyder, C. Scheu, R. He, S. Zhang, *Advanced Energy Materials* **2023**, 2204321, DOI 10.1002/aenm.202204321.

[2] R. Bueno Villoro, M. Wood, T. Luo, H. Bishara, L. Abdellaoui, D. Zavanelli, B. Gault, G. J. Snyder, C. Scheu, S. Zhang, *Acta Materialia* **2023**, 118816, DOI 10.1016/j.actamat.2023.118816.



Ruben Bueno Villoro
Max Planck Institute
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