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Engineering Thermal and Electrical Interfaces and Grain Boundaries in Thermoelectric Materials

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Abstract

To devise strategies for improving the thermoelectric performance of materials, it is essential to understand the coupled charge and thermal transport mechanisms. In heavily doped semiconductors, we often expect ionised impurity scattering to dominate electrical transport, especially when mobility increases with temperature. However, the inadequacy of this description in thermoelectric materials, such as the new high-performance n-type Mg_3Sb_2, becomes apparent when trying to consistently explain various experimental observations, such as enhanced mobilities in larger grain samples and sharp crossovers to metal-like mobilities which decrease with temperature. The underlying cause of such complications is largely associated with the conventional Mathiessen’s Rule which interprets or models all charge carrier scattering as homogeneous events. The inhomogeneous nature of materials caused by grain boundaries must be taken into account to rethink engineering strategies to further improve thermoelectric materials.

Prevailing models for thermal transport treat interfaces and grain boundaries as structure-less, even though at the atomic scale, they are better described as arrays of various types of linear defects. Allowing for this inherent structure, several fundamental characteristics of heat transport arise, such as diffraction conditions when heat carrying phonons scatter off the periodic, linear defect arrays present in grain boundaries. Furthermore, a dimensionality crossover is observed in diffusive heat transport, where phonons with a wavelength longer than the linear defect spacing see the interface simply as a structure-less planar defect.

Biography

Dr G. Jeffrey Snyder is a Professor of Materials Science and Engineering at Northwestern University. His interests are focused on materials physics and chemistry of thermoelectric materials, which include band engineering, design of complex Zintl compounds and use of nanostructured composites. His interdisciplinary approach stems from studies of solid state chemistry at Cornell University and the Max Planck Institute for Solid State Research, applied physics at Stanford University and thermoelectric materials and device engineering at NASA/Jet Propulsion Laboratory and the California Institute of Technology.

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