MAR13-2012-020020

Abstract for an Invited Paper
for the MAR13 Meeting of
the American Physical Society

Anharmonicity and its application in earth abundant thermoelectrics

DONALD MORELLI, Michigan State University

Recently very exciting improvements in the thermoelectric figure of merit have been reported in bulk nanostructured chalcogenides, mostly due to lattice thermal conductivity suppression by nanoscale-level interfaces. A critical issue in these types of structures is maintaining good electrical conductivity while blocking phonon transport. While so-called "endotaxial" nanostructuring, for example, can substantially maintain electron transport across interfaces, generally nanocomposite structures display reduced electrical conductivity which can counteract or in some cases overwhelm the improvements in figure of merit due to thermal conductivity reduction. Additionally, the thermal stability of nanostructured materials at operating temperatures at a significant fraction of the melting point is a concern. Here we describe another approach to reducing lattice thermal conductivity based on designing materials with large lattice anharmonicity. Anharmonic phonon vibrations are the source of intrinsic thermal resistivity in solids and manifest themselves in large Grüneisen parameters. We show that one class of compounds, those containing antimony atoms with a lone pair configuration, exhibits a strongly anharmonic phonon spectrum that leads to intrinsically small lattice thermal conductivity. We have applied this concept to ternary copper-antimony-chalcogenide semiconductors and find that the family of compounds based on the tetrahedrite crystal structure can exhibit thermoelectric figure of merit rivaling that of conventional materials like PbTe. The tetrahedrite family is the most widespread sulfosalt mineral on Earth and we show that the mineral itself can be used directly as a source material for earth abundant thermoelectrics. This may pave the way for many new, low cost applications of thermoelectrics in waste heat recovery and power generation.