

Center for Revolutionary Materials for Solid State Energy Conversion (RMSSEC)
EFRC Director: Donald T. Morelli
Lead Institution: Michigan State University

Mission Statement: *To investigate the underlying physical and chemical principles of advanced materials for the conversion of heat into electricity.*

The *Center for Revolutionary Materials for Solid State Energy Conversion* will focus on solid state conversion of thermal energy to useful electrical power, both to increase the efficiency of traditional industrial energy processes and to tap new unused sources of energy such as solar thermal. Additionally materials with enhanced thermoelectric properties will find application in high efficiency, environmentally benign climate control systems. Our team represents some of the most experienced and capable researchers spanning all aspects of thermoelectric science from the design, synthesis and characterization of materials through the development of thermoelectric devices and systems. We will undertake a broad-based effort in semiconductor energy conversion materials utilizing and combining experimental, theoretical, and computational efforts. While ultimately the solution to the energy challenge is a technological one, beginning to solve this problem will take a serious effort at understanding physical processes at an elemental level. Our focus, therefore, will be on the fundamental aspects of thermoelectricity, which have their origin in physical processes occurring on the atomic scale. A major focus of our effort will be in the synthesis of new forms of matter, including both single phase alloys and compounds and composite structures created using nanoscience.

In order to meet the overall objective and mission of our Center, we have chosen to attack this problem from several different perspectives in terms of materials and fundamental processes. However these approaches share two common guiding principles and unifying objectives:

- i. meet the challenge of lowering the thermal conductivity of thermoelectric materials to a minimum possible value;
- ii. target the much more difficult task of increasing the thermoelectric power factor by manipulation of the electronic density of states of materials systems.

Ultimately, by working together in this Center we aim to develop design rules to predict properties of advanced thermoelectric materials, and realize these structures through innovative synthesis and advanced structural as well as chemical characterization.

We have organized our EFRC to have six main thrusts. The first four thrusts are directed at four broad categories of materials. In addition to these materials thrusts, our Center will recognize the importance of the characterization of the physical properties of new thermoelectric materials. Further, while the research is fundamental in nature, our aim is ultimately to develop new thermoelectric materials for use in devices with high conversion efficiency for power generation spanning the temperature range 0 - 700°C. Such thermoelectric materials and the devices and systems built up from them are expected to have myriad applications, including, for instance, auxiliary generators, waste heat recovery systems for vehicles, and solar thermal energy conversion systems. For these reasons, we also include effort aimed at understanding fundamental scientific issues related to thermoelectric devices and systems.

The six main thrusts of the Center are:

- I. cubic nanostructured chalcogenides
- II. self-assembled nanostructures
- III. transition metal alloys with gaps and wells in the electron density of states
- IV. anharmonic solids with low intrinsic thermal conductivity
- V. thermoelectric and mechanical characterization of new thermoelectric materials
- VI. fundamental scientific issues related to thermoelectric devices and systems

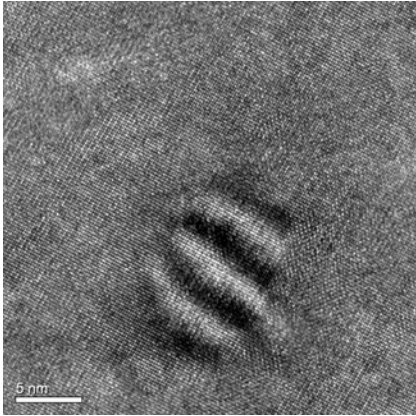


Figure 1 High resolution TEM image showing spinodally decomposed regions in PbTe-16%PbS.

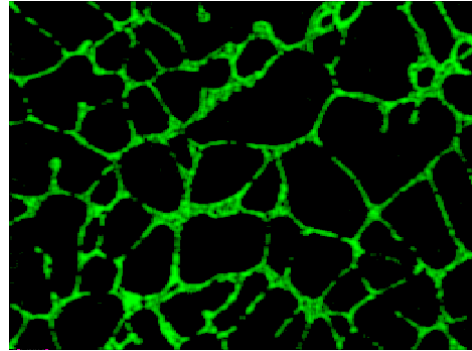


Figure 2 Auger map of boron (green) decorating grain boundaries in a Co-Si alloy.

Work in these thrusts will be highly interdisciplinary and will involve all aspects of the experimental, theoretical, and computational capabilities available to us. For example, synthesis of bulk nanostructured chalcogenides (**Figure 1**) can be modeled computationally, structurally studied using advanced TEM and laser-assisted tomography, and characterized for thermoelectric and thermomechanical properties. An important part of our effort will involve the use of facilities at the Oak Ridge National Laboratory High Temperature Materials Lab (ORNL- HTML); an example is the Auger mapping capability illustrated in **Figure 2**.

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