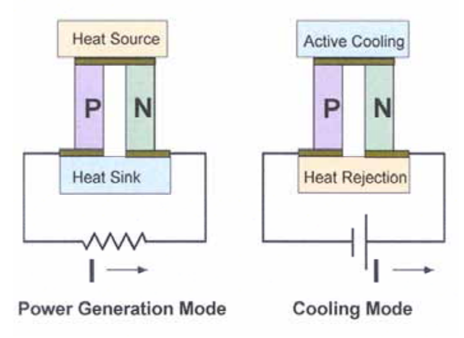
Measurements and Standards for Thermoelectric Materials

Objective

Our goal is to develop standard reference materials (SRMs), measurement methodologies, and comprehensive data sets (Seebeck coefficient, electrical conductivity, thermal conductivity) for thin film and bulk thermoelectric materials to enable the development of these materials for applications involving waste heat recovery and solid-state cooling. Our approach will facilitate comparison of thermoelectric data between leading laboratories, and accelerate the commercialization of these materials.



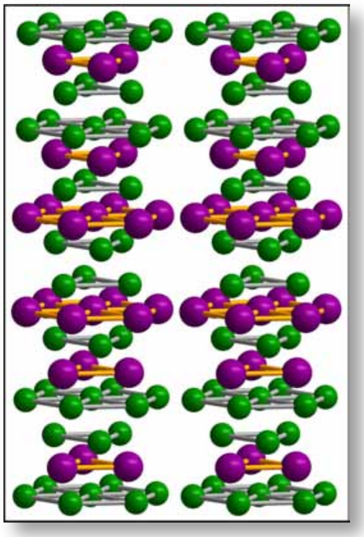
Impact and Customers

- Thermoelectric SRMs and measurement methods will allow for inter-laboratory validation of data, thereby accelerating the selection and optimization of thermoelectric materials. This will lead to more rapid commercialization of thermoelectric materials for waste heat recovery and solid-state cooling applications.
- The widespread use of thermoelectric converters for vehicular waste heat recovery would lead to a 10% improvement in fuel efficiency, translating to a fuel savings of $150 per year for every automobile, as well as decreased CO_2 emissions.

- Improved cooling of microelectronic devices would result in greater operational efficiency and reliability of integrated circuits, which are the major products of the $43B U.S. semiconductor industry.
- Customers for thermoelectric materials and devices include the automotive and consumer products industries, the military, NASA, and the energy sector.

Approach

Our approach is to develop standard reference materials, measurement methods, and combinatorial methodologies to accelerate the commercial introduction of thermoelectric materials to the market place. Especially for the case of thin film thermoelectric materials, there are currently no methods to accurately and reproducibly (laboratory to laboratory) measure the material properties that determine thermoelectric conversion efficiency, i.e., Seebeck coefficient (*S*), resistivity (ρ), and thermal conductivity (κ). High-throughput combinatorial methodologies will be employed to generate comprehensive data sets (*S*, ρ, k) for industrially relevant bulk and thin film thermoelectric materials. We will also collaborate with industrial, university and government laboratories to generate the appropriate data sets and standard reference materials.

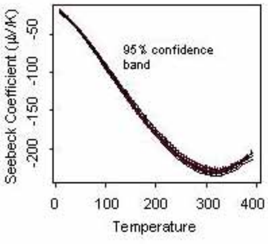


Accomplishments

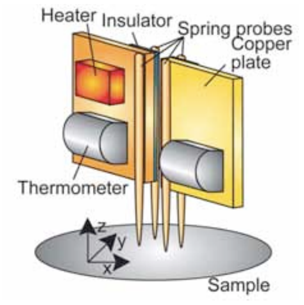
We have accomplished three goals this year: completion of a standard reference material (SRM3451) for the low-temperature Seebeck coefficient (10K to 390K); development of a set of automatic screening tools for measurements of the thermoelectric properties of thin films; and crystallographic measurements of novel thermoelectric materials.

Based on the Seebeck coefficient round robin data generated from twelve laboratories on two candidate materials, Bi_2Te_3 and constantan (a Cu-Ni alloy), we have chosen Bi_2Te_3 as our prototype SRM. Certification measurements were performed using two different techniques (a steady state primary measurement, and a secondary transient measurement) on randomly selected samples. The certified Seebeck coefficient values are provided from 10K to 390K. The availability of this SRM will enable accurate instrument calibration, and therefore meaningful inter-laboratory comparison of data. SRM 3451 is expected to be available to the public in FY 2009.

The set of automatic scanning tools consists of one for measurement of the power factor (S^2/ρ), and another for thin film thermal conductivity (κ). The power factor scanning tool consists of a probe and an automated translation stage to move it in the x, y, and z directions. Measurements take as little as 20 seconds, to determine both the electrical conductivity and Seebeck coefficient at each sample point; thus, over a thousand points can be measured within 6 hours.

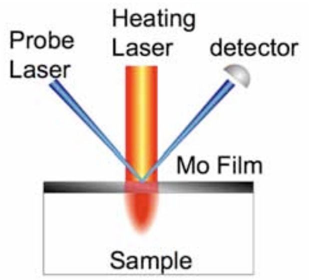


Temperature-dependent S-values for SRM 3451



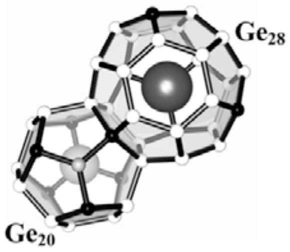
Power Factor scanning tool

Based upon the success of the power factor tool, a thin film thermal conductivity tool, based on the frequency domain thermoreflectance technique, was developed. This tool can rapidly and locally (10 μm spot size) measure the thermal conductivity of combinatorial, composition-spread films. The sample, a thermoelectric film coated with a thin molybdenum layer, is locally heated by an intensity-modulated laser; the thermal response of the film is detected by the reflected beam of a second (probe) laser. Evaluation of the phase lag between the thermoreflectance and the heating laser signals enables one to determine the thermal effusivity, b, equal to $(\kappa c d)^{1/2}$, where κ is the thermal conductivity, c is the specific heat, and d the density. Using a two-layer thermal-mathematical model, the thermal conductivity of a $Ba_2YCu_3O_{7-x}$ film was determined. The measured value, 11.96 $J(Kms)^{-1}$, is within about 10% of the reported value of 12.87 $J(Kms)^{-1}$. With the availability of this tool, future mapping of the thermoelectric figure of merit, $ZT = S^2/\rho\kappa$, is possible.



Thermal conductivity measurement geometry

Finally, in collaboration with the University of South Florida, and the Naval Surface Warfare Center, we successfully determined the local structure of Cu in a novel type-II clathrate, $Cs_8Na_{16}Ge_{136-x}Cu_x$, using X-ray absorption spectroscopy.



$Cs_8Na_{16}Ge_{136-x}Cu_x$ polyhedra framework

Cu was confirmed to dope preferably in the most distorted tetrahedral Ge site. Thus, it is likely that the values of S, ρ and κ can be modified by doping.

Learn More

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Publications

Lowhorn N, Wong-Ng W, Zhang W, Lu J, Otani M, Green M and Tranh TN R*ound-Robin Studies of Two Potential Seebeck Coefficient Standard Reference Materials* Appl. Phys. A (Materials Science & Processing), 94: 231 (2009)

Mansour AN, Beekman M, Wong-Ng W and Nolas GS *Local Structure of Cu in* $Cs_8Na_{16}Cu_5Ge_{131}$ *Type II Clathrate* J. Solid State Chem., 182:107 (2009)

Otani M, Thomas E, Wong-Ng W, Schenck PK, Lowhorn ND, Green ML and Ohguchi H *A High-throughput Screening System for Thermoelectric Materials Exploration Based on a Combinatorial Film Approach* Jap. J. App. Phys., in press (2009)

Otani M, Lowhorn ND, Schenck PK, Wong-Ng W and Green M *A High-throughput Thermoelectric Screening Tool for Rapid Construction of Thermoelectric Phase Diagrams* Appl. Phys. Lett., 91:132102 (2007)