Sustainability Focus Topic
Room 5 & 6 - Session SU+AS+EM+MS-WeM
Piezoelectrics, Thermoelectrics, and Superconductors

Moderators: George Nolas, University of South Florida, Kimberly Cook-Chennault, Rutgers University

8:20am **SU+AS+EM+MS-WeM-2 Investigation into Novel p-type Thermoelectric Materials*, Dean Hobbis, K Wei, G Nolas,*** University of South Florida

Novel thermoelectric materials are in high demand due to the ability to directly convert waste heat into electrical power, a process that has limitless applications both privately and commercially. Currently n-type thermoelectric materials have been more vastly studied than p-type and have been optimized to higher Figures of Merit (ZT). A thermoelectric module requires both n-type and p-type materials, therefore the efficiency of the module is characterized by the combination of ZT values. This means the optimization of p-type thermoelectric materials is extremely important to the commercial viability of thermoelectric technology. Furthermore, the particular synthesis method is also of importance for applications in industry. In skutterudites, for example, methods of fractional filling are typically used to improve thermoelectric efficiency by promoting phonon scattering to reduce thermal conductivity in the material, but most of the elements used as filler are electron donors. Nevertheless, Br is an electron acceptor when used as a filling atom [1]. In quaternary chalcogenides, thermal conductivity can be intrinsically low due to the crystal structure so methods to improve electrical transport is often employed through alloying and substitution on different atomic sites. Certain antimonides also possess intrinsically low thermal conductivity. Furthermore, differing processing conditions can influence the transport properties significantly, resulting in different ZT values. In this talk we present our latest work on these material systems, including new data that shows substantial improvement In ZT with composition and processing conditions.

[1] Nolas et al. *Mat. Res. Soc. Symp.* 626, **2001**, Z10.1.1

8:40am **SU+AS+EM+MS-WeM-3 Thermoelectrics for Sustainable Energy Harvesting*, Mary Anne White,*** Dalhousie University, Canada **INVITED**

Thermoelectrics can convert heat to power. The key to this process is the combined electrical (high electrical conductivity and Seebeck coefficient) and thermal (low thermal conductivity) properties. Although thermoelectrics have been used commercially for more than 50 years, new materials with higher efficiency could make their use more widespread. A large fraction of energy consumed is actually wasted as heat, so efficient conversion of this waste heat to useable power would be a great advantage to humanity. After a general introduction to thermoelectrics, this presentation will focus on improvement of thermoelectrics via sustainable approaches, including consideration of sustainability of the elements, and recent work focusing on elements with high availability.

9:20am **SU+AS+EM+MS-WeM-5 Toward a Greener World: The (Re)search for Lead-Free Piezoelectrics*, Xiaoli Tan,*** Iowa State University **INVITED**

Piezoelectricity refers to the linear coupling, in the direct effect, between mechanical stress and electric displacement, and in the converse effect, between mechanical strain and applied electric field. The proportionality constants are the piezoelectric coefficients which are equivalent between the direct and the converse effects. For the past six decades ceramics based on $Pb(Zr_{1-x}Ti_x)O_3$ (PZT) perovskite oxides have been the workhorse of piezoelectric technology due to their excellent properties, ease of processing, and low cost. The high piezoelectric performance of PZT is primarily resulted from the intrinsic lattice distortion and the ferroelectric domain switching. However, environmental concerns with lead have stimulated worldwide intensive efforts in the search for lead-free piezoelectric ceramics.

The research efforts on lead-free piezoelectric ceramics have been largely concentrated on three solid solution families: $BaTiO_3$-based, $(K_{0.5}Na_{0.5})NbO_3$-based, and $(Bi_{1/2}Na_{1/2})TiO_3$-based compositions. $BaTiO_3$-based ceramics exhibit excellent piezoelectric coefficients, but their applications are limited by their low Curie points (~100 °C). $(K_{0.5}Na_{0.5})NbO_3$-based compositions possess high piezoelectric coefficients and relatively high Curie points (> 200 °C), but have stringent requirements on the processing conditions. $(Bi_{1/2}Na_{1/2})TiO_3$-based polycrystalline ceramics develop giant electrostrains (up to 0.70%), but usually require a very high electric field.

In this presentation, an overview of the recent development in the search and research on lead-free piezoelectric ceramics will be given. Their chemical compositions, structure evolutions, and mechanisms for property optimization will be discussed. In addition, two specific investigations will be presented. The first one is on the microstructural response to poling electric fields in the $(Bi_{1/2}Na_{1/2})TiO_3$–$BaTiO_3$ solid solution. With the *in situ* transmission electron microscopy technique, it is directly observed that poling fields can either destroy or create morphotropic phase boundaries and the associated strong piezoelectric property. The second investigation is on the development of a giant electrostrain of 0.70% at 50 kV/cm at room temperature in $\{[Bi_{1/2}(Na_{0.84}K_{0.16})_{1/2}]_{0.96}Sr_{0.04}\}(Ti_{0.975}Nb_{0.025})O_3$. This polycrystalline ceramic with randomly oriented grains is even better than some single crystals in terms of some electromechanical properties. *In situ* transmission electron microscopy examination indicates that the giant electrostrain is originated from the reversible phase transitions under applied electric fields.

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11:20am **SU+AS+EM+MS-WeM-11 Thermal Annealing Effects on the Thermoelectric Properties of Si/Si+Sb Thin Films*, Satilmis Budak*, *Z Xiao, M Curley, M Howard, B Rodgers, M Alim,*** Alabama A&M University

Thermoelectric devices were prepared from multi-nanolayered Si/Si+Sbthin films using DC/RF magnetron sputtering system. Thermoelectric devices were annealed at different temperatures to form quantum (nano) structures in the multilayer thin films to increase the Seebeck coefficients and electrical conductivity and decrease thermal conductivity. The prepared devices were characterized using Seebeck coefficient measurement; four probe van der Pauw measurement resistivity and the laser thermal conductivity systems. The surface morphology of the fabricated thermoelectric films is characterized using Scanning Electron Microscope (SEM+EDS).

Acknowledgement

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11:40am **SU+AS+EM+MS-WeM-12 Critical Current by Design*, George Crabtree, U Welp,*** Argonne National Laboratory*; K Kihlstrom,* University of Illinois at Chicago*; A Koshelev,* Argonne National Laboratory*; A Glatz,* Northern Illinois University*; I Sadovskyy, W Kwok,* Argonne National Laboratory **INVITED**

We introduce a new approach for rational design of superconducting critical currents, using time-dependent Ginzburg-Landau simulation to predict the critical current produced by an arbitrary mixed pinning landscape. Time dependent Ginzburg-Landau simulations automatically take into account vortex flexibility, the variation of coherence length with temperature and field, the mutual interaction of vortices and the interaction of vortices and defects. Core pinning by an arbitrary mixed pinning landscape is included by lowering the superconducting condensation energy at points, along lines and within finite nanoscale regions corresponding to specific pinning defects. We show results for several real-world cases that verify predictive ability, outline a program for unfolding the interaction of multiple pinning defects and for maximizing the critical current in targeted temperature and field ranges

Vortices in High Performance High Temperature Superconductors, W. K. Kwok et al., Reports on Progress in Physics. 79, 116501 (2016)

Toward Superconducting Critical Current by Design, Ivan A. Sadovskyy et al, Advanced Materials 28(23), 4593-4600 (2016)

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