MM 22: Functional Materials I

Time: Tuesday 10:15–11:30 Location: H 1029

MM 22.1 Tue 10:15 H 1029

Optimizing thermoelectric Properties: Microstructure Analysis of $AgPb_{18}SbTe_{20}$ — •Susanne Perlt[1], Thomas Höche[2], Jayaram Dadda[3], and Eckhard Müller[3] — [1]Leibniz Institute of Surface Modification, Leipzig — [2]Fraunhofer Institute for Mechanics of Materials, Halle — [3]German Aerospace Center, Institute of Materials Research, Köln

Given the looming shortage of natural resources, there is a growing interest in renewable energy in recent years. The feasible recovery of waste-heat energy as it is generated by industrial and vehicle engines has led to increasing research interest in thermoelectrics (TE). In order to get TE materials with high performance, i.e. with a large figure of merit ZT, one needs to tune electronic and phononic properties. A promising candidate is the quaternary compound $AgPb_mSbTe_{2+m}$ (Lead-Antimony-Silver-Tellurium, LAST-m). Its excellent performance is mainly based on a low value of the thermal conductivity κ - widely believed to be caused by self-assembled nanostructures. This study reports microstructure investigations at two different length scales. The micrometer scale was evaluated by SEM to analyze volume fraction and number of secondary phases as well as the impact of processing parameters on the homogeneity of bulk samples. Site-specific liftout of TEM lamellae from thermoelectrically characterised samples was made to investigate the structure on the nanometer scale. High-resolution TEM was performed to reveal shape and size distribution of nanoprecipitates. An attempt is made to derive a structure-property relationship.

MM 22.2 Tue 10:30 H 1029

Reference materials for traceable measurements of thermoelectric properties from 300 K to 900 K — Frank Edler[1], •Ernst Lenz[1], and Pawel Ziolkowski[2] — [1]Physikalisch Technische Bundesanstalt, Berlin, Germany — [2]German Aerospace Center - Institute of Materials Research, Germany

Thermoelectric generators for converting wasted heat directly into electric energy are of increasing interest during the last years. The efficiency of those generators is normally expressed by the dimensionless figure of merit which scales with the square of the Seebeck coefficient. However, traceable reference materials for Seebeck coefficients in the temperature range of 300 K to 900 K are still not available. The intention of the project "Metrology for Energy Harvesting" founded by the European metrology organization is to provide those reference materials [1].

A metallic nickel copper alloy (CuNi44) and a semicoducting iron disilicide ($Fe_{0.95}Co_{0.05}Si_2$) will be presented as two possible reference materials. A relative uncertainty of about 2% for the Seebeck coefficient can be shown under utilization of an improved measurement system. The enhancement of the measuring system will be achieved by using gold/platinum thermocouples and a Pt-100 thermometer.

[1] http://www.empronline.eu/energycall/index.html

MM 22.3 Tue 10:45 H 1029

First-principles study of native point defects in the thermoelectric material Bi_2Te_3 — •Adham Hashibon and Christian Elsässer — Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

The thermoelectric properties of Bi_2Te_3, which is the currently preferred thermoelectric material for energy conversion applications at room temperature, are strongly affected by the nature and concentration of native point defects. However, knowledge of the formation energies of point defects and the manner by which they affect thermoelectric properties is still incomplete. We present a systematic study of formation energies and electronic densities of states for native point defects in Bi_2Te_3 [1] using first-principles calculations based on density functional theory. Formation energies are calculated assuming the dilute limit of defects by employing an ab-initio thermodynamics approach. Results for the formation energies of the most prominent native point defects, namely vacancies and anti-site defects on the Bi, Te1, and Te2 sub-lattices of the Bi_2Te_3 structure will be presented and their impact on the thermoelectric properties will be discussed.

[1] Adham Hashibon and Christian Elsässer, Phys. Rev. B 84, 144117 (2011)

MM 22.4 Tue 11:00 H 1029

Dynamic stabilisation of polar oxide growth: the case of MgO(111) — •Philip Hasnip and Vlado Lazarov — University of York, York, UK

Intrinsic polar materials such as metal-oxides are some of the most commonly used materials in electronic, magnetic and chemical applications. Along the polar direction, these materials consist of oppositely charged ionic planes and this polarity dominates the growth process. Attempts to grow polar oxides in their polar direction often result in surface faceting, surface reconstructions, adatoms or surface metallisation as the system attempts to heal the polarity and prevent a divergent electrostatic dipole.

By using MgO(111) as a model system for polar oxide film growth, we show by ab initio calculations that H can act as a surfactant, stabilising the growth dynamically without disrupting the growth or becoming trapped in the film. The continuous presence of H during the growth of a MgO(111) film efficiently removes the microscopic dipole moment, thus enabling the growth of perfect fcc-ordered MgO(111) films. These theoretical predictions are confirmed experimentally by molecular beam epitaxy single crystal growth of MgO(111) on SiC(0001).

MM 22.5 Tue 11:15 H 1029

Three displacively excited coherent phonons in infinite BN nanotubes — •Bernd Bauerhenne, Eeuwe Zijlstra, and Martin Garcia — Theoretische Physik - Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

BN nanotubes are isostructual to carbon nanotubes with boron and nitrogen atoms occupying the even and odd sublattices, respectively. They are described by the so called wrapping vector, which defines how the hexagonal sheet is cut off and rolled up. The wrapping vector also divides the tubes into the three groups: armchair, zizag and chiral. In particular, we investigate the excitation of a (5,0) zigzag BN nanotube with an intense ultrashort laser pulse by means of ab initio molecular dynamics simulations on laser-excited potential energy surfaces. Our results show that only three phonon modes are simultaneously excited. We identify these three modes as the radial breathing mode, the radial buckling mode and the longitudinal bond stretching mode. The frequencies of the three modes show a softening for increasing laser intensity. The analysis of our results show, that we can describe all effects of the laser excitation by a three-dimensional harmonic oscillator. Using this model we analyse the possibility to steer the excitation of the three modes by using, instead of one, two or three pump laser pulses.