DS 13: Thermoelectric Thin Films and Nanostructures I

Time: Tuesday 10:30–13:00 Location: H8

DS 13.1 Tue 10:30 H8

Thermoelectric investigations on nanocomposite PbTe with different inclusions — •Gert Homm[1], Denis Petri[3], Sabine Schlecht[2], and Peter J. Klar[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität, Gießen, Germany — [2]Institut für Anorganische und Analytische Chemie, Justus-Liebig-Universität, Gießen, Germany — [3]Institut für Chemie und Biochemie, Freie Universität Berlin, Berlin, Germany

We investigated different series of nanogranular so called LAST (LeadAntimonySilverTelluride) samples where either the composition of the inclusion of particles was varied or the PbTe matrix itself was doped isovalently by different elements. Inclusion particles of $BiSbTe_3$, $AgSbBiTe_2$ and $AgSbTe_2$, respectively, were distributed into a nanoparticulate matrix of PbTe by co-ball-milling of the two components and compacting/annealing of the resulting composite material. This is a very easy and economic way of nanostructuring. The resulting nanogranularity of the material is supposed to exhibit a lower thermal conductivity than the corresponding bulk material but possess comparable electrical conductivity. The thermopower and the electrical conductivity was measured in the range of 50-300 K before and after annealing of the specimens. The changes of the thermoelectric properties due to doping of the PbTe matrix as well as of the nanograins will be discussed. The effects of the annealing with respect to structural changes as well as dopant diffusion will be explained. (SPP 1386)

DS 13.2 Tue 10:45 H8

Experimental and theoretical investigations of PbTe-based nanocomposites with different inclusion phases — Denis Petri[1], Christoph Erk[2], Gert Homm[3], Markus Piechotka[3], Peter J. Klar[3], Sabine Schlecht[2], and •Beate Paulus[4] — [1]Freie Universität Berlin, Institut für Chemie und Biochemie, Fabeckstraße 34-36, 14195 Berlin — [2]Justus-Liebig-Universität Gießen, Institut für Anorganische und Analytische Chemie, Heinrich-Buff-Ring 58, 35392 Gießen — [3]Justus-Liebig-Universitä t Gießen, I. Physikalisches Institut, Heinrich-Buff-Ring 16, 35392 Gießen — [4]Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustraße 3, 14195 Berlin

Nanocomposite thermoelectric materials made by co-ball-milling of lead telluride and an added inclusion phase of Sb_2Te_3, $BiSbTe_3$, Bi_2Te_3 or $AgSbTe_2$ were investigated. A cold-pressing/annealing approach was applied to the resulting powders and the thermopower and the electrical conductivity of the products were measured in the temperature range of 50-300 K. The two quaternary phases $Pb_{10}BiSbTe_{13}$ (n-type) and $Pb_{10}AgSbTe_{12}$ (p-type) show the most promising power factors within the series of nanocomposites investigated. These experimental investigations are supported by first principle calculations for the bulk and the surfaces on the different materials.

DS 13.3 Tue 11:00 H8

Conductivity anisotropy of layered BiTe-SbTe-heterostructures — •Bogdan Yavorsky[1], Nicki Hinsche[1], Martin Gradhand[1,2], Peter Zahn[1], and Ingrid Mertig[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, D-06099 Halle — [2]MPI für Mikrostrukturphysik, Weinberg 2, D-06120 Halle

Transport properties of ordered bismuth and antimony tellurides are studied theoretically based on first-principle electronic structure calculations using a screened Korringa-Kohn-Rostoker Greens function method. The anisotropy of the electron mobility both in the bulk materials and in layered BiTe-SbTe-heterostructures is analyzed within the relaxation time approximation of the Boltzmann theory. The influence of doping on the electrical conductivity is discussed applying the rigid band approximation.

DS 13.4 Tue 11:15 H8

Evidence of Multiphase Nature of β-Zn_4Sb_3 by means of Surface Scanning Techniques — •Titas Dasgupta[1], Christian Stiewe[1], Ralf Hassdorf[1], Lothar Böttcher[1], Hao Yin[2], Bo Iversen[2], and Eckhard Müller[1] — [1]German Aerospace Center (DLR), Institute of Materials Research, Linder Höhe, 51147, Cologne, Germany — [2]University of Aarhus, Department of Chemistry, Langelandsgade 140, DK-8000, Aarhus, Denmark

β-Zn_4Sb_3 has been considered as a promising candidate for thermogenerator applications for long due to its high thermoelectric figure of merit (ZT) reaching up to ∼1.3 at intermediate temperatures. The high ZT is a result of the unusually low thermal conductivity (κ) observed in this material. The cause of this low κ is still under debate. Reports on structural analyses reveal a disordered structure with presence of interstitial Zn atoms to be the likely cause of the low κ. Also, soft phonon modes have been observed in this material due to the presence of Sb dimers which can also lead to the observed low κ. Thus the present work investigates the surface homogeneity and microstructure of β-Zn_4Sb_3 based on Seebeck Microprobe (PSM) and Scanning Electron Microscopy (SEM) studies. PSM measurements indicate the presence of local structures with slightly varying but distinct Seebeck (S) values. SEM studies also reveal the presence of local structures arising due to dopant contrast.Based on these observations, the possibility of the presence of multiple phases within β-Zn_4Sb_3 is discussed.

DS 13.5 Tue 11:30 H8

Thermoelectric $CoSb_3$ thin films on amorphous SiO_2 substrates — •Marcus Daniel, Christoph Brombacher, Gunter Beddis, and Manfred Albrecht — Chemnitz University of Technology, Institute of Physics, Germany

Since energy efficiency is becoming more and more important and novel nanostructured materials as well as new material groups have recently been introduced, the field of thermoelectricity is particularly in the focus of current research activities. One of the promising materials for future applications is $CoSb_3$ in its skutterudite phase. In this study, 30nm thick $CoSb_x$ films with different Sb content x have been deposited by MBE onto thermally oxidized Si(001) substrates. The deposition temperature was varied between room temperature and 300°C. In addition, samples deposited at room temperature have been annealed under UHV condition for one hour at different temperatures up to 700°C. The composition of these films was investigated by RBS and it was found that the Sb content of the deposited films is strongly dependant on the substrate temperature/annealing temperature. Structural investigations by XRD reveal the existence of the desired skutterudite phase in a narrow composition range and the influence of the preparation parameters on the phase formation will be discussed. In addition, the topography and electric conductivity was measured by AFM and four probe measurements, respectively. It was found that the morphology of the samples dominates the electrical conductance.

DS 13.6 Tue 11:45 H8

Doped NiTiSn as a n- + p-type thermoelectric material pair in almost one material — •B. Balke, S. Ouardi, M. Schwall, and C. Felser — Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany

Excellent n-type XNiSn (ZT_{max}=1.5) and p-type XCoSb (ZT_{max} = 0.7) (X = Ti, Zr, Hf) high temperature thermoelectrics were reported recently and reproduced by several groups in Asia (Toshiba, Toyota) and US. But to reach the goal to develop a thermoelectric converter (TEC) beyond the state-of-the-art for power generation one has to overcome several difficulties. The demands are environmental friendliness, low-cost and future availability of raw materials, high efficiency, operating temperature 100 - 700°C + short time excess temperature up to 800°C, possibility of industrial processing, and a thermoelectric material pair (n- + p-type) with very similar coefficients of thermal expansion and good thermoelectric compatibility. The half-Heusler materials class does meet nearly all requirements including a high power factor, but a general challenge in improving half-Heuslers is to reduce the comparatively high thermal conductivity. We produced and investigated the thermoelectric properties of doped NiTT'Sn(T = Ti, Zr, Hf, and T' = Sc, Y, V, Nb) and we were able to reach both goals, reducing the comparatively high thermal conductivity and designing a thermoelectric material pair (n- + p-type) in almost one material. *This work was financially supported by the Stiftung für Inovation Rheinland Pfalz.*

DS 13.7 Tue 12:00 H8

Enhanced Thermoelectric Figure of Merit in Edge Disordered Zigzag Graphene Nanoribbons — •Haldun Sevincli and Gianaurelio Cuniberti — Institute for Materials Science, TU Dresden, 01062 Dresden, Germany

We investigate electron and phonon transport through edge disordered zigzag graphene nanoribbons based on the same methodological tool of nonequilibrium Green functions [1]. We show that edge disorder dramatically reduces phonon thermal transport while being only weakly detrimental to electronic conduction. The behavior of the electronic and phononic elastic mean free paths points to the possibility of realizing an electron-crystal coexisting with a phonon-glass. The calculated thermoelectric figure of merit (ZT) values qualify zigzag graphene nanoribbons as a very promising material for thermoelectric applications.

[1] H. Sevincli and G. Cuniberti, arXiv:0908.3207

DS 13.8 Tue 12:15 H8

Calculation of the Seebeck-coefficient using the NEGF formalism in a 1D-model — •Michael Bachmann, Michael Czerner, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

We present a 1D model that can be used to calculate electron transport through interfaces of heterostructures. The model is based on the non-equilibrium Green's function (NEGF) formalism in the single band effective mass approximation. The effect of phonon scattering is taken into account by adding a self energy to the Hamiltonian. We obtain the Seebeck-coefficient within this model by applying a temperature difference and simultaneously adjusting the voltage to prevent a net current flow. The ratio of this voltage and the difference in temperature is the Seebeck-coefficient. We perform all calculations self consistently with respect to the Poisson equation. (SPP 1386)

DS 13.9 Tue 12:30 H8

Order-N method for calculating thermal transport at the mesoscale — •Wu Li[1,2], Haldun Sevincli[2], Stephan Roche[3,2], and Gianaurelio Cuniberti[2] — [1]Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, China — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — [3]CEA, Institute for Nanoscience and Cryogenics, INAC, SP2M, Lsim, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France

We develop an order-N method for calculating the phonon transport in mesoscopic systems using the real space Kubo approach in the harmonic approximation. The advantage of our method over the Green function method is that we can compute the phonon transport properties of quasi-one dimensional structures as wide and as long as the experimentally relevant sample sizes within much shorter computation times. As a test case of this method, we calculate the elastic phonon mean free paths (MFP) of isotopically disordered carbon nanotubes (CNT). Our MFP values are in excellent agreement with the ones obtained from the Green function approach except for the very low energies. For such low energies, we use the analytic expression derived from perturbation theory. We apply the method to edge disordered graphene nanoribbons (GNR). We show that the phonon thermal conductance is reduced by more than two orders of magnitude due to edge disorder.

DS 13.10 Tue 12:45 H8

Strained and rolled up silicon: Electronic structure calculations of a promising thermoelectric material — •Nicki Hinsche, Bogdan Yavorski, Peter Zahn, and Ingrid Mertig — Martin-Luther-Universität, Institut für Physik, Von-Seckendorff-Platz 1, 06120 Halle/S.

Starting from bulk silicon, we studied the valley splitting due to symmetry breaking that occurs in rolled-up Si. Valley splitting in Si was studied recently because of tetragonal distortion and quantum well effects in heterostructures [1,2]. The new aspect in nowadays experimentally accessible rolled-up Si tubes is that symmetry breaking occurs in all spatial directions [3]. As a result, splitting of the six-fold degenerate conduction-band minimum is expected to be lifted. This has a strong influence on the transport properties as well. In detail, the anisotropy of the effective masses of charge carriers contributing to the conductivity in different directions will be studied in dependence on the applied strain. The electronic structure is calculated self consistently within the framework of density functional theory. The transport properties of the promising thermoelectric material will be studied in the diffusive limit of transport applying the Boltzmann theory in relaxation time approximation.

[1] Dziekan et al. Physical Review B 75, 195213 (2007) [2] Boykin et al. Physical Review B 70, 165325 (2004) [3] Cavallo et al. Journal of applied physics 103, 116103 (2008)