DS 15: Thermoelectric Materials

Time: Tuesday 9:30–12:15 Location: H8

Invited Talk DS 15.1 Tue 9:30 H8

Heterostructures with Targeted Nanoarchitecture and Tunable Properties — •David Johnson — University of Oregon, Department of Chemistry and Materials Science Institute, Eugene, OR, USA

By controlling the composition of an amorphous intermediate on the nanoscale we can kinetically control the self-assembly of new nanostructured compounds consisting of two or more compounds with different crystal structures that are precisely interleaved on the nanoscale. We have used this approach to synthesize hundreds of new metastable heterostructures with designed nanostructure, including structural isomers. Many of these materials have unprecedented physical properties, including the lowest thermal conductivities ever reported for a fully dense solid, systematic structural changes dependent on nanostructure, and charge density wave transitions. The designed precursors enable diffusion to be followed and quantified over distances of less than a nanometer, providing insights to the mechanism that gives control of the nanoarchitecture of the final product. We believe the ability to prepare entire families of new nanostructured compounds permits a new "thin film metallurgy" or *nanochemistry* in which nanostructure and composition can both be used to tailor physical properties, interfacial structures can be determined for precisely defined constituent thicknesses, and interfacial phenomena and modulation doping can be systematically exploited.

DS 15.2 Tue 10:00 H8

Symmetrical and non-symmetrical TiNiSn/HfNiSn superlattices — •Paulina Komar[1,2], Emigdio Chávez Angel[1], Christoph Euler[1], Gregor Fiedler[3], Benjamin Balke[4], Peter Kratzer[3], and Gerhard Jakob[1,2] — [1]Institute of Physics, University of Mainz, Mainz, Germany — [2]Graduate School Materials Science in Mainz, Mainz, Germany — [3]Faculty of Physics, University of Duisburg-Essen, Duisburg, Germany — [4]Institute of Inorganic and Analytical Chemistry, University of Mainz, Mainz, Germany

The goal of our work is to reduce the thermal conductivity by phonon scattering at the superlattice (SL) interfaces and enhance $ZT = \frac{S^2\sigma}{\kappa}T$. For symmetrical SLs (TiNiSn:HfNiSn ratio=1 and variable SL period) we observe a very good agreement between the cross-plane thermal conductivity measured by the 3ω method and a calculation based on Boltzmann transport theory down to a SL period of 3 nm. At the SL period of 3 nm a crossover between the particle- and the wave-like transport of phonons takes place and, therefore, κ increases for decreasing periods [1]. An investigation of non-symmetrical SLs (variable TiNiSn:HfNiSn ratio and constant SL period) reveal that not only the SL period and the number of interfaces have an influence on κ, but the ratio of materials with higher and lower κ influences the thermal conductivity as well. Additionally, a systematic improvement of the in-plane Seebeck coefficient is observed.

We gratefully acknowledge financial support by DFG (Ja821/4-2) and (GSC 266).

[1] P. Hołuj *et al*. Phys. Rev. B 92, 125436 (2015).

DS 15.3 Tue 10:15 H8

Full thermoelectric characterization of individual silver-nanowires — •Rüdiger Mitdank[1], Danny Kojda[1], Zhi Wang[2], Johannes Ruhhammer[2], Michael Kroener[2], Peter Woias[2], Martin Albrecht[3], and Saskia F. Fischer[1] — [1]Novel Materials Group, Institut für Physik der Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [2]Laboratory for Design of Microsystems, University of Freiburg - IMTEK, 79110 Freiburg, Germany — [3]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2 , 12489 Berlin, Germany

A full characterization of the thermoelectric properties of nanowires (NWs) requires information about the Seebeck coefficient as well as the electrical and thermal conductivity. The temperature normalized ratio of both conductivities is known as Lorenz number L and is discussed for Ag-NWs in [1]. In order to determine the thermoelectric figure of merit of Ag-NWs, individual Ag-NWs are transferred to a micro machined measurement platform (TNCP) and contacted by electron beam induced deposition (EBID) with platinum. The focus of this talk is directed to the discussion of the temperature-dependent Seebeck coefficient of Ag-NW's. The thermovoltage of Ag-NWs was measured with respect to Pt between 4 K and 300 K. The Seebeck coefficient S changes the sign at T = 150 K and exhibits a minimum at T = 70 K. This zero-crossing and the influence of the phonon drag are discussed. As a result, the figure of merit S*S/L is discussed for the temperature-range between 4 K and 300 K.

[1] D. Kojda et. al. Phys. Rev. B, 91, 024302 (2015)

DS 15.4 Tue 10:30 H8

Surface Effects on Thermoelectric Properties of Single Crystalline Semiconducting Nanowires — •Danny Kojda[1], Rüdiger Mitdank[1], Anna Mogilatenko[2], William Töllner[3], Zhi Wang[4], Michael Kröner[4], Peter Woias[4], Kornelius Nielsch[3], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, D-12489 Berlin — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, D-12489 Berlin — [3]Institut für Angewandte Physik, Universität Hamburg, D-20355 Hamburg — [4]Laboratory for Design of Microsystems, University of Freiburg - IMTEK, D-79110 Freiburg

Bismuth telluride nanowires (Bi_2Te_3 NWs) are proposed to reveal a thermoelectric figure of merit ZT that is influenced by confinement and surface effects. To determine the role of surface effects we consider individual single crystalline NWs as model system of a high surface-to-volume-ratio for which grain boundary scattering is negligible. We demonstrate the state-of-the-art of the combination of the structural, chemical, and temperature-dependent complete thermoelectric characterization for individual single crystalline $Bi_{0.39}Te_{0.61}$ NWs, which only differ in surface morphology. With the 3ω-method a reduction of the thermal conductivity of about 50 % is measured in a diameter varied NW with respect to a NW with a constant diameter [1]. For homogenous, diameter varied and single indented NWs finite element simulations are performed to interpret the measurement results [2].

[1] D. Kojda *et al.*, Semicond. Sci. Technol. **29**, 124006 (2014).
[2] D. Kojda *et al.*, Phys. Status Solidi A, DOI:10.1002/pssa.201532464.

15 min. break.

DS 15.5 Tue 11:00 H8

Full- and half- Heusler phase coexistence in phase separated Z_{2-x}TiSb (Z=Co,Ni) thermoelectrics. — •Joaquin Miranda, Heiko Schoberth, Thomas Gruhn, and Heike Emmerich — Lehrstuhl für Material- und Prozesssimulation, Universität Bayreuth, Universitätsstraße 30, D-95447 Bayreuth, Germany

During the last year, we have successfully employed ab-initio Density Functional calculations and Monte Carlo simulations to show that some thermoelectric half-Heusler alloys show phase separation [1-3]. Recently, we have studied transition metal alloys with the formula Z_{2-x}TiSb (Z=Co, Ni), where x sets the concentration for a half (if x=1) or full (if x=0) Heusler material. We show that the materials undergo a complex phase separation containing half/full Heusler superstructures. This separation is assumed to have beneficial effects on the charge and heat transports mechanism and to lead to higher figures of merit in thermoelectrics. The interplay of kinetics and transport on the bulk as well as the role of the inter-phases are still under investigation. Here we show simulations that clarify the individual contributions.

1.- Nanophase separation in CoSb-based half-Heusler thermoelectrics: A multiscale simulation study. Phys. Status Solidi A (2015).

2.- Miscibility gap in the phase diagrams of thermoelectric half-Heusler materials CoTi_{1-x}Y_xSb (Y = Sc, V, Mn, Fe). Journal of Electronic Materials (2015).

3.- Ab-initio study of domain structures in half-metallic CoTi_{1-x}Mn_xSb and thermoelectric CoTi_{1-x}Sc_xSb Half-Heusler alloys. Journal of Alloys and Compounds, Vol. 650,25,728 (2015).

DS 15.6 Tue 11:15 H8

Electronic topological transition in epitaxially strained delafossite $PtCoO_2$ — •Markus E. Gruner[1,2], Ulrich Eckern[3], and Rossitza Pentcheva[2,1] — [1]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Technical University Munich — [2]Faculty of Physics and Center for Nanointegration, CENIDE, University of Duisburg-Essen — [3]Institute of Physics, University of Augsburg

The hexagonal delafossites $PdCoO_2$ and $PtCoO_2$ exhibit highly

anisotropic transport properties including large negative values of the thermopower S_{zz} perpendicular to the hexagonal plane [1], which is of interest for thermoelectric energy conversion or sensor applications. By means of DFT calculations combined with semiempirical Boltzmann transport theory in the single relaxation time approximation we explore the effect of strain on the thermoelectric properties of both systems. We demonstrate that, despite their rather similar structural response, the isoelectronic compounds differ significantly in their transport behavior under tensile and compressive expitaxial strain [2]. This is related to specific changes of the Fermi surface involving an electronic topological transition, which occurs in $PtCoO_2$ at moderate compressive strain. Combining our first-principles results with available experimental data, we estimate a maximum ZT of 0.25 obtained for $PtCoO_2$ under $-4\,\%$ epitaxial strain. Funding by the DFG (TRR80) is gratefully acknowledged.

[1] K.P. Ong, D.J. Singh, P. Wu, Phys. Rev. Lett. 104, 176601 (2014)
[2] M.E. Gruner, U. Eckern, R. Pentcheva, arXiv:1511.09087

DS 15.7 Tue 11:30 H8

Optimized thermoelectric performance of n-type half-Heusler TiNiSn by addition and substitution with Mn — •Enkhtaivan Lkhagvasuren, Siham Ouardi, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Half-Heusler compounds have attracted considerable attention as high temperature thermoelectric materials. The state of the art n-type half-heusler compounds are based on TiNiSn. Key to their thermoelectric high efficiency is an intrinsic phase separation by Hf substitution. In the present study, the carrier concentration of the n-type half-heusler compound TiNiSn is optimized by addition and substitution of the low-cost Mn. The power factor is increased and the lattice thermal conductivity reduced with increasing Mn concentration.

DS 15.8 Tue 11:45 H8

Calculation of thermal conductivity across an interface using beam matching — •Debanjan Basu and Peter Bloechl — Institute for Theoretical Physics, Clausthal University of Technology

Designing efficient thermoelectric materials requires nanostructures with low thermal conductivity. Our goal is to study thermal transmission in multilayered structures on a mode-by-mode basis. This requires us to determine the "complex bandstructure", which describes propagating as well as evanescent phonon modes inside each layer. We also describe how to extract the matching conditions from Newton's equations of motion for the atoms at the interface between two layers.

This work is funded by the DFG Schwerpunktprogramme 1386.

DS 15.9 Tue 12:00 H8

Thermoelectric properties of half-Heusler heterostructures from ab initio calculations — •Peter Kratzer and Gregor Fiedler — Faculty of Physics, University Duisburg-Essen, 47048 Duisburg, Germany

Semiconducting half-Heusler alloys have recently emerged as a class of thermoelectric materials with outstanding performance in the medium-to-high-temperature range. Heterostructures promise further reduction of the thermal conductivity due to phonon scattering at interfaces. Here, both the electronic and phononic spectra of half-Heusler compounds based on Ti, Zr, and Hf are calculated using density functional theory (DFT). With this input, thermoelectric properties are obtained. We demonstrate how the thermal conductivity of a superlattice can be estimated in dependence on its period, by using the mean free path of phonons in bulk materials plus an extension of the diffuse mismatch model. The results are compared to experiment (PRB 92 (2015), 125436). Moreover, we demonstrate that, in a short-period superlattice, a high power factor may be retained, while the thermal conductivity is reduced compared to single-phase half-Heusler crystals.