DS 17: Thermoelectric Materials

Time: Monday 17:45–19:00 Location: CHE 89

DS 17.1 Mon 17:45 CHE 89

Thermal conductivity of Half-Heusler superlattices — Paulina Komar[1,3], Niklas Reuter[1], Emigdio Chavez-Angel[1], Sven Heinz[1,3], Benjamin Balke[2], and •Gerhard Jakob[1,3] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [2]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [3]Graduate School Materials Science in Mainz, 55128, Germany

Variable designs of TiNiSn/HfNiSn superlattices (SLs) and nonperiodic multilayers were investigated to find the most effective way to reduce the crossplane thermal conductivity κ at room temperature. The latter property was determined using a differential 3ω method. The research started from investigation of the relation between κ and the SL period while keeping the ratio of the two materials in the SL period equal to unity. To obtain information exceeding that from the bare interface density, a series of films with varying layer thickness ratios was investigated. Moreover, we discuss the design of non-periodic multilayers and their influence on the thermal conductivity. For the latter materials we developed a software to simulate x-ray diffraction patterns of non-periodic structures.
The main conclusion is that the nanostructuring helps to reduce the thermal conductivity and contributes to enhanced figure of merit ZT compared to bare TiNiSn and HfNiSn films.
We gratefully acknowledge financial support by DFG (Ja821/4-2) and the Graduate School of Excellence Material Science in Mainz (GSC 266).

DS 17.2 Mon 18:00 CHE 89

Electronic and thermoelectric properties of polar $LaNiO_3/SrTiO_3(001)$ superlattices — •Benjamin Geisler[1], Ariadna Blanca-Romero[2], and Rossitza Pentcheva[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg, Germany — [2]Department of Chemistry, Imperial College London, London, SW7 2AZ, United Kingdom

Advances in layer-by-layer fabrication techniques have made it possible to grow epitaxial transition metal oxide superlattices with atomic precision. We combine DFT+U calculations and Boltzmann transport theory to analyze the implications of the interface-dependent polar discontinuity in $LaNiO_3/SrTiO_3(001)$ superlattices on the structural, electronic, and thermoelectric properties. While $(LaO)^+/(TiO_2)^0$ interfaces result in an n-type superlattice, $(NiO_2)^-/(SrO)^0$ interfaces lead to p-type doping. We find that significant octahedral tilts are induced in the $SrTiO_3$ region and that the La-Sr distances act as a fingerprint of the interface type. In contrast to the paradigmatic $LaAlO_3/SrTiO_3$ system, the electrostatic doping is mainly accommodated in the metallic NiO_2 layers. We explain the electronic structure within the $SrTiO_3$ band gap in terms of an orbital-selective quantization of Ni-3d-derived quantum well states. Complex cylindrical Fermi surfaces emerge which show a tendency towards nesting that depends on the interface polarity. Finally, we demonstrate that the thermoelectric response of our oxide superlattices can be selectively controlled by a targeted interface design.

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DS 17.3 Mon 18:15 CHE 89

Design of thermoelectrically highly efficient Heusler compounds using phase separations and nano-composites under an economic point of view — •Benjamin Balke — Johannes Gutenberg-Universität Mainz

Half-Heusler compounds are one of the most promising candidates for thermoelectric materials for automotive and industrial waste heat recovery applications. In this talk, I will give an overview about our recent investigations of phase separations in half Heusler thermoelectrics, focusing on the ternary system TiNiSn-ZrNiSn-HfNiSn. I will show how we adapted this knowledge to design a p-type Heusler compound which exhibits a ZT that is increased by 130% compared to the best published bulk p-type Heusler. I will also present how we used the phase separation to design thermoelectric highly efficient nano-composites of different single-phase materials. Since the price for Hafnium was doubled within the last 15 months, our research focused on the design of half-Heusler compounds without Hafnium. I will present a very recent calculation on ZT per € and efficiency per € for various materials followed by our latest very promising results for n-type Heusler compunds without Hafnium resulting in 20 times higher ZT/€ values. These results strongly underline the importance of phase separations as a powerful tool for designing highly efficient materials for thermoelectric applications that fulfill the industrial demands for a thermoelectric converter.

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pattern formation in the half-Heusler NiTi_{x-1}Zr_xSb_{1-y}Sn_y — •Joaquin Miranda, Thomas Gruhn, and Heike Emmerich — Material- und Prozesssimulation, Bayreuth University. Universitaetstr 30, DE 95447, Bayreuth

Domain formations offer the possibility to reduce the lattice thermal conductivity in thermoelectrics. In this view, We employed ab-initio Density Functional calculations and Monte Carlo simulations to investigate the thermoelectric NiTi_{x-1}Zr_xSb_{1-y}Sn_y presents phase separation and rich patterning when is simultaneously alloyed Ti with Zr and Sb with Sn. We found that the material undergoes multiple phase separations as the temperature is lowered. First Ti and Zr phase separated at near 650 K but Sn and Sb tend to remain homogeneously distributed until temperatures around 300 K are reached. Within this temperature range (300-650 K) it is observed a slight preference of Zr-Sn (or Ti-Sb) nearest neighbors formation. Below 300 K both neighbors are increased, giving place to a second phase separation of richer Sn regions embedded in Zr volumes and Sb regions in Ti volumes; interestingly showing a meta-crystal structure preference of neighboring Zr and Sn atoms. We discuss the relevance of these observations within the context of thermoelectrics.

DS 17.5 Mon 18:45 CHE 89

Defects in Heusler compounds for thermoelectric applications. — •Gerhard H. Fecher[1], Benjamin Balke[2], and Claudia Felser[1] — [1]Max Planck Institute - CPFS, Dresden, Germany — [2]Johannes Gutenberg University, Mainz, Germany

It turned out that semi-conducting Heusler compounds with $C1_b$ structure and 18 valence electrons are reliable materials for thermoelectric applications, in particular for generators. The materials are mostly based on Ni for n-type or Co for p-type thermoelectrics. Examples are TNiSn or TCoSb where (T =Ti, Zr, Hf) is a transition metal or a combination of transition metals e.g.: $Hf_{0.35}Zr_{0.35}Ti_{0.3}$. The latter mixture leads already to chemical disorder, as different elements share the same position of the $C1_b$ structure. Further defects are anti-site disorder caused by a swap of two different atoms (e.g.: Ti $\leftrightarrow$Sn), off-stoichiometry by excess or deficiency of one of the elements ($TiNi_{1\pm x}Sn$) or Frenkel defects (e.g.:Ni $\leftrightarrow \square$). First principles calculations were performed for Heusler compounds exhibiting such defects and the influence of the defects on the electronic structure was studied. The main emphasis was on the changes of the band gap and the occurrence of states inside of the gap. The effects of the different defects on the electronic transport properties will be discussed.