# DS 10: Thermoelectric materials

Time: Tuesday 9:30–11:00 Location: H 0111

DS 10.1 Tue 9:30 H 0111

**Complete thermoelectric material characterization at high temperatures** — •Hendrik Kolb[1], Titas Dasgupta[2], Johannes de Boor[1], Knud Zabrocki[1], and Eckhard Müller[1,3] — [1]Institute of Materials Research, German Aerospace Center — [2]Dept. of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay — [3]Institute of Inorganic and Analytical Chemistry, Justus-Liebig-Universität Gießen

Thermoelectricity is the direct conversion of thermal energy into electrical energy and can be used for the recovery of waste heat into electrical power. For an efficient research process a quick characterization is crucial to see the effects of the material manufacturing process on the thermoelectric properties. The three thermoelectric key quantities can strongly be temperature dependent, which makes a complete characterization over a wide temperature range necessary. The special feature of our system is the additional direct zT measurement by the Harman method independently from the single measurements to verify the results. The better comparability of the measured properties is one main advantage in a simultaneous measurement, because all quantities are measured at one temperature step. Additionally the measurement uncertainty which can easily reach more than 20% in the zT measurement due to methodical or geometrical differences in different setups is reduced. We show results for a complete high temperature characterization of thermoelectric materials up to 650 K and show good agreement with reference data. Also, we demonstrate the influence of radiation losses on thermal conductivity measurement.

DS 10.2 Tue 9:45 H 0111

**Enhanced transport properties of rutile oxides** — •Denis Music and Jochen M. Schneider — Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, 52074 Aachen, Germany

Oxide based thermoelectrics offer potential for high efficiency thermoelectric conversion for harvesting electricity from heat, but suffer from a low power factor due to the low electrical conductivity. We used quantum mechanical calculations to identify alloying elements for RuO2 with enhanced Seebeck coefficient. We probed all 3d and 4d transition metals as well as all lanthanides and identified Fe and La to be the most promising candidates as a manifold increase in Seebeck coefficient was predicted. This materials design proposal was then critically evaluated by measuring the Seebeck coefficient of sputter-deposited thin films. Furthermore, the electrical and thermal conductivity was measured. Saturated RuO2 with Fe and La exhibit not only a fourfold increase in the Seebeck coefficient, but also a decrease in thermal conductivity. This yields the highest power factor reported for RuO2 despite a twofold decrease in the electrical conductivity. Hence, the ab initio predictions regarding the Seebeck coefficient are validated by experiments. Furthermore, Fe and La lead to grain refinement and a more porous morphology. Our results suggest that maximizing the structural distortion of RuO2 by dilute alloying with selected transition metals and lanthanides can increase the Seebeck coefficient and decrease the thermal conductivity by fostering quantum confinement and phonon scattering, respectively. Other rutile oxides, such as MnO2, will also be discussed.

DS 10.3 Tue 10:00 H 0111

**Reduced thermal conductivity of TiNiSn/HfNiSn superlattices** — •Paulina Holuj[1,3], Christoph Euler[1], Tino Jaeger[1], Benjamin Balke[2], and Gerhard Jakob[1,3] — [1]Institute of Physics, University of Mainz, Staudinger Weg 9, 55128, Germany — [2]Institute of Inorganic and Analytical Chemistry, University of Mainz, Staudinger Weg 9, 55128, Germany — [3]Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128, Germany

Thermoelectric materials possess the ability to convert unused heat to electricity. The efficiency of their operation depends on the dimensionless figure of merit $ZT = \frac{S^2\sigma}{\kappa}$ that contains only material dependent parameters (S - Seebeck coefficient, $\sigma$ - electrical conductivity, $\kappa$ - thermal conductivity). The goal of our work is to reduce thermal conductivity and doing so we aim to enhance ZT. Reduction of $\kappa$ is achieved by scattering of phonons at interfaces of superlattices (SL) made out of TiNiSn and HfNiSn half-Heusler materials. Based on x-ray diffraction we assume to have sharp interfaces between constituent layers. In the current study we observe a systematic reduction of the thermal conductivity as the period of the SLs is decreasing with a clear minimum at about 3 nm and a further increase of $\kappa$ due to formation of an artificial crystal.

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DS 10.4 Tue 10:15 H 0111

**Nanostructured SiGe thin films obtained through MIC processing** — •Marc Lindorf[1], Hartmut Rohrmann[2], and Manfred Albrecht[1] — [1]University of Augsburg, Universitätsstraße 1, 86159 Augsburg, Germany — [2]Oerlikon Advanced Technologies AG, Iramali 18, 9496 Balzers, Liechtenstein

In times of growing energy consumption thermoelectric devices pose an opportunity for energy harvesting. However commercially available thermoelectric materials show a deficit in efficiency governed by low ZT values. New approaches like nanostructuring [1] try to increase the efficiency, but often lack industrial applicability due to high cost and low production speed. This work presents results on sputter deposited multilayer stacks of $Si_{80}Ge_{20}(10\,nm)/[Al(d_{Al})/Si_{80}Ge_{20}(10\,nm)]_{50}/SiO_2(200\,nm)/Si$. Crystallization and Al dopant activation is achieved by post-annealing through metal induced crystallization (MIC) [2]. This approach allows grain size control via annealing temperature and Al interlayer thickness $d_{Al}$ in the nanometer regime. Results will be presented regarding structural and thermoelectric properties.

[1] Y. Lan et al.,*Adv. Funct. Mater.* **20**, 357-376 (2010).
[2] Z. M. Wang et al.,*Phys. Rev. Lett.* **100**, 125503 (2008)

DS 10.5 Tue 10:30 H 0111

**The Influence of a Distinct Diameter Variation on the Thermal Conductivity of Individual Bismuth Telluride 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]AG Neue Materialien, Humboldt-Universität zu Berlin, D-10099 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

Calculations on indented nanowires (NWs) have shown that surface morphology can affect the thermal conductivity $\lambda$ by phonon backscattering [1]. In order to determine the role of a distinct diameter variation, two $Bi_{0.39}Te_{0.61}$ NWs from the same batch are investigated by means of a combined full-thermoelectrical, structural and chemical characterization. Both NWs have the same chemical composition and the same direction of growth along the [110] direction. The NWs differ in their morphology. One NW shows a strong diameter variation between 190 nm and 320 nm and the other has a diameter of 187 nm with smooth sidewalls. At room temperature $\lambda$ was determined by the $3\omega$-method and a reduction in the indented NW by about 50 % with respect to the smooth NW was observed. Hence, NW-vacuum interfaces perpendicularly arranged to the direction of transport can lead to a reduced $\lambda$ in NWs [2]. [1] A. Moore *et al.*, 2008 APL, **93** 083112. [2] D. Kojda *et al.*, 2014 Semicond. Sci. Technol., **29** 124006.

DS 10.6 Tue 10:45 H 0111

**Enhanced thermoelectric efficiency of *p*-type Half-Heuslers by intrinsic phase separation and carrier concentration optimization.** — •Elisabeth Rausch[1,2], Claudia Felser[2], and Benjamin Balke[1] — [1]Institut für Anorganische und Analytische Chemie, Johannes Gutenberg-Universität, Mainz, Germany — [2]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

State of the art *p*-type Half-Heusler compounds (space group $F\bar{4}3m$) for thermoelectric applications are found in the $MCoSb_{0.8}Sn_{0.2}$ ($M$ = Ti/Zr/Hf) system. The outstanding properties are achieved by a nanostructuring approach via ball milling followed by a rapid consolidation method. We, herein report on a alternative approach to reduce the thermal conductivity, which is by an intrinsic phase separation. A optimum ratio of Ti to Hf in combination with an adjustment of carrier concentration via Sn substitution lead to a record thermoelectric figure of merit $ZT = 1.15$ for $Ti_{0.25}Hf_{0.75}CoSb_{0.85}Sn_{0.15}$. Our

study is complemented by a long-term stability test under thermal cycling conditions in the interesting temperature range for automotive applications.