# DS 24: Thermoelectric Materials

Time: Wednesday 14:45–17:00 Location: H32

DS 24.1 Wed 14:45 H32

**Investigations on novel thermoelectric materials using a high temperature Hall-measurement-setup** — •Hans-Fridtjof Pernau, Markus Bartel, Frank Menzel, Alexandre Jacquot, Martin Jägle, and Kilian Bartholome — Fraunhofer IPM

Novel thermoelectric materials especially for medium and high temperature application are in the focus for waste heat recovering systems not only in automotive applications. Beside the accurate determination of all thermoelectric properties and thereby the ZT-value a detailed understanding of the processes inside the materials are needed. Hall-measurements are the well-known tool to investigate carrier concentration and mobility within metals, semiconductors and of course thermoelectric materials. Up to now most commercial setups are only suitable for temperatures up to 400°C. The full characterization of high temperature materials like oxides or silicides require measurement temperatures of 600°C and above. Therefore Fraunhofer IPM developed a high temperature Hall-measurement-setup which allows measurements in this range. We will present first high temperature measurements on different materials and sample geometries performed with our new IPM-HT-Hall setup.

DS 24.2 Wed 15:00 H32

**Thermoelectric properties of laser-assisted wet-chemically doped group-IV nanoparticles** — •Benedikt Stoib[1], Anton Greppmair[1], Tim Langmann[1], Nils Petermann[2], Hartmut Wiggers[2], Martin Stutzmann[1], and Martin S. Brandt[1] — [1]Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching — [2]Institut für Verbrennung und Gasdynamik, Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg

We present recent studies on the morphology and the thermoelectric properties of thin films of laser-sintered group-IV nanoparticles. The structure size in the macro-porous network is in the sub-$\mu$m regime and can be controlled by the laser fluence used for sintering. Doping was achieved by immersing the nanoparticle film prior to sintering in a liquid containing the dopants. Conductivity and thermopower measurements provide insight into the doping efficiency. For the doping with group-V elements we find a threshold concentration, above which the conductivity can be increased by several orders of magnitude up to 100 S/cm, using different dopant concentrations in the dopant solution. Thermopower measurements show that the laser-sintered thin films are indeed n-type after this procedure, reaching a maximum Seebeck coefficient of -270 $\mu$V/K. We present the extension of this doping method to SiGe and Si and discuss relevant materials properties affecting the efficiency of the doping process.

[1] B. Stoib et al., Phys. Stat. Solidi A, doi 10.1002/pssa.201228392 (2012)

DS 24.3 Wed 15:15 H32

**Nanoscale Heat Transport from Self-Organised Ge Hut and Dome Clusters into Si(001)** — •Tim Frigge, Boris Krenzer, Verena Tinnemann, Annika Kalus, Friedrich Klasing, Anja Hanisch-Blicharski, and Michael Horn-von Hoegen — University of Duisburg-Essen and CENIDE, Duisburg, Germany

The nanoscale heat transport from self-organized Ge hut and dome clusters into Si substrates was determined by ultrafast time-resolved electron diffraction in reflection geometry. Within a temperature range between 400°C and 600°C Ge grows epitaxially in form of kinetically self-limited hut and dome clusters. In-situ deposition of 8ML Ge at 550°C under UHV conditions on Si(001) results in huts of 2 nm height and 20 nm width and domes with a height of 6 nm and a diameter of 50 nm. The clusters were excited in a pump-probe setup by 50 fs-laser pulses at a wavelength of 800 nm and probed by ultrashort electron pulses. Electron diffraction patterns were recorded at different delay times between the pump and probe pulses The observed transient drop of spot intensity is explained by the Debye-Waller effect and reflects the temperature increase from 25 K to 125 K. The cooling rate is determined from the exponential recovery of intensity: huts cool within 50 ps while the larger domes cool three times slower in 150 ps. This is in clear contrast to temperature dependent numerical simulations and reflects that size effects can reduce the heat transfer in nanoscale heterosystems by more than a factor of 8.

DS 24.4 Wed 15:30 H32

**Thermal conductivity of SiGe-based nanostructures** — •Katrin Bertram[1], Bodo Fuhrmann[1], Nadine Geyer[2], Alexander Tonkikh[2], Nicole Wollschläger[2], Peter Werner[2], and Hartmut S. Leipner[1] — [1]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle- Wittenberg, 06120 Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

A low thermal conductivity of thermoelectric materials is necessary to achieve enhanced figure of merits ZT for thermoelectric generators and Peltier coolers. Regarding theoretical predictions, nanostructured materials such as superlattices, quantumdot superlattices or nanowires, are able to show a higher figure of merit than bulk materials. The reduction of thermal conductivity in superlattices is achieved by diffuse interface scattering of the phonons at the interfaces. With a mismatch of the phonon dispersions the scattering of short-wavelength phonons is enhanced due to localized phonon states. Some theoretical work predicted a further decrease in thermal conductivity with nonperiodic superlattice structures. In this study, we have investigated the thermal conductivities of Si-Ge based superlattices. Periodic and nonperiodic $Si_m$-$Ge_n$ superlattices with stacks of m Si and n Ge layers of various thicknesses were grown by molecular beam epitaxy on (111) Si substrates. The influence of periodicity was investigated. Further investigations were done on nanowire arrays grown from these superlattices. A comparison between the different approaches for the reduction of thermal conductivity will be presented.

DS 24.5 Wed 15:45 H32

**Thermoelctrical Measurements on Single $Bi_2Te_3$ Nanowires** — •Danny Kojda[1], Rüdiger Mitdank[1], Zhi Wang[2], Michael Kröner[2], Peter Woias[2], William Töllner[3], Kornelius Nielsch[3], and Saskia F. Fischer[1] — [1]Novel Materials, Humboldt-Universität zu Berlin, D-10099 Berlin — [2]IMTEK, University of Freiburg, D-79110 Freiburg — [3]University of Hamburg, D-20355 Hamburg

Nanowires (NWs) made of $Bi_2Te_3$ are expected to improve the thermoelectric efficiency. In order to investigate the thermoelectric properties (Seebeck coefficient, electrical and thermal conductivity), as well as the crystal structure via TEM for one and the same NW, a special measurement device was fabricated by means of silicon micromachining [1]. This device contains two symmetric Si cantilevers (with a 4 $\mu$m gap) where the NW is deposited in between via dielectrophoresis and contacted in four point geometry via electron beam assisted deposition of Pt. Thin Pt micro-heaters and Pt-thermometers are situated near the NW to create and measure a temperature gradient. In the bath temperature range $T_B = 4.2$ K-300 K we measured the temperature dependent resistance of a single $Bi_2Te_3$-NW, observing metallic behavior. We also measured the Seebeck voltage between the NW-endings and a resistance change of the heated thermometer lead as function of the heating current and bath temperature. With this we are able to calculate tempeature dependent the Seebeck coefficient. It has an absolute maximum of $-35\,\mu$V/K at about 200 K.

[1] Z. Wang *et al.*, Sens. and Actuat. A: Phys. (188; p. 417-426; 2012)

DS 24.6 Wed 16:00 H32

**Reduced thermal conductivity in Half Heusler superlattices** — •Tino Jaeger[1], Christoph Euler[1], Christian Mix[1], Michael Schwall[2], Benjamin Balke[2], Sascha Populoh[3], Anke Weidenkaff[3], Claudia Felser[2], and Gerhard Jakob[1] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany — [2]Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany — [3]Empa-Eidgenössische Materialprüfung und -forschungs Anstalt Festkörperchemie und Katalyse, Ueberlandstrasse 129, 8600 Duebendorf, Switzerland

Besides bulk applications that are well-established in industry, thin film technology moves into focus. Self-sustaining sensors and on-chip cooling represent the most emerging fields of application. As valid for the conventional techniques, enhancing ZT would open new prospects in commercial usage. For thin films, the fabrication of superlattices enables a unique type of nanostructuring. To sustain electronic behavior from layer to layer, subsequently deposited materials must have a structural similarity. XRD and transport measurements have shown that the Half-Heusler alloys TiNiSn and $Zr_{0.5}Hf_{0.5}NiSn$ are appropriate in doing so. Increased cross-plane ZT in this material system is requested by additional interface scattering. Depressed thermal conductivity has been obtained by 3omega method. The measurement was performed by a home-made assembly using a passive circuit and a lock-in amplifier. We gratefully acknowledge financial support by DFG Ja821/4-1 with in the priority program SPP 1386.

DS 24.7 Wed 16:15 H32

**Growth and characterization of the low-temperature properties of $MoSi_2$ thin films** — •Mehrdad Baghaie Yazdi, Maximilian Fries, and Lambert Alff — Technische Universität Darmstadt, Materialwissenschaft, Dünne Schichten, Darmstadt, Deutschland

$MoSi_2$ is considered to be one of the best high-temperature electric conductors, often used as heating element in furnaces. Its oxidation resistance at elevated temperature makes it a good candidate as a thin film electrode for various applications. However, $MoSi_2$ also shows intriguing low-temperature properties when grown as a thin film. Woerlee *et al.* [1] attributed a low-temperature anomaly to the Kondo effect. In a new set of experiments we have studied the growth properties of radio-frequency magnetron sputtered $MoSi_2$ on polycrystalline $Al_2O_3$. We have characterized the thin films by X-ray diffraction and scanning electron microscopy. Based on low-temperature electrical transport measurements we propose a novel nanocrystal network conduction model as alternative scenario.

[1] P. H. Woerlee *et al.*, Appl. Phys. Lett. **44, 876 (1984).**

DS 24.8 Wed 16:30 H32

**Acoustic phonon propagation in cobalt antimony skutterudites** — •Chuan He[1], Martin Grossmann[1], Martin Schubert[1], Marcus Daniel[2], Manfred Albrecht[2], and Thomas Dekorsy[1] — [1]University of Konstanz, Germany — [2]Chemnitz University of Technology, Germany

Cobalt antimony skutterudites are interesting due to their promising thermoelectric properties. Filling foreign atoms in its cage-like structure is considered beneficial to their thermoelectric properties. The undoped CoSb3 samples and Co4Sb12 samples with different Yb concentration we studied are fabricated using molecular beam epitaxy and characterized by femtosecond pump and probe spectroscopy with an asynchronous optical sampling system. The transient reflectivity signal is strongly dependent on the Yb concentration. For highly doped samples fast electron-phonon coupling is observed.

DS 24.9 Wed 16:45 H32

**The ineffectiveness of energy filtering at grain boundaries for thermoelectric materials** — •Michael Bachmann, Michael Czerner, and Christian Heilger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

We present results that show the ineffectiveness of energy filtering at grain boundaries [1]. Our results are based on a model that we developed to describe electron transport in nanograined materials. For the band structure we use a one band effective mass model. The transport is calculated using the Landauer formalism. The grain boundaries are described using the model by Seto [2]. In this model additional trapping states in the grain boundary are assumed that causes a space charge accumulation in the grain boundary. This space charge distribution leads to a formation of a double Schottky barrier. It is believed that such barriers can increase the efficiency of thermoelectric materials by energy filtering effects. Since in our model the space charge distribution depends on the doping concentration and therefore also the barrier, we are able to calculate the electron transport in dependence of the doping concentration. For low doping concentration we obtain a energy filtering effect, but for high doping concentration that are necessary for effective thermoelectric material the barrier height and width is too small to have an impact on the transport. Therefore, we conclude that electrostatic barriers play no role for thermoelectric devices.

[1] M.Bachmann, M. Czener and C.Heiliger, Phys. Rev. B 86, 115320
[2] J. Seto, J.Appl. Phys. 46 5247 (1975)