DS 60: Thermoelectric Materials, Thin Films, and Nanostructures II (Focused Session – Organisers: Nielsch, Rastelli, Balke)

Time: Friday 14:00–15:45 Location: GER 37

DS 60.1 Fri 14:00 GER 37

Harman measurements on laser-annealed thin films of Si and Ge nanoparticles — •Benedikt Stoib[1], Martin S. Brandt[1], Nils Petermann[2], Hartmut Wiggers[2], and Martin Stutzmann[1] — [1]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching — [2]Institut für Verbrennung und Gasdynamik, Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg

We discuss Harman measurements of the thermoelectric figure of merit ZT for thin films made of nanoscale Si, Ge and SiGe particles. The particles are prepared by plasma decomposition of silane and/or germane in a microwave plasma reactor and have a size of around 25 nm in the case of SiGe particles. Thin films are prepared by a drop-casting process on quartz substrates, followed by an annealing step with a high intensity pulsed laser. Films with μm-range thicknesses are subjected to a specific current cycle at varying temperature. The Harman method is known to directly yield the thermoelectric figure of merit ZT under certain conditions. In this contribution, we show temperature-dependent measurements suggesting values of $ZT > 0.3$ at 650 K for SiGe. The presented data are discussed taking into account possible parasitic effects.

DS 60.2 Fri 14:15 GER 37

3ω measurements of half-Heusler thin films using a passive circuit — •Christian Mix, Tino Jäger, and Gerhard Jakob — Institut für Physik, Universität Mainz, Staudinger Weg 7, 55128 Mainz

One possibility to increase the thermoelectric Figure-of-Merit of thin films is to decrease the thermal conductivity, by replacing the thin film with a superlattice of the same thickness. This is one of the major challenges in ongoing research. For this purpose a 3ω-measurement system is built up to obtain the thermal conductivity of thin films. To nullify influences of active elements, a setup including a wheatstone bridge is used. Different aspects of the measurement system like the influence of thermal penetration depth and the energy losses by atmosphere are discussed. Additionally, first results on Half-Heusler thin films and superlattices are presented.

DS 60.3 Fri 14:30 GER 37

Cross-plane thermal conductivity of Ge/Si multilayers — •Peixuan Chen, Jianjun Zhang, Fabio Pezzoli, Mathieu Stoffel, Christoph Deneke, Armando Rastelli, and Oliver Schmidt — Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany

One of the approaches to increase the efficiency of a thermoelectric converter is the reduction of the lattice thermal conductivity k of the employed materials. By using multilayers of Ge nanodots separated by Si barriers we have shown that it is possible to precisely control the thermal conductivity of the resulting nanostructured material by simply varying the thickness of the Si spacer [1]. Here, we study the dependence of k of Ge/Si layers on the amount of deposited Ge. By gradual increasing the amount of deposited Ge, flat Ge/Si multilayers with different Ge thickness and nanodot Ge/Si multilayers with different dot density were obtained. We performed thermal conductivity measurements by using the 3-omega method and found that: (i) in the case of Ge/Si flat multilayers the total thermal resistance increases and k decreases with increasing Ge amount; (ii) in the case of Ge/Si nanodot multilayers, the change of total thermal resistance and thermal conductivity is smaller than the error bar. In order to study the effect of alloying and interface sharpness, we have performed postgrowth annealing on the nanodot multilayers. By gradual increase of the annealing temperature, the thermal conductivity of Ge/Si film increases and finally approaches the values of GeSi alloys.

[1] G. Pernot et al., Nature Materials 9, 491 (2010)

DS 60.4 Fri 14:45 GER 37

Half Heusler thin film superlattices — •Tino Jaeger[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, Universität Mainz, Staudinger Weg 7, 55128 Mainz, Germany — [2]Institut für Anorganische Chemie und Analytische Chemie, Universität Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [3]EMPA -Eidgenössische Materialprüfung und -forschungsanstalt, Festkörperchemie und Katalyse, Ueberlandstrasse 129, 8600 Duebendorf, Switzerland

Due to rising energy costs and carbon dioxide concentration in the atmosphere thermoelectric materials have moved into focus. Recently, the efficiency of thermoelectric materials is to be increased by nanostructuring. So, Seebeck coefficient and electrical conductivity are increased or/and thermal conductivity is reduced. Here, DC magnetron sputtering is used for epitaxial deposition of thin films containing Half-Heuslers. As bulk materials, TiNiSn and $Zr_{0.5}Hf_{0.5}NiSn$ exhibit promising thermoelectric properties. It is shown that TiNiSn and $Zr_{0.5}Hf_{0.5}NiSn$ are suitable to be epitaxially deposited on top of each other. Therefore, both Half-Heusler materials can be used for superlattice structures to decrease the thermal conductivity perpendicular to the surface. The relation between crystal quality and in-plane thermoelectric properties is been shown.

DS 60.5 Fri 15:00 GER 37

Investigations on the optimum Zr to Hf ratio in $Zr_{1-x}Hf_xNiSn$ as n-type thermoelectric materials — •Michael Schwall and Benjamin Balke — Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany

Excellent XNiSn (X=Ti, Zr, Hf) n-type thermoelectric materials (ZTmax= 1.5) were reported from several groups in Asia and the USA. The best reported half-Heusler materials exhibit thereby always the same Zr to Hf ratio. Because of the demands on a thermoelectric converter (TEC) like environmental friendliness, low-cost and future availability of raw materials, we investigated the effect of varying the Zr to Hf ratio and the effect of Ti substitution on the X-position. The best Zr to Hf ratio was then substituted with the best Ti value. We will present the results of the thermal transport measurements, the structure analysis of the materials and outgoing from these results some ideas for further investigations to increase the ZT.

DS 60.6 Fri 15:15 GER 37

Electronic structure and thermoelectric properties of doped Heusler compounds $CoTi_{1-x}M_xSb$(M = Sc,V) — •S. Ouardi[1], G. H. Fecher[1], B. Balke[1], X. Kozina[1], M. Schwall[1], G. Stryganyuk[1], S. Ueda[2], K. Kobayashi[2], and C. Felser[1] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany — [2]NIMS Beamline Station at SPring-8, National Institute for Materials Science, Hyogo 679-5148, Japan.

Heusler compounds are considered to be promising thermoelectric materials because of their potential role in the realization of environmentally friendly technology. Complex $C1_b$ compounds such as CoTiSb are promising thermoelectrical materials. The substitutional series of Heusler compounds $CoTi_{1-x}T'_x$Sn (T'= Sc, V) were synthesized and experimentally investigated with respect to their electronic structure and transport properties. The results show the possibility to create n-type and p-type thermoelectrics within one compound. The carrier concentration and temperature dependence of electrical conductivity, Seebeck coefficient, and thermal conductivity were investigated. Hard X-ray photoelectron spectroscopy was carried out to study the details of the electronic structure and relate it to the transport properties. Massive *"in gap"* states are found in pure CoTiSb that contain about 0.07 electrons per cell. This proves that the electronic states close to the Fermi energy play a key role on the behavior of the transport properties. *This work was financially supported by the Federal Ministry of Economics and Technology (0327876D thermoHEUSLER).*

DS 60.7 Fri 15:30 GER 37

Electronic structure and thermoelectric properties of doped Heusler compounds. — •G. H. Fecher, S. Ouardi, and C. Felser — Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany

Different substitutional series of Heusler compounds $XTi_{1-x}Y_xZ$ (where X = Co, Ni, Y = Sc, V and $0 < x < 0.2$, and Z = Sn, Sb) were investigated by ab-initio calculations of their electronic structure, mechanical, optical, and transport properties. Different theoretical methods were applied. The results from the ground state electronic structure calculations were used together with Boltzmann transport theory to calculate the thermoelectric transport properties. The mixed

compounds with random site occupancy were treated by the virtual crystal and coherent potential approximations. It is found that the in-gap states observed for the pure compound arise from anti-site disorder by partially filling the vacant site of the lattice by Ti through swap and contain about 0.1 electrons per cell. This "self-doping" results in the excellent thermoelectric properties of the pure material. The calculated carrier concentration and temperature dependence of electrical conductivity, Seebeck coefficient, and thermal conductivity were calculated in the range from 10 K to 300 K and agree very well with the experimental observation. The sign of the Seebeck coefficient changes from negative for V to positive for Sc substitution. The calculations reveal that the high n-type and low p-type power factors are explained by differences in the chemical disorder scattering induced electric resistivity.