DS 41: Thermoelectric materials III: Heterostructures (Focused session – Organizers: Meyer, Heiliger)

Time: Friday 9:30–11:15 Location: H 2032

DS 41.1 Fri 9:30 H 2032

Phonon transport from *ab initio* in $ZnO_{1-x}S_x$ and $ZnS_{1-x}O_x$ — Michael Bachmann, •Michael Czerner, Saeideh Edalati-Boostan, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

We present results from *ab initio* calculations of $ZnO_{1-x}S_x$ and $ZnS_{1-x}O_x$. We focus our investigations on the Phonondensity of states and the inter atomic force constants in these systems. Furthermore the inter atomic force constants are used in an atomistic Green's function method [1] to obtain the phonon transmission function of the system. The transmission function can then be used to calculate the thermal lattice conductance within the linear response regime. Having the lattice conductance we can estimate the usability of such systems for thermoelectric applications.

DS 41.2 Fri 9:45 H 2032

Experimental determination of the thermoelectric figure-of-merit and optimal annealing condition of electrodeposited films. — •Hans-Fridtjof Pernau, Martin Jägle, Alexandre Jacquot, Benjamin Bayer, Karina Tarantik, Olivia Herm, Harald Böttner, Jan König, and Kilian Bartholomé — Fraunhofer Institut für Physikalische Messtechnik IPM, Heidenhofstr. 8, 79110 Freiburg, Deutschland

Thermoelectric characterization tools developed at the Fraunhofer-IPM can not only be used for the characterization of thermoelectric properties, but also for optimization purposes. For example, thin film samples can be monitored on-line during annealing. These tools optimiza-tion technique is applicable for sputtered or electroplated films. An overview on the 3-omega method in combination with other measurement techniques allowing a determination of the figure of merit will be given.

This work presents the on-going efforts of the Fraunhofer-IPM to measure the thermoelectric figure of merit of electrodeposited or sputtered films and the fast determination of optimal an-nealing conditions.

DS 41.3 Fri 10:00 H 2032

Epitaxial growth and control of sodium content in Na_xCoO_2 thin films grown by pulsed laser deposition — •Sandra Hildebrandt, Philipp Komissinskiy, Marton Major, Wolfgang Donner, and Lambert Alff — Institut für Materialwissenschaft, Technische Universität Darmstadt, 64287 Darmstadt, Germany

A variety of interesting phenomena such as large thermoelectric power and (possibly) unconventional superconductivity of the water-intercalated compound are observed in sodium cobaltate Na_xCoO_2 depending on sodium content[1,2]. We have grown c-axis oriented Na_xCoO_2 thin films on $SrTiO_3$(100) using pulsed laser deposition. The sodium stoichiometry of the films is controlled within $0.38 < x < 0.84$ by varying the post-deposition annealing conditions in oxygen. Thus, low sodium content ($x < 0.5$) can be achieved without the commonly used chemical deintercalation of Na using a Br_2- (or I_2-) based solution. X-ray diffraction analysis demonstrates that the Na_xCoO_2 films grow in two twin domains rotated by 15 and 45 degrees relative to [100] $SrTiO_3$. After annealing for 15-20 minutes single-crystalline films are obtained with a full width at half maximum of the (002) reflection below 0.2 degrees.

1. I. Terasaki, Y. Sasago, and K. Uchinokura, Physical Review B **56**, 12685 (1997).

2. K. Takada, H. Sakurai, E. Takayama-Muromachi, F. Izumi, R. A. Dilanian, and T. Sasaki, Nature **422**, 53 (2003).

This study was supported by DFG through project AL560/6-1.

DS 41.4 Fri 10:15 H 2032

Thermal conductivity in $Pr_{1-x}Ca_xMnO_3$ and $SrTiO_3$ thin film systems — •Stefanie Wiedigen[1], Thilo Kramer[1], Manuel Feuchter[2], Kodanda R. Mangipudi[1], Jörg Hoffmann[1], Marc Kamlah[2], Cynthia A. Volkert[1], and Christian Jooss[1] — [1]Institute for Materials Physics, University of Göttingen, Germany — [2]Institute for Applied Materials, Karlsruhe Institute of Technology, Germany

Epitaxial multilayers and superlattices are one recent approach for the design of efficient thermoelectrics. To study the effect of phonon blocking and scattering on thermal conductivity of oxide multilayers, a combination of two perovskites with promising thermoelectric properties is selected: the orthorhombic $Pr_{1-x}Ca_xMnO_3$ and the cubic $SrTiO_3$. In order to investigate the effect of microstructure, interfaces and acoustic impedance mismatch on thermal conductivity κ high preparation quality is needed. Our thin films were prepared by ion-beam and magnetron sputtering. Structural analysis is done by XRD and TEM and will be presented in combination with thermal conductivity measurements using the 3ω method. Single layers of $Pr_{1-x}Ca_xMnO_3$ show low κ values and no significant increase of thermal conductivty with increasing doping. In homoepitaxial single layers of $SrTiO_3$ preparation conditions have a high impact on κ, most probably due to different concentrations of point defects. $Pr_{1-x}Ca_xMnO_3/SrTiO_3$ multilayers show a κ decreases systematically with increasing number of double layers. The results are discussed in the light of the theoretically calculated phonon dispersion and the experimentally observed microstructure.

DS 41.5 Fri 10:30 H 2032

Thermoelectric Transport in strained Si and Si/Ge heterostructures — Nicki F. Hinsche[1], Ingrid Mertig[1,2], and •Peter Zahn[1] — [1]Martin-Luther-Universität, Institut für Physik, Von-Seckendorff-Platz 1, D-06120 Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle

Starting from bulk silicon, we study the change in thermoelectric properties due to symmetry breaking in strained Si which might be applied in nanostructured thermoelectrics.

In detail, the anisotropy of the electrical conductivity, the thermopower and the resulting power factor in the in-plane and cross-plane directions are studied in dependence on doping level, temperature, and strain in [001] and [111] direction. Our results show that tetragonal [1] and rhombohedral [2] distortions have a strong influence on the thermoelectric transport properties. The electronic structure is calculated self-consistently within the framework of density functional theory. The transport properties are studied in the diffusive limit applying the Boltzmann theory in relaxation time approximation [3].

Furthermore, we present results for strained Si/Ge heterostructures, showing an enhanced power factor in cross-plane direction under electron doping as suggested by Koga *et al.* [4].

[1] N. F. Hinsche, I. Mertig, and P. Zahn, *J. Phys.: Cond. Matt.* **23**, 295502 (2011). [2] N. F. Hinsche, I. Mertig, and P. Zahn, *to be published.* [3] I. Mertig, *Rep. Prog. Phys.* **62**, 237 (1999). [4] T. Koga, X. Sun, S. B. Cronin, and M. S. Dresselhaus, *Appl. Phys. Lett.* **75**, 2438 (1999).

DS 41.6 Fri 10:45 H 2032

Electric Characterization of Si/Ge Superlattices — •Markus Trutschel[1], Katrin Bertram[1], Bodo Fuhrmann[1], Alexander Tonkikh[2], Peter Werner[2], and Hartmut S. Leipner[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Interdisziplinäres Zentrum für Materialwissenschaften, Heinrich-Damerow-Str. 4, D-06120 Halle, Germany. — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany.

Si/Ge superlattices are expected to have an increased figure of merit due to their two dimensional structure. The enhancement in the figure of merit can be attributed to a decreased thermal conductivity due to phonon scattering at the interfaces between the Si/Ge layers. For this reason applications are aspired in cross plane direction.

The measurement of electrical properties in cross plane direction of thin films with thicknesses in the nanometer range is strongly affected by measurement uncertainties. In this work, we studied the requirements of the electrical conductivity measurement cross plane using a modified transmission line model (TLM). For this purpose, a suitable mesa structure for TLM measurements was developed. In order to obtain more precise results, a finite element model was performed to simulate the current density distribution in the sample. Additionally we present experimental results in comparison to the calculated values.

We thank the BMBF for financial support.

DS 41.7 Fri 11:00 H 2032

Thermoelectric Transport in Bi_2Te_3/Sb_2Te_3 heterostructures — •Nicki F. Hinsche[1], Bogdan Yu. Yavorsky[1], Ingrid Mertig[1,2] und Peter Zahn[1] — [1]Martin-Luther-Universität, Institut für Physik, Von-Seckendorff-Platz 1, D-06120 Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle

Bi_2Te_3/Sb_2Te_3-heterostructures show a remarkable enhancement of the thermoelectric figure of merit compared to the bulk materials [1]. While gaining much attention in the last decade, the physical origin of this enhancement is still under debate. To contribute on this, we studied the electronic structure of Bi_2Te_3/Sb_2Te_3 heterostructures with a fully relativistic screened Korringa-Kohn-Rostoker Greens function method. The thermoelectric transport properties in-plane and cross-plane were calculated within the relaxation time approximation of the Boltzmann theory. The influence of composition, interfacial strain, and doping on the anisotropic thermoelectric properties were studied in detail [2,3].

[1] R. Venkatasubramanian, E. Siivola, T. Colpitts, and B. O'Quinn, *Nature* **413**, 597 (2001). [2] N. F. Hinsche, B. Yu. Yavorsky, I. Mertig, and P. Zahn, *Phys. Rev. B* **84**, 165214 (2011). [3] B. Yu. Yavorsky, N. F. Hinsche, I. Mertig, and P. Zahn, *Phys. Rev. B* **84**, 165208 (2011).