DS 12: Poster Session II: Functionalized semiconductor nanowires (jointly with HL); Resistive switching (jointly with DF, KR, HL); Thermoelectric materials

Time: Monday 17:00–20:00 Location: Poster B1

DS 12.1 Mon 17:00 Poster B1

Optical properties of Sn-doped CdS nanowires — •Marcel Wille[1], Sebastian Geburt[1], Robert Röder[1], Mengyao Zhang[2], Jia Grace Lu[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]Department of Physics and Electrical Engineering, University of Southern California, Los Angeles, USA

Nanowires (NWs) are promising candidates for future optoelectronic applications due to their possibility of light generation, waveguide properties and light amplification in a Fabry-Perot resonator. The controlled modification of their electrical and optical properties, for example by doping, will continue the consequent progress in NW research. The in-situ doping during the VLS synthesis is a difficult task due to the restricted solubility of dopants in gold (Au), which is typically used as catalyst. Therefore, we investigate an alternative catalyst (Sn) in order to succeed in successful doping during growth. SEM an TEM were performed to analyse the morphology of CdS NWs synthesized under usage of Sn as catalyst. The stoichiometry and successful doping with Sn was proven by EDX point measurements and mappings. In micro-PL, macro-PL and CL measurements at low and room temperatures the NBE, DLE and DAP (donor-acceptor pair) transitions were investigated to state about the optical properties. The occurring DAP transition, which was proven by power- and temperature dependent PL measurements, indicates the successful incorporation of Sn into the CdS NWs.

DS 12.2 Mon 17:00 Poster B1

Tailoring CdS nanowire lasing resonators — •Robert Röder[1], Sebastian Geburt[1], Andreas Johannes[1], Markus Glaser[2], Alois Lugstein[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena — [2]Institut für Festkörperelektronik, TU Wien, Floragasse 7, A-1040 Wien

The nanophotonics research for the development of on-chip optical components has to be intensified due to the forthcoming limits of conventional electronic integrated circuits. Semiconductor nanowires mark the physical size limit of a multimode photonic laser system. Thus, they are promising for circumventing these limits via optical data transmission and processing. The green spectral range around 2.4 eV is made accessible by high quality VLS synthesized cadmium sulfide nanowires (CdS NW) acting as Fabry-Pérot laser resonators with a remarkable low threshold of 10 kW/cm^2 at room temperature [Geburt et al, Nanotechnology 23, 365204 (2012)]. The resulting task for the processing of CdS nanolasers with reproducible properties remains in defining the resonator: The mode spacing can be adjusted by reducing the cavity length. The reflectivity of the guided modes can be enhanced as well by polishing the facet ends. Thus, preparation techniques for tailoring the resonator are demonstrated using focused ion beams (FIB) and a focused laser beam.

DS 12.3 Mon 17:00 Poster B1

Luminescence decay dynamics of colloidal CdSe quantum dots in different environments — •Michael Diez[1], Stephanie Bley[1], Dongchao Hou[1], Sebastian Resch[2], Siegfried Waldvogel[2], Jürgen Gutowski[1], and Tobias Voss[1] — [1]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen, Germany — [2]Institute of Organic Chemistry, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

The functionalization of semiconductor surfaces with colloidal quantum dots has gained substantial interest because of its wide application in optical sensing and energy harvesting. The quantum dots can be selectively attached to semiconductor surfaces with the help of linker molecules. We have studied the luminescence decay dynamics of colloidal CdSe quantum dots functionalized with ω-mercapto alkanoic acid in different environments. As optical excitation source we use a frequency-doubled Ti:sapphire laser ($\lambda = 350\,nm$, $\Delta t = 60\,fs$, $f = 82\,MHz$ and $E_{pulse} = 12\,nJ$). We detect the luminescence signal with a streak camera and an attached spectrometer ($\Delta t < 2\,ps$, $\Delta\lambda < 0.2\,nm$). For colloidal CdSe quantum dots in aqueous solution, we find that the luminsescence decay time can be well fitted with a biexponential decay (shorter decay time $t_1 \approx 200\,ps$, longer decay time $t_2 \approx 3\,ns$). Furthermore, we discuss the importance of surface and bulk states for the observed biexponential decay and study the change of t_1 and t_2 for quantum dots attached to different oxide surfaces. The observed results will allow for the optimization of quantum dot properties for specific optoelectronic applications.

DS 12.4 Mon 17:00 Poster B1

Einfluss der Prozessparameter auf das Wachstum von ZnO-Nanodrähten — •Matthias Ogrisek, Andreas Johannes und Carsten Ronning — Friedrich-Schiller-Universität, Jena, Deutschland

ZnO Nanostrukturen können sehr einfach über Gasphasentransport und -Abscheidung in einem horizontalen Rohrofen synthetisiert werden. In den vergangenen Jahren stand hier insbesondere die Herstellung von ZnO Nanodrähten über den Vapor-Liquid-Solid (VLS) Mechanismus im Fokus. Dabei ist das Verständnis über die wechselseitigen Einflüsse der einzelnen Prozessparameter auf die resultierenden Nanostrukturen nicht vollständig geklärt. ZnO Nanodrähte und andere Strukturen wurden durch thermisches Verdampfen von ZnO:C Pulver (carbothermal method) auf verschiedenen Substraten (SiO2, AZO) gewachsen. Die sich gegenseitig beeinflussenden Prozessparameter erlauben dabei das Wachstum von Nanodrähten bei sehr unterschiedlichen Bedingungen. Untersucht wurden die erzeugten ZnO Nanostrukturen mittels Rasterelektronenmikroskopie (REM) und Photolumineszenz-Spektroskopie (PL). Über den Vergleich der Bandkantennahen- und Defektbandemission lassen sich Rückschlüsse auf die relative Defektkonzentration ziehen.

DS 12.5 Mon 17:00 Poster B1

Growth of GaAs nanowires using the ANKA portable MBE system — •Jean-Wolfgang Hornung[1], Emmanouil Dimakis[2], Philipp Schroth[1], Lutz Geelhaar[2], and Tilo Baumbach[1] — [1]Karlsruhe Institute of Technology, Institute for Photon Science and Synchrotron Radiation, Karlsruhe, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

We present results on first growth experiments with the portable Molecular Beam Epitaxy (PMBE) System at ANKA performed at the PDI in Berlin. This system enables the growth of nanostructures in the (In,Ga)As-material system and in-situ monitoring of growth processes using synchrotron radiation at various synchrotron radiation facilities such as ANKA, ESRF, PETRA III. The properties of such NWs are of great importance for the fabrication of high performance electronic devices such as vertical transistors and solar cells.

For future time-resolved XRD-measurements on single NWs, the control of the axial growth rate and number density is very important. We show that by changing the growth parameters (growth temperature, V/III-ratio) we were able to influence these properties. In particular we grew self-catalyzed GaAs-Nanowires (NWs) on Si(111) substrates covered with thin oxide layers of different thicknesses. In-situ the growth process was monitored using RHEED measurements. Ex-situ the samples were characterized by SEM measurements.

We gratefully acknowledge the help of C. Hermann, A.-K. Bluhm and H. - P. Schönherr at PDI, as well as the support by Dr. B. Krause and H.-H. Gräfe at ANKA.

DS 12.6 Mon 17:00 Poster B1

Structural and resistive switching properties of $SrTiO_3$ deposited by RF sputtering — •Benjamin Roessler, Jura Rensberg, Frank Schmidl, and Carsten Ronning — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Strontium titanate ($SrTiO_3$) exhibits bipolar resistive switching between a high- and a low-resistance state when applying an appropriate electric field. The possibility to deposit $SrTiO_3$ at room temperature by magnetron sputtering on silicon substrates without buffer layers makes it one of the promising candidates for future nonvolatile data memory application. Therefore, we deposited polycrystalline $SrTiO_3$ on p-Si(100) as well as p-Si(110) at room temperature with a fixed oxygen-to argon content ratio of 1:2. The microstructure as well as the crystalline quality of the films was analyzed using cross-sectional electron microscopy and X-ray diffraction analysis. For both substrates

a broad grain size distribution was found for the as-deposited films. To improve the crystalline quality post-deposition annealing was performed up to temperatures of 1000°C. In this contribution we discuss the structural changes and electrical properties of $SrTiO_3$, i.e. the resistive switching properties as a function of the annealing temperature.

DS 12.7 Mon 17:00 Poster B1

Memory Effects in Resistive Ion-beam Modified Oxides — •S. Gemming[1,2], D. Blaschke[1,2], K. Potzger[1], P. Zahn[1], A. Bogusz[2], H. Schmidt[2], T. Mikolajick[3], S. Slesazeck[3], H. Wylezich[3], B. Abendroth[4], D. C. Meyer[4], S. Rentrop[4], R. Dittmann[5], K. Skaja[5], R. Waser[5], J. Rensberg[6], C. Ronning[6], N. A. Spaldin[7], and D. Basov[8] — [1]HZ Dresden-Rossendorf, D-01314 Dresden — [2]TU Chemnitz, D-09107 Chemnitz — [3]TU Dresden, D-01062 Dresden — [4]TU Bergakademie Freiberg, D-09596 Freiberg — [5]FZ Jülich, D-52425 Jülich — [6]Friedrich Schiller University Jena, D-07743 Jena — [7]ETH Zürich, CH-8092 Zürich, Switzerland — [8]U.C. San Diego, La Jolla CA 92093-0354, U.S.A.

The Virtual Institute 'Memriox' establishes a joint research initiative in the field of ion-tailored oxide-based memristive elements, to be pursued within a novel and unique combination of core competences from the Helmholtz centers Dresden-Rossendorf and Jülich and their university partners in Dresden, Freiberg, Jena, San Diego, and Zürich. A nanoscale memristive element may prove the concept of the ultimate future non-volatile memory cell with a resistance set directly by electric currents. The Virtual Institute aims at stepping beyond the established layer-by-layer control of intrinsic defects during the synthesis of memristive homojunctions. The project is financed by the Initiative and Networking Funds of the Helmholtz Association (VH-VI-442).

DS 12.8 Mon 17:00 Poster B1

Transmission X-ray microscopy of resistively switched epitaxial Fe-doped SrTiO3 MIM structures — •Holger Wasmund[1], Annemarie Köhl[1], Peter Guttmann[2], Katja Henzler[2], Stephan Werner[2], Sebastian Schmelzer[1], Regina Dittmann[1], and Rainer Waser[1] — [1]FZ Jülich, PGI-7, Germany — [2]HZB, Institute for soft Matter and functional Materials, Germany

There exists strong experimental evidence that the resistance change in transition metal oxides is caused by a valency change on a nanoscale. Transmission X-ray microscopy exhibit the potential of observing bulk spectral information of the sample with a spatial resolution of 25nm unlike other methods which exclusively probe the surface e.g. XPS. One central issue in TXM probe preparation is the sample thickness which should not exceed 100nm. As a first approach we studied polycrystalline STO devices on SiN membranes which were switched in two different resistive states. To analyse epitaxial grown STO devices we prepared SRO|STO|Pt MIM structures on top of NGO substrates with an intermediate sacrifical layer by pulsed laser deposition and sputtered Pt electrodes. A chromium adhesion layer and a carbon film were deposited on top of the stack in order to serve as a carrier foil, followed by a selective etching step of the sarifical layer to release the specimen from the substrate. XAS spectra measurements at the Ti L edge and the Fe L edge for electrode pads in different resistive states were realized at the U41 beamline at Bessy II. We observed significant changes in the Ti spectra which are indications for a valency change in a filament like region.

DS 12.9 Mon 17:00 Poster B1

Adaptive Robot learning via (simulated) memresistive Elements — •Marius Schirmer and Andy Thomas — Bielefeld University, Bielefeld, Germany

Memristors are new circuit elements that fill the gap in relations between the circuit variables flux ϕ and charge q. Like their name consisting of *Mem*ory and Res*istor* presumes, they are resistors with memory. The resistance depends on the current *i(t)* that was applied to an element earlier. This behavior is similar to the synapse of a living nerve cell and therefore networks of memristors can be used as neuronal networks in hardware circuits.

To visualize the learning process of such a memresistive neuronal network we used a *Lego Mindstorms NXT* robot and designed an interface for using memristors that can be connected to the *NXT brick*. We also designed a circuit board that is simulating memresistive behavior. The Software written in Java allows several different learning tasks.

DS 12.10 Mon 17:00 Poster B1

Thermal conductivity measurements using the Raman shift method — •Simon Filser, Benedikt Stoib, Martin Stutzmann, and Martin S. Brandt — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching

With the aim to determine the in-plane thermal conductivity of laser-sintered thin films of SiGe nanoparticles [1], we study the applicability of a contactless optical method employing the temperature-dependent frequency shift of the LO phonon mode, as observed by Raman spectroscopy, as a measure for the local temperature. We present our results on a variety of model systems such as, e.g., bulk Si, free-standing Si films and rectangular cantilevers validating the method. The pressure-dependent influence of parasitic thermal conduction through the ambient atmosphere is studied, indicating a small effect for single crystalline material, but a significant contribution for the macro-porous laser-sintered system studied here. Free-standing samples of laser-sintered Si nanoparticle thin films were fabricated either by scanning electron microscope-based micro-manipulation or via a liquid-transfer technique. The results of Raman mapping of such membranes are consistent with the sample morphology and provide insight into the thermal transport.

[1] B. Stoib et al., Appl. Phys. Lett., **100**, 231907 (2012)

DS 12.11 Mon 17:00 Poster B1

A real space method for third-order IFCs and phonon relaxation times for Si from first principles — •Marcel Giar, Michael Bachmann, and Christian Heiliger —)I. Physikalisches Institut, Justus-Liebig-Universität, D-35392 Giessen, Germany

We present a real space method to obtain third-order phonon anharmonicities from first principles calculations. The anharmonic interatomic force constants (IFCs) of third order are determined from a real space method involving small displacements of atoms inside a supercell. We calculate the anharmonic IFCs from force fields due to the displaced atoms using the Vienna *Ab Initio* Simulation Package (VASP). We determine the third-order anharmonicities of the potential for the case of silicon (Si). From these the phonon relaxation times for Si are obtained for different phonon branches.

DS 12.12 Mon 17:00 Poster B1

Phonon Transport in Si-Isotope-Multilayer — •Michael Bachmann, Michael Czerner, Robert Henrich, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

In thermoelectrics the maximum achievable efficiency is linked to the material parameters by the so called figure of merit. There are in principle four different material parameters, which can be divided into three electronic parameters and one phononic parameter. The three electronic parameters are the electric conductivity, the Seebeck coefficient, and the thermal conductivity of the electrons. The phononic parameter is the thermal conductivity of the lattice. In silicon the electronic parameters are suitable for thermoelectric applications, but the high lattice thermal conductivity prevents the application of pure silicon in thermoelectric devices. Si-isotope-multilayers are a promising structure, where the lattice thermal conductivity can be decreased and the electronic parameters remain unaffected. We present phonon transport calculations based on an atomistic Greens function method for $^{28}Si/^{29}Si$ and $^{28}Si/^{30}Si$ isotope-multilayers. These results show that a periodic arrangement of the layer-system cannot decrease the phonon thermal conductivity substantially, whereas a random arrangement of the layer-system can lead to a strong decrease in the phonon conductivity.

DS 12.13 Mon 17:00 Poster B1

Glancing Angle Deposited Silicon/Germanium Nanostructures for Electronic Applications — •Christoph Grüner and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, D-04318 Leipzig, Germany

Obtaining control over the physical properties of semiconductors is a big challenge for future electronics. The use of nanostructures can provide this control, since quantum mechanical and surface effects become important. Nanostructured thin films can show higher optical absorption or reduced reflectivity, higher thermal resistivity and altered electrical properties compared to bulk material. Most preparation techniques for such structures, like etching or VLS growth, are limited by a small window of usable materials or process conditions. With Glancing Angle Deposition (GLAD) it is possible to produce nanostructures from a wide range of materials and with highly customizable shapes, such as slanted and vertical wires, spirals or zig-zag

structures. In this technique a highly oblique incidence of deposited material causes small obstacles to cast shadows during the high vacuum deposition, so that areas behind them do not receive material. This leads to the growth of a highly porous thin film. The shape of the individual structures can be influenced by a controlled substrate rotation. We present silicon/germanium GLAD heterostructures with different shapes, a varying germanium distribution and adjustable doping. We also show some approaches to prepare electrical contacts to nanostructure arrays for device integration.

DS 12.14 Mon 17:00 Poster B1

Thermoelectric characterization of $Sn_1(V)_2(VI)_4$ substitutional systems — •Stefan Jakobs[1], Felix Rolf Lutz Lange[1], Karl Simon Siegert[1], Peter Jost[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA - Fundamentals of Future Information Technology, RWTH Aachen University, Germany

The environmental impact of global warming and the steady rise of the world-wide energy demand requires an increased efficiency of energy consumptive applications.

Thermoelectric generators may contribute to increased efficiency since they are able to convert waste heat into electrical energy. The conversion efficiency of thermoelectric materials is characterized by the dimensionless figure of merit $zT = \frac{\alpha^2\sigma}{\kappa}T$. Hence, to gain large zT values, it is mandatory to have a high electrical conductivty σ, a large Seebeck coefficient α and a low thermal conductivity κ. Since charge carriers also contribute to thermal transport, low lattice thermal conductivities are crucial for a high thermoelectric performance.

Thin film $(IV)_1(V)_2(VI)_4$ chalcogenides allow access to a metastable rocksalt phase. While one sublattice consists of Te, the cation site is randomly occupied by Sn, Sb and 25% of vacancies. This unconventionally high degree of disorder in combination with the large amount of vacancies is favourable for low lattice thermal conductivities [1].

Here, we present the thermoelectric properties of $Sn_1Sb_2Te_4$ and $Sn_1Bi_2Te_4$ thin films prepared under different annealing conditions.

[1] E. R. Sittner *et al.*, *Phys Status Solidi* **A**, DOI 10.1002/pssa.201228397

DS 12.15 Mon 17:00 Poster B1

Transport through nano sized pillars — •Thorben Bartsch, Alina Wetzel, David Sonnenberg, Christian Heyn, and Wolfgang Hansen — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Jungiusstraße 11, 20355 Hamburg, Germany

We fabricate GaAs nanopillars with typical lengths between 4-8 nm and diameters of about 100 nm using molecular beam epitaxy [1]. The pillars are linked to a GaAs substrate on one end and to a GaAs layer of variable thickness at the other end. The epitaxial growth of the structure ensures that there are no crystal interfaces at these contacts. The pillars are embedded in a matrix of AlAs that can be selectively removed with hydrofluoric acid.

When the AlAs matrix is removed, the pillars open a gap between the GaAs layer and the substrate [1]. Appling a thermal gradient across the gap, thermal transport through the pillars can be studied. Using the 3-omega method we verified that the thermal transport through the pillars is ballistic in a temperature range at least up to 150 K [2]. Here influences from variations of the heterostructure geometry, especially from variable top layer thicknesses are discussed.

Moreover, in case of doped structures, charge transport through the pillars between two charge reservoirs held at different electric potential can be studied. We present first results of electronic transport experiments. At low temperature, the conductance is found to strongly depend on the strength and orientation of a magnetic field.

[1] Ch. Heyn et al., Appl. Phys. Lett. 98, 033105 (2011)
[2] Th. Bartsch et al., Phys. Rev. Lett. 108, 075901 (2012)

DS 12.16 Mon 17:00 Poster B1

Thermoelectric Transport Properties of GeTe Rich GeTe-Sb_2Te_3 Thin Films — •Felix R. L. Lange[1], Ernst-Roland Sittner[1], Karl Simon Siegert[1], Peter Jost[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA - Fundamentals of Future Information Technology, RWTH Aachen University, Germany

Phase change materials (PCM) are a class of alloys that can be reversibly and rapidly switched between the amorphous and the crystalline state. Since these two states differ significantly in their physical properties such as reflectivity and resistivity they are well suited for future nonvolatile data storage applications. Some PCM along the pseudo-binary line between GeTe and Sb_2Te_3 exhibit a rather unusual combination of physical properties which render these alloys a potential p-type thermoelectric. These alloys allow access to a meta-stable cubic phase where one lattice site is randomly occupied by Ge, Sb and a certain amount of structural vacancies. Only recently Siegrist *et al.* identified disorder in these alloys as the cause of a metal to insulator transition. The degree of disorder can be affected by two independent parameters: stoichiometry and annealing conditions. Since disorder affects both, electrical and vibrational degrees of freedom, this opens up a pathway to tailor electrical and thermal transport properties independently. Using this concept we report enhanced thermoelectric efficiencies for GeTe rich GeTe-Sb_2Te_3 thin films prepared under different annealing conditions [1].

[1] E. R. Sittner *et al.*, *Phys Status Solidi* **A**, DOI 10.1002/pssa.201228397 (2012)

DS 12.17 Mon 17:00 Poster B1

Thermoelectric power factor and full ZT characterization of Bi2Te3-nanowires — •Rüdiger Mitdank[1], Danny Kojda[1], Zhi Wang[3], William Toellner[2], Kornelius Nielsch[2], Peter Woias[3], and Saskia F. Fischer[1] — [1]Novel Materials, Institute of Physics, Humboldt Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [2]Institute of Applied Physics, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany — [3]) IMTEK, University of Freiburg, D-79110 Freiburg

Thermoelectric (TE) properties of single Bi2Te3 nanowires (NW) were investigated using a TNCP (Thermoelectric characterization platform) which allows the determination of the Seebeck coefficient S, the conductivity σ and the thermal conductivity. The NW is deposited between 2 thin and freestanding Si-cantilevers. On each cantilever, 2 Pt-electrodes are arranged serving as microheater and thermometer. The calibration of the TNCP is discussed. In the temperature range 4,2K $<$ T $<$ 300K, the conductivity and the thermopower were measured. The function σ(T) corresponds to a rather metallic behaviour. The thermopower exhibits a maximum near 200 K. For a conductivity of nearly 1000S/cm the thermopower S(300K) varied between -35 μV/K and -50 μV/K. Experiments to determine the thermal conductivity are discussed.

DS 12.18 Mon 17:00 Poster B1

Thickness-dependent thermoelectric properties of BiSb thin films — •Heiko Reith[1,2], Friedemann Voelklein[2], and Michael Huth[1] — [1]Physikalisches Institut, Goethe-University, Frankfurt am Main, Germany — [2]IMtech, Hochschule Rhein Main, Ruesselsheim, Germany

We investigated the thermoelectric properties of BiSb thin films in the thickness range between 50 nm and 500 nm. For the determination of the thermoelectric properties we measured the Seebeck-coefficient and the thermal and electrical conductivity to obtain the figure of merit of the films. The thermal conductivity was measured using a specially designed microchip. For the electrical conductivity and Seebeck-measurement a four point structure deposited on a Si/Si_3N_4-wafer was used. The BiSb films were deposited onto these substrates using a thermal evaporation process. During the deposition of the films the substrates and microchips were placed next to each other and the thickness was detected by a quartz microbalance. Afterwards the thickness was measured with a surface profilometer. We present the used measurement techniques and results. From the measurement results we determine the figure of merit of the films and discuss the results using finite size effect models.

DS 12.19 Mon 17:00 Poster B1

Unexpected temperature dependence of thermal boundary conductance for epitaxial Bi(111) films on Si(001) — •Verena Tinnemann, Tim Frigge, Boris Krenzer, Anja Hanisch-Blicharski, Friedrich Klasing, Annika Kalus, and Michael Horn-von Hoegen — Faculty of Physics and Center for Nanointegration CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Ultrafast time-resolved reflection high energy electron diffraction was used to study the heat transfer from epitaxial Bi(111) films into the Si(001) substrate. Films with thicknesses in the range from 25 nm to 120 nm were prepared in-situ under UHV conditions. In a pump-probe setup the Bi films were excited by 50 fs-laser pulses with a wavelength of 800 nm. Short electron pulses were created by photoemission, accelerated to 7 keV, and focused by an electrostatic lens. For variable time delays between laser pump and electron probe diffraction pat-

terns were recorded. The transient drop of spot intensity is explained in terms of the Debye-Waller effect and reflects the instant heating and subsequent cooling of the Bi films. The thermal boundary conductance of the interface is then determined from the exponential cooling of the film. We show that the thermal boundary conductance increases by more than 35% if the substrate temperature is increased from 80 K to 300 K. This is not explained by numerical simulations of the heat transport using temperature dependent parameters. For the 120 nm thick Bi-film a bi-exponential intensity is observed and explained by diffusion in the film and across the interface.

DS 12.20 Mon 17:00 Poster B1

Structural and electrical properties of thermoelectric $Fe_xCo_{1-x}Sb_3$ thin films — Ayham Dalla, •Marcus Daniel, Andreas Liebig, Fabian Ganss, Gunter Beddies, and Manfred Albrecht — Chemnitz University of Technology, Institute of Physics

Increasing interest in efficiency enhancement of existing energy sources led to an extended research in the field of thermoelectricity. A suitable thermoelectric material like $CoSb_3$ is characterised by a high power factor and a low thermal conductivity. To control and improve the power factor a targeted electrical doping is necessary to achieve charge carrier densities up to 10^{20} cm^{-3}. In case of $CoSb_3$ controlled doping can be obtained by a partially substitution of Co by Fe atoms. In this study, 30 nm thick $Fe_xCo_{1-x}Sb_y$ films have been deposited via MBE onto thermally oxidized Si(100) substrates at room temperature. The samples were post-annealed in ultra-high vacuum for one hour at 450°C. Two sample series with varying Fe content ($0<x<0.5$) were fabricated, a Sb rich ($y = 3.3$) and a Sb deficient series ($y = 2.5$). The composition was verified by RBS and the XRD analysis confirmed $CoSb_3$ as major phase. A systematic decrease of the extracted lattice parameter with increasing Fe content indicated the substitution of Co by Fe atoms. The electrical characterization was performed in a temperature range between 4 K and 300 K. Both series show an increase in charge carrier concentration with increasing Fe content, and thus a decrease in resistivity. The temperature dependence of the resistivity revealed for both sample series a change from semiconducting to metallic behaviour at a critical charge carrier concentration.

DS 12.21 Mon 17:00 Poster B1

Measurement setup fpr simultaneous determination of electrical conductivity, Hall coefficient and Seebeck coefficient. — •H. Kolb, J. de Boor, A. Sesselmann, T. Dasgupta, G. Karpinski, and E. Müller — DLR, Institute of Materials Research, Cologne

Thermoelectric materials can convert heat directly into usable electrical energy. An important aim in thermoelectric research is to find and optimize suitable materials and improve their performance to get higher efficiency. For a complete characterization it is in general required to do several different measurements in different apparatuses which can be challenging and time consuming. Therefore we developed a measurement system that can measure three of the thermoelectric key quantities (electrical conductivity, Seebeck- and Hall coefficient) simultaneously from room temperature up to 1000K, which is a typical temperature region for many potential applications of these materials. All three quantities are coupled via the charge carrier concentration and therefore a simultaneous measurement is important for a deep insight in the charge carrier transport in the sample. This is particularly important for thermally instable materials, where consecutive measurements can easily lead to misinterpretations. Four sheathed thermocouples arranged in a van der Pauw geometry are pressed by small springs on a round sample for electrical contact. This special arrangement allows for the electrical measurements, while the thermocouples allow for a determination of the Seebeck coefficient if an additional temperature gradient is applied. We will discuss technical details, features and limitations of the setup.

DS 12.22 Mon 17:00 Poster B1

Anomalous enhancement of the thermoelectric figure of merit by V co-doping in $SrTiO_3$ — •Udo Schwingenschlögl and Mousumi Upadhyay-Kahaly — KAUST, PSE Division, Thuwal, Saudi Arabia

The effect of V co-doping in Nb-$SrTiO_3$ and Pr-$SrTiO_3$ is studied by full-potential density functional theory. While in Nb-$SrTiO_3$ a high carrier density counteracts a high thermoelectric figure of merit, the trend is inverted by V co-doping. A similar but even more pronounced effect is found in Pr-$SrTiO_3$. The mechanism leading to this behavior is explained in terms of a local spin-polarization introduced by the V ions. Our results indicate that magnetic co-doping can be a prominent tool for improving the thermoelectric figure of merit.

Reference: Applied Physics Letters **100**, 193110 (2012)

DS 12.23 Mon 17:00 Poster B1

The effect of interfaces on the thermoelectric properties of laterally microstructured ZnO-based thin-films — •David Hartung, Florian Gather, Achim Kronenberger, Martin Eickhoff, Bruno K. Meyer, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen

A series of samples was laterally microstructured with a self-aligned pattern transfer method consisting of alternating stripes of ZnO grown by molecular-beam epitaxy and radio-frequency sputtered Ga-doped ZnO stripes. The MBE-grown ZnO thin film samples were laterally microstructured by photolithography followed by ion-beam etching in order to obtain different lateral arrangements of stripes of defined interface geometry. In a second step the free regions between the stripes of MBE-grown ZnO were sputtered with Ga-doped ZnO. A lift-off step completes the micro-fabrication of a planar alternating ZnO/ZnO:Ga bar structure on each sample.

Throughout the series the bar width and hence the number of interfaces was kept constant, but the interface profile was varied yielding different interface lengths and geometries.

We measured in-plane as a function of temperature the Seebeck coeffificient S and the electrical conductivity σ of the samples with the transport direction perpendicular to the stripe direction.

The measured data were compared to simulated data using an empirical network model.

DS 12.24 Mon 17:00 Poster B1

Thermoelectric properties of $ZnO_{1-x}S_x$ thin films — •Florian Gather, Achim Kronenberger, Peter J. Klar, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen

We investigated the thermoelectric properties of rf-sputtered $ZnO_{1-x}S_x$ thin films on sapphire substrates. Due to its good availability and its non-toxicity, $ZnO_{1-x}S_x$ is a promising candidate for thermoelectric applications. The electric conductivity σ, the Seebeck coefficient S and carrier concentrations of a series of hydrogen doped samples and aluminum doped samples respectively were determined in in-plane direction over a wide temperature range. For the investigation of the influence of the sulphur concentration x on the thermal conductivity κ we employed the 3-omega method on a series of undoped thin-films. The measurements reveal a reduced κ in cross-plane direction of the samples containing sulphur compared to zinc-oxide samples. Using Raman spectroscopy we found indications for local phonon modes of oxygen in zinc-sulfide and of sulphur in zinc-oxide, respectively. These local phonon modes cause the reduction of κ observed in the experiments. Both sample series are compared in terms of crystal quality and grain size using XRD-analysis and atomic force microscopy.