DS 43: Poster II: Thin Film Chalcogenide Photovoltaics; Thermoelectric Materials, Thin Films, and Nanostructures

Time: Wednesday 15:00–17:30 Location: P2

DS 43.1 Wed 15:00 P2

Aspects of designing an optimized molybdenum back contact in CIGS-technology — •Michael Oertel, Stefan Götz, Jakob Haarstrich, Heinrich Metzner, Udo Reislöhner, Carsten Ronning, and Werner Wesch — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany

In $Cu(In,Ga)Se_2$(CIGS)-solar cell and module production, the sputtering of the molybdenum back contact is the first step in nearly all process lines. We present our results of experiments to elucidate the different aspects which have to be kept in mind when depositing the molybdenum back contact by dc-magnetron sputtering. These aspects include: I) The adhesion of the molybdenum to the glass substrate as well as the adhesion of the CIGS-layer to the molybdenum, II) electrical conductivity, III) sodium diffusion and IV) the specific contact resistance of the molybdenum to the aluminium doped zinc oxide (Al:ZnO) window layer. We present our three layer design of the back contact which combines an optimized adhesion to both the substrate and the absorber and also a high electrical conductivity. X-ray diffraction measurements (XRD) are employed to characterize each single layer. We also discuss I-U-measurements of $CuInSe_2$-solar cells made in a sequential absorber layer process in order to study the sodium transport behaviour of molybdenum back contacts sputtered at different argon sputter pressures. The sodium content in the absorber and the different back contact layers is measured by secondary ion mass spectroscopy (SIMS). A lowest value of the specific contact resistance between the Mo and the Al:ZnO of $(1.37 \pm 0.14) \cdot 10^5 \Omega\mathrm{cm}^2$ was determined.

DS 43.2 Wed 15:00 P2

Characterisation of Cu_2ZnSnS_4 — •Jan E. Stehr[1], Detlev M. Hofmann[1], Bruno K. Meyer[1], Folker Zutz[2], Christine Chory[2], Ingo Riedel[2], and Jürgen Parisi[2] — [1]1st Physics Institute, Justus-Liebig-University Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [2]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Carl-von-Ossietzky-Straße 9-11, 26129 Oldenburg, Germany

Cu_2ZnSnS_4 (CZTS) is an interesting material for thin film photovoltaic applications. It has a band gap energy in the required range (~ 1.5 eV) and avoids the cost intensive Indium being part of the solar-cell-absorbers based in $CuInS_2$. We investigated CZTS nanoparticles prepared by wet chemistry and deposited in the form of thin films on glass substrates by optical absorption and magnetic resonance spectroscopies. Optical absorption starts at about 1.3 eV which indicates that some centres causing sub-band-gap absorption are present in the material. Low temperature EPR spectra reveal the presence of Cu^{2+} by the observation of the typical 4 line spectrum caused by the hyperfine splitting. Regarding the precursors used for synthesis one expects copper to be in the valence state of 1 (Cu^+) thus the result may give a first experimental hint on the origin of the intrinsic p-type conductivity of the material.

DS 43.3 Wed 15:00 P2

Modeling the Thermal Conductance of Silicon Phononic Crystal Plates — •Stefanie Thiem[1] and Joel Moore[2] — [1]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]Department of Physics, University of California, Berkeley, CA 94720, USA

Silicon phononic crystal plates with void pores have been found to posses enhanced figures of merit ZT, which make them potentially interesting for the construction of thermoelectric devices. We developed a method to compute the phonon thermal conductivity for these materials using the Landauer formula. This requires the calculation of the complete dispersion relation for the holey silicon plates. Thereby, we determine the elastic band structure by a plane-wave expansion method with a supercell approach.

DS 43.4 Wed 15:00 P2

Thermal conduction in correlated multilayer structures — •Stefanie Wiedigen[1], Kodanda R. Mangipudi[1], Manuel Feuchter[2], Christian Jooss[1], Cynthia A. Volkert[1], and Marc Kamlah[2] — [1]Institut für Materialphysik, Georg-August-Universität Göttingen, Germany — [2]Institut for Materials Research II, Karlsruhe Institute of Technology, Germany

High-efficient thermoelectric devices require effective methods of suppressing thermal conductivity, e.g. by complex materials, multilayer structures or nanoscale patterning to enhance the figure of merit Z. The goal of this collaborative work is to understand the anisotropic and size dependent thermal conductivity in multilayer structures. Because of correlation effects, e.g. perovskite oxides are promising new thermoelectric materials. Thin films of these materials are measured with the 3ω method which is a common and reliable measurement technique for thin film and multilayer thermal conductivity. However, measuring complex geometries requires an extension of the standard method. Improvement of the experimental setup is related to new heater concepts and patterned layer configurations. This needs support by finite element simulations with respect to the detailed thermal and electric conditions due to lack of analytical solutions. Another important requirement is the selection of multilayer materials and their geometry. We study phonon dispersion in a two component singly-periodic infinite multilayer system using continuum finite element models. The results will be presented in terms of the effect of the elastic constants and thickness on the phonon band gap variation.

DS 43.5 Wed 15:00 P2

Nb Substitution in Zr0.5Hf0.5NiSn based Compounds. — •Schwall Michael and Benjamin Balke — Johannes-Gutenberg University Mainz

This work reports about the structural and physical properties of the Heusler alloy (Zr0.5Hf0.5)1-xNbxNiSn with varying Nb concentration. The structure of the(Zr0.5Hf0.5)1-xNbxNiSn solid solution was investigated by means of X-ray diffraction. It is found that the alloys exhibit the C1b structure for all Nb concentration. The physical properties were studied using the PPMS from low temperature to room temperature. It was shown that the thermoelectric properties like the dimensionless Figure of Merit is increased 5 times by substituting(Zr0.5Hf0.5) with Nb to 0.09 at 300 K and the Powerfactor is increased 10 times to 1.8 mW/K2m at 300K.

DS 43.6 Wed 15:00 P2

The potential of phase change materials for thermoelectric applications - An investigation of alloys along the pseudo binary line from GeTe to SnTe — •Felix Lange, Hanno Volker, Karl Simon Siegert, and Matthias Wuttig — 1. Physikalisches Institut IA, RWTH Aachen University

Thermoelectric generators make use of the Seebeck effect which is an intrinsic property of any non dielectric solid. Materials with a high conversion efficiency are characterized by a high figure-of-merit $ZT = \sigma S^2/\kappa$, where σ is the electrical conductivity, S the Seebeck coefficient and κ the thermal conductivity.

We have recently shown that phase change materials employ resonant bonding [1] which results in a delocalization of carriers and an anharmonic potential [2]. The delocalization of carriers leads to high electrical conductivity while the anharmonic potential enhances the probability for phonon-phonon interactions such as umklapp processes. Hence, phase change materials are promising candidates for thermoelectric applications.

Therefore alloys along the pseudo binary line from GeTe to SnTe are investigated. It is shown, that the electrical conductivity can be tailored by gradually adding Sn. The disorder on the Ge-Sn sublattice causes a low thermal conductivity which develops a minimum for $Ge_2Sn_2Te_4$.

[1] K. Shportko *et al.*, Nature Materials **7**, 653-658 (2008)
[2] D. Lencer *et al.*, Nature Materials **7**, 972-977 (2008)

DS 43.7 Wed 15:00 P2

Laser-induced electronic transport through electrochemically-fabricated point-contacts — •Bastian Kopp, Daniel Benner, Markus Schmotz, Zhiwei Yi, Johannes Boneberg, Paul Leiderer, and Elke Scheer — Universität Konstanz

Aim of this work is to study the effects of laser illumination on electrochemically-fabricated metallic point-contacts. By electron-beam lithography we pattern nanoscale metallic electrodes separated by a gap of roughly 500nm. This gap is then closed by electrochemical deposition of a second metal [1]. After removal of the electrolyte solution atomic-size contacts with conductance in the range of 10 to 100 G_0 are obtained. We present results measured on contacts consisting of various metal combinations including Au, Ag and Pt. We observe a distinct change of the conductance of these contacts upon laser irradiation. We study the spatial and wavelength dependence of the conductance change. The amplitude and sign of the signal depend on both the position of irradiation and the applied voltage. Our results can qualitatively be explained by thermoelectric effects with corrections for small conductance values.

[1] F.-Q. Xie, Phys. Rev. Lett. **93**, 128303 (2004)

DS 43.8 Wed 15:00 P2

A set-up for 3ω measurements on semiconductor nanowires and the role of electron-phonon decoupling — •Johannes Gooth[1,2], Phillip Wu[1], Sofia Fahlvik Svensson[1], Johannes Kimling[2], Kornelius Nielsch[2], and Heiner Linke[1] — [1]Division of Solid State Physics, Lund University, Sweden — [2]Applied Physics and Microstructure Research Center Hamburg, University of Hamburg, Germany

To characterise the performance of thermoelectric materials, the so called "figure of merit" ZT is an important value. We present a device for ZT measurements in semiconductor nanowires by using a microheater for the thermopower measurement and use of the the 3ω method to measure the thermal conductivity. A double-resist technique is used to suspend CBE-grown InAs nanowires wires above a substrate. Whereas near room temperature the 3ω method is very well established, questions arise about the coupling of electrons and phonons during the self-heating process at lower temperatures. To obtain a better understanding, we model the situation using a two temperature model, and we aim to compare our experimental results to a measurement method which is not based on self heating.

DS 43.9 Wed 15:00 P2

Ab initio investigations of inter atomic force constants and phonon dispersion relations at ZnO interfaces — •Michael Bachmann, Saeideh Edalati Boostan, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

ZnO/ZnS nanostructures are a promising material for thermoelectric applications due to the expectation of a strong phonon scattering at the interface but a high transmission of electrons through the interface. Since the heat conductance due to phonons reduces the efficiency of thermoelectric elements the understanding of phonon transport across interfaces is an important feature to improve thermoelectric devices. We present ab initio calculations of the inter atomic force constants for ZnO/ZnO interfaces. From these force constants we calculate the dynamic matrix and the dispersion relation as well as the phonon density of states. These calculations help us to first understand the thermal transport in sputtered ZnO films which is the basis for further investigations of the ZnO/ZnS nanostructure.

DS 43.10 Wed 15:00 P2

Reduction of the Lattice Thermal Conductivity in One-Dimensional Quantum Dot Superlattices due to Phonon Filtering — Denis L. Nika[1], Evghenii P. Pokatilov[1], Alexander A. Balandin[2], Vladimir M. Fomin[3], •Armando Rastelli[3], and Oliver G. Schmidt[3] — [1]Laboratory PMSMM, Department of Theoretical Physics, Moldova State University, MD-2009 Chisinau, Republic of Moldova — [2]Nano-Device Laboratory, Department of Electrical Engineering, University of California–Riverside, CA 92521 Riverside, U.S.A. — [3]Institute for Integrative Nanosciences, IFW-Dresden, D-01069 Dresden, Germany

One-dimensional quantum-dot superlattices (1D-QDS) consisting of acoustically mismatched materials Si/Ge, Si/plastic, Si/SiO_2 and Si/SiC are shown to possess sub-1 W $m^{-1}K^{-1}$ thermal conductivity in a temperature range from 50 K to 400 K. The phonon energy spectra are calculated in the framework of the molecular dynamic Face-centered Cubic Cell model. A significant reduction of the lattice thermal conductivity in 1D-QDS structures in comparison with homogeneous rectangular Si quantum wires is explained by the fact that the 1D-QDS structures act as effective phonon filters eliminating a significant number of phonons from thermal transport. The work was supported by the IB BMBF Project MDA 09/007 and ASM-BMBF Project 10.820.05.02GA.

DS 43.11 Wed 15:00 P2

Thermal conductivity measurements on nano air gaps. — •Thorben Bartsch, Matthias Schmidt, Christian Heyn, and Wolfgang Hansen — Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany

Nano air gaps in thermoelectric devices are an attempt to enlarge the efficiency of thermoelectric devices by drastically lowering of the thermal conductivity [1]. We present thermal conductivity measurements on GaAs based nano air gap heterostructures. The investigated structure is grown by molecular beam epitaxy. It is composed of a 50 nm GaAs layer which quasi hovers above the underlying GaAs substrate. The GaAs layers are held in position by GaAs nanopillars. Two samples have been studied with an air gap of 4 and 6 nm thickness, respectively. The measurements were performed for temperatures between 20 K and 300 K via the 3ω - method. The thermal conductivity values are up to three orders of magnitude smaller than the corresponding bulk thermal conductivity. [1] T. Zeng, Appl. Phys. Lett. 88, 153104 (2006).

DS 43.12 Wed 15:00 P2

3ω-measurements on ZnO/ZnS thin film structures — •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 thermal conductivity of rf-sputtered ZnO/ZnS thin film layer structures. For this purpose a 3ω measurement system has been set up. It is based on a passive bridge circuit to eliminate the 1ω voltage component to facilitate a reliable measurement of the 3ω component. The samples can be heated as well as cooled, so that measurements can take place in a temperature range from 80 K to 400 K. In addition to the experimental setup, first measurements on ZnO/ZnS thin film layers will be presented. These will be carried out in a heater on top configuration and with different heater lengths on the same samples. The different ΔT curves are compared and the cross-plane thermal conductivities of the films will be evaluated for different temperatures.

DS 43.13 Wed 15:00 P2

Thermal conductivity and thermoelectric properties of a suspended GaAs/AlGaAs heterostructure — •Matthias Schmidt, Andrea Stemmann, and Wolfgang Hansen — Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany

We study low-temperature magnetothermoelectric properties of two-dimensional electron systems (2DEGs) embedded in a thin suspended membrane consisting of a modulation doped GaAs/AlGaAs heterostructure grown by molecular beam epitaxy. Electron-beam lithography is used to pattern the top of the membrane featuring a microscaled Hall bar, thermometers, and a Joule heater on top. The heater at the central region of the membrane generates a strong thermal gradient between the hot and the cold end side of the 34 μm long Hall bar including the 2DEG. A temperature difference of more than 5 K can be achieved at a mean temperature well below 10 K. We present heat conductivity and magnetothermopower measurements. The results show that the specific thermal conductivity of the membrane is qualitatively and quantitatively different with respect to the bulk value. Observed magnetothermopower is similar to results of earlier publications on GaAs/AlGaAs heterostructures. However, in contrast to previous results our measurements of the zero-field thermopower reveal that thermodiffusion is the main source of the thermopower at temperatures up to 3 K until the phonon drag dominates the run of the thermopower. This value is significantly higher than reported for non-suspended heterostructures [1].

[1] R. Fletcher et al., *Phyical Review B* 14991 (1994)

DS 43.14 Wed 15:00 P2

In-plane transport of artificially structured CVD ZnO/ZnO:Ga and ZnS/ZnO:Ga barstructures with different interface design — •Gert Homm, Steve Petznick, Sebastian Eisermann, Torsten Henning, Martin Eickhoff, Bruno K. Meyer, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig Universität, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Series of different bar-shaped samples consisting of lateral arrangements of either alternating ZnO:Ga and ZnO stripes or ZnO:Ga and ZnS stripes were fabricated from rf-sputtered layers or epitaxial layers. Photolithography techniques and wet-chemical or ion-beam etching followed by a second sputtering process were used to transfer the pattern. The bar-shaped structures have dimensions of a few micrometers and are oriented parallel to the applied temperature gradient and thus to the transport direction. The structure of the interfaces is varied to create controlled interface roughnesses. This enables one to gain information about the extension of the interface region and the transport mechanisms along the interfaces by measuring the Seebeck coefficient and the electrical conductivity of series of samples with different interface structures.

DS 43.15 Wed 15:00 P2

Doping of hydrogenated a-Si and a-Ge nanostructures — •Christoph Grüner, Jens Bauer, Chinmay Khare, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung, Permoserstrasse 15, D-04318 Leipzig, Germany

Nanostructured semiconductor thin films promise high performance in future thermoelectric applications. Glancing angle deposition (GLAD) is a recent technique to fabricate self-organized nanostructures. Based on shadowing at oblique incidence angle separated nanocolums evolve, which can be shaped by substrate rotation about its normal. As a result vertical nanospirals, nanoscrews, or nanocolumns are formed. By variing the incidence angle the deposition can be further customized. Amorphous hydrogenated silicon and germanium layers and nanostructures were grown by electron-beam evaporation at room temperature. Antimony and boron were used for in-situ doping by effusion cells. Hydrogenation is done with a hydrogen atom beam source. Hydrogen passivates the dangling bonds of the amorphous materials and thus it is used to enhance the electrical properties of doped a-Si and a-Ge films. We will present the influence of hydrogen on the dopant concentration and the electrical resistivity in a-Si and a-Ge thin films. The effect of Sb and B segregation will be discussed with respect to the hydrogen flux. The chemical composition is investigated by SIMS profiles. Furthermore, rapid temperature annealing experiments were performed for electrical activation of the dopants. Also the influence of hydrogenation and doping on the appearance and distribution of nanostructures is shown.

DS 43.16 Wed 15:00 P2

Measurements of the in-plane thermal conductivity of thin films using a microstructured heater and sensor arrangement — •David Hartung, Achim Kronenberger, Steve Petznick, Torsten Henning, Bruno K. Meyer, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany

The aim of this work is to characterise the lateral heat flow in a thin semiconductor layer on a glass substrate. Cover-glass is used for the heater and sensor arrangement. The masurement area is 0.5 mm × 0.5 mm where sensor and heater are deposited. A broad Au wire along the middle axis of this measurement area serves as the electric heater, three narrow Au wires at different distances from, but parallel to the heater wire, serve as temperature sensors. The arrangement was defined by photolithography on to the grass-substrate. Thin films of insulating ZnS and ZnO are deposited on to the measurement by RF-sputtering. First results of the measurements will be presented.

DS 43.17 Wed 15:00 P2

Thermal properties of phase change materials — •Karl Simon Siegert, Carl Schlockermann, Peter Zalden, and Matthias Wuttig — 1. Physikalisches Institut IA, RWTH Aachen University, 52064 Aachen

Many chalcogenic alloys such as GeTe or $Ge_1Sb_2Te_4$ offer unique physical properties which justify their classification as so called phase change materials (PCM). All of these materials share the following attributes: high contrast between the amorphous and the crystalline state in both electrical resistivity and optical reflectivity combined with fast crystallization speed in the order of ns [1]. This special combination of properties make PCMs favorable for modern data storage applications. As the switching between states is induced by temperature, detailed knowledge of the thermal properties is needed for further improvement of PCM based data storage devices.
This work contributes to the thermal characterization of phase change materials. Several PCM thin films were sputter deposited on silicon substrates. Using different experimental techniques, the specific heat (DSC measurements) and the cross plane thermal conductivity (differential 3ω) of the films were measured. Further data processing revelead the thermal diffusivity and the main heat conduction channels of the materials. Additionally, the influence of thermal interface resistances within a PC-dielectric dual-layer system was determined by thickness series.
[1] Bruns et al., Nanosecond switching in GeTe phase change memory cells, APL 2009

DS 43.18 Wed 15:00 P2

Investigation of thermal and electrical properties of individual nanostructures using specially designed microchips — •Daniel Huzel[1,2], Heiko Reith[1,2], Matthias C Schmitt[1,2], Friedemann Völklein[1], Roland Sachser[2], and Michael Huth[2] — [1]Institut für Mikrotechnologien (IMtech), Hochschule RheinMain, Am Brückweg 26, D-65428 Rüsselsheim — [2]Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str. 1, D-60438 Frankfurt am Main

Our work focuses on the determination of thermal and electrical transport properties of individual thermoelectric nanostructures, in particular single nanowires. The Seebeck coefficient, electrical and thermal conductivity depend strongly on material, composition, crystallinity and geometric structure. To measure these coefficients, specially designed microchips have been developed and employed. FEM simulations demonstrate that the temperature profiles of the microchips show appropriate temperature gradients for Seebeck effect measurements and heat sink conditions for thermal conductivity investigations. Results of measurements on bismuth, bismuth-telluride and -antimonide nanowires are presented. The microchips have also been used for thermoelectric measurements on nano-granular metals prepared by focused electron beam induced deposition (FEBID).