HL 21: Poster IB (Oxide semiconductors; II-VI and group IV semiconductors; Nanotubes and Buckyballs)

Presenters are kindly requested to be near their poster for at least one hour in the time between 17:00-19:00 or to leave a note about their availability for discussions.

Time: Monday 15:00–20:00 Location: Poster B

HL 21.1 Mon 15:00 Poster B

Multi-beam sputtering approach for creation of material libraries — •Martin Becker, Angelika Polity, and Bruno K. Meyer — 1st Physics Institute, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Ion beam sputter deposition (IBSD) has been under focus of research for a number of years due to the flexibility it provides in the deposition of novel thin film materials. One of the characteristics, making IBSD unique, is the ability to deposit multi-component or multi-layered materials using a multi-target single ion gun scheme. This is accomplished by sequentially positioning selected targets in front of the ion source. Furthermore the demand of new combinatorial capabilities for both the synthesis of new solid state opto-electronics and optimization of existing materials has driven the interest in multi-beam arrangements. Important materials for applications include semiconductors, transparent conductors, energy storage materials and more.

We report on the application of single beam and combinatorial approach to the specific material type of transparent conducting oxides (TCOs). In this case, libraries are generated by ion beam sputtering. The application of a combinatorial approach to this materials area can greatly accelerate the rate of discovery and optimization of new materials and the optimization of devices. Initial collection of characterization tools for investigation of optical and structural properties includes UV/VIS/NIR transmission/reflection, Raman scattering and X-ray diffraction.

HL 21.2 Mon 15:00 Poster B

An X-ray photoelectron spectroscopy (XPS) study on intrinsic and nitrogen doped tin oxides — •Fabian Michel, Benedikt Kramm, Martin Becker, Jie Jang, Angelika Polity, and Bruno K. Meyer — 1. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Gießen

This work is an XPS study on intrinsic and nitrogen doped tin oxide. We fabricated SnO_x thin films by ion beam sputtering and epitaxial growth. By sputtering we produced a series with varying stoichiometrie by changing the oxygen flow and/or the substrate temperature. Using the second method we made a series of SnO_2 with different nitrogen concentrations. By X-ray photoelectron spectroscopy (XPS) we identified the phases in the SnO_x thin films. Therefore, we took a look at the relative atomic concentration of tin and oxygen in the stoichiometrie series and especially at the relative atomic concentration of nitrogen in the samples produced by epitaxial growth. We also investigated the variation of the valence band position in relation to the treatments mentioned above. Thus we analyzed the chemical shifts of the photoelectron and the Auger electron lines. Furthermore the effects of the nitrogen doping on the valence band maximum and on the work function were investigated using ultraviolet photoelectron spectroscopy (UPS).

HL 21.3 Mon 15:00 Poster B

Ohmic contacts to In2O3 single crystals — •Maryam Nazarzadehmoafi[1], Mattia Mulazzi[1], Christoph Janowitz[1], Stephan Machulik[1], Zbigniew Galazka[2], and Recardo Manzke[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany — [2]Leibniz Institut für Kristallzüchtung, Max Born Str. 2, 12489 Berlin, Germany

It is known that the barrier formation at the interface between metals and ionic semiconductors usually follows the Schottky-Mott rule. In contrast, this model fails for the several metal-In2O3 interfaces, and this is commonly attributed to an electron accumulation layer at the surface of In2O3, believed to prevent the Schottky contact formation. In order to have a deeper insight into the metal-In2O3 contacts, the barrier heights of In and Cu on the melt-grown In2O3(111) single crystals were studied by means of ARPES at room temperature (RT) and low temperature (LT). The growth of Copper on In2O3 (111) is ordered and homogenous at RT, as suggested by the presence of a distinct surface state for thick Cu films. In the case of Indium, we observed an electronic state near the Fermi level at small coverages, blurring out for increasing the metal thicknesses, what is a signature of an interface state. The ohmic behavior of both interfaces is evident at RT and LT for both metals, contrary to the prediction of the Schottky-Mott rule, with a stronger discrepancy for Cu/In2O3. We interpret the results in terms of surface electron and hole-doping of the semiconductor and with the presence of a significant density of electronic states within the band gap that is responsible for the reduction of the barrier height.

HL 21.4 Mon 15:00 Poster B

Investigations on simple copper vacancies and split vacancies in Cu_2O based on density functional theory — •Raphael Knecht and Christian Heiliger — 1. I. Physikalisches Institut, Justus Liebig University Giessen, Germany

We present investigations on simple copper vacancies V_{Cu} and split vacancies V_{Cu}^{split} in Cu_2O based on density functional theory. Both defects are simulated in a 2x2x2 supercell of Cu_2O. We determine the influence of these defects on structural and electronic properties using the LDA+U functional and compare them with properties of defect free Cu_2O. Since both vacancies come along with an electron hole state, we further investigate the localization of this defect state. In order to do so we calculate Born effective charges, magnetic moments and density-differences for both defect structures.

HL 21.5 Mon 15:00 Poster B

Ab initio Raman Spectra of $Zr_{1-x}Ce_xO_2$ and of Ceria with oxygen vacancies — •Michael Bachmann and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

Although the phase diagram of $Zr_{1-x}Ce_xO_2$ has been investigated a while ago with Raman spectroscopy [1] it is still not fully understood. We perform DFT supercell calculations of $Zr_{1-x}Ce_xO_2$ for different phases. For each concentration we average over a number of supercells with different configurations. We present the concentration dependence of the lattice constants, the band gaps, and the Raman spectra. All quantities are obtained by thermodynamic and statistic weighting. Furthermore, we use a supercell approach to calculate the Raman spectra of ceria with oxygen vacancies as a function of the oxygen vacancy concentration.

[1] Yashima et al. J.Am. Ceram. Soc. 77 1067 (1994)

HL 21.6 Mon 15:00 Poster B

Ab-initio Electronic Structure of Different Tin Oxides — •Bianca Eifert and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

Tin forms two stable oxides, a monoxide and a dioxide, which are already used in application fields ranging from electrochemistry to optoelectronics. Tin dioxide (SnO_2) is a wide-bandgap n-type semiconductor, while tin monoxide (SnO) is usually regarded as a semimetal or a small-bandgap p-type semiconductor. At higher temperatures, SnO disproportionates into Sn and SnO_2, and oxides of other stoichiometries are sometimes observed in experiments during this reaction. This variety of oxide phases with very different electronic properties makes the tin/oxygen system an interesting candidate for electronic components such as p/n junctions, which could be constructed from just two types of atoms. The present work contributes to the theoretical understanding of different tin oxides phases, their stability, and their electronic and optical properties by performing DFT calculations of the structural properties, bandstructures, and Raman spectra of these phases.

HL 21.7 Mon 15:00 Poster B

Ab initio study on structural and optical properties of copper oxide compounds — •Markus Heinemann, Marcel Giar, Bianca Eifert, and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-Universität, Gießen, Germany

Due to its promising electronic properties, nontoxicity, and vast abundance the p-type semiconductor copper oxide and its related com-

pounds are of broad research interest for various applications ranging from optoelectronics to solar cell design [1]. In this work we use density functional theory (DFT) calculations to investigate structural, electronic, and optical properties of the copper oxide compounds Cu2O, CuO, and Cu4O3. We show that numerical methods beyond the local density approximation are necessary to correctly describe the electronic structure of these compounds and compare different approaches to the exchange- correlation functional. For Cu2O a hybrid functional approach yields best results while for CuO and Cu4O3 the LDA+U method succeeds [2]. We further discuss the performance of self-consistent quasiparticle calculations within the framework of the GW approximation for all three compounds. Optical properties are evaluated by assessing the dielectric function from which optical absorption spectra are derived. We compare these quantities to recent experimental data [1]. As the conduction mechanism for CuO is still under discussion we investigate the influence of the formation of various point defects in this material using a supercell approach.

[1] Meyer et al., pss(b) 249, 1487 (2012)
[2] Heinemann et al., Phys. Rev. B 87, 115111 (2013)

HL 21.8 Mon 15:00 Poster B

NIR-VUV dielectric function of (Al,In,Ga)$_2$O$_3$ thin films — •Rüdiger Schmidt-Grund, Chris Sturm, Christian Kranert, Hannes Krauss, Holger von Wenckstern, Michael Bonholzer, Jörg Lenzner, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

We present the dielectric function spectra of (Al,In,Ga)$_2$O$_3$ thin films in a wide composition range obtained by means of spectroscopic ellipsometry in the spectral range from near NIR to vacuum UV and temperatures between 10K and room temperature [1]. By model analysis of the experimental data using a parametric model dielectric function approach we derive the refractive index dispersion in the visible spectral range and the energies of electronic transitions as a function of the composition and temperature. For In incorporation in β-Ga$_2$O$_3$ we found that the electronic structure for x<0.3 is dominantly that of monoclinic β-Ga$_2$O$_3$ and for x>0.7 that of the cubic bcc-In$_2$O$_3$ [2]. In the intermediate composition range, the DF reveals strong signatures of rh-In$_2$O$_3$ or rh-In$_2$O$_3$II. For increasing In and Al concentration we found a redshift respective a strong blueshift of the transition energies. The thin films with compositional spread were deposited on 2" a-plane sapphire and MgO substrates by means of pulsed laser deposition using segmented targets (consisting of half-segments of binary aluminum oxide respective indium oxide and binary gallium oxide) [3].

[1] R. Schmidt-Grund et al., APL **105**, 111906 (2014); JAP **116**, 053510 (2014). [2] C. Kranert et al., JAP **116**, 013505 (2014). [3] H. von Wenckstern et al., Cryst. Eng. Comm. **15**, 10020 (2013).

HL 21.9 Mon 15:00 Poster B

Bipolar Oxide heterodiodes comprising In$_2$O$_3$ thin films — •Steffen Lanzinger, Daniel Splith, Peter Schlupp, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

Recently, the interest on In$_2$O$_3$ extends beyond application as transparent electrode and properties of semiconducting In$_2$O$_3$ thin films were reported. Different measurements revealed that In$_2$O$_3$ tends to form a surface electron accumulation layer, which makes the formation of rectifying contacts non-trivial. Recently, by using reactively sputtered Schottky contacts, highest rectification of about 3 orders of magnitude at room temperature was achieved, which is not sufficient for most applications (e.g. field-effect transistors). Therefore, the exploitation of pn-heterodiodes presents an additional, interesting approach towards higher rectification.

We investigated nominally undoped In$_2$O$_3$ thin films with a compensated In$_2$O$_3$:Mg surface layer with different thickness (0 nm, about 10 nm and about 100 nm). The thin films were deposited by pulsed-laser deposition at 600°C and 0.016 mbar. On top, NiO and ZnCo$_2$O$_4$ were deposited at room temperature, forming pn-heterojunction diodes with the In$_2$O$_3$. Those diodes were investigated by current-voltage measurements (IV) at room temperature. Best rectifications of p-NiO/n-In$_2$O$_3$ and p-ZnCo$_2$O$_4$/n-In$_2$O$_3$ are with 4 orders of magnitude better than that of best Schottky barrier diodes on In$_2$O$_3$ thin films grown by molecular beam epitaxy. Further, temperature-dependent IV and the breakdown behavior of the diodes will be discussed.

HL 21.10 Mon 15:00 Poster B

Lattice dynamics of β-Ga$_2$O$_3$ mono-crystals — •Marcel Weinhold, Thomas Sander, and Peter Jens Klar — Justus-Liebig-University Giessen, Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen

Ga$_2$O$_3$ has attracted great interest, due to its potential use in UV transparent electrodes, photodetectors, and field-effect transistors (FETs). On top of that, Ga$_2$O$_3$ offers the opportunity to grow single crystalline substrates. In spite of that, the knowledge about its lattice vibration modes is still limited. We performed Raman studies of monoclinic Ga$_2$O$_3$ single crystals and performed a corresponding group theoretical analysis of the Raman activity of the vibrational modes. These results are compared with the Raman spectra obtained at room temperature of ($\bar{2}$01) and (010) oriented β-Ga$_2$O$_3$ grown by the edge-defined film-fed growth method (EFG). To identify the symmetry characteristics of the phonons, the samples were rotated about the axis defined by the excitation laser light coming in at normal incidence. Furthermore, the dependence of the Raman spectra on excitation wavelength in the UV to IR range will be presented.

HL 21.11 Mon 15:00 Poster B

Stark-Effect Measurements on Giant Rydberg Excitons in Cuprous Oxide — •Johannes Thewes[1], Julian Heckötter[1], Marc Assmann[1], Tomasz Kazimierczuk[2], Dietmar Fröhlich[1], and Manfred Bayer[1] — [1]Institut für Physik, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Faculty of Physics, University of Warsaw, Poland

We report on Stark-effect measurements of Giant Rydberg excitons[3] in Cu_2O with quantum numbers up to $n = 25$. These excitons have extensions up to 2 μm. As known from hydrogen, the dipole matrix elements for $\Delta n = 0$ and $\Delta l = \pm 1$ grow quadratically with n. In Cu_2O, P-excitons are dipole-allowed. Due to the electric field-induced coupling of P-excitons to S- and D-excitons we observe P/S and P/D resonances in fields as low as $10\,V cm^{-1}$. Measurements are done on a 30 μm sample with a single frequency dye laser (ΔE = 1 neV) at temperatures down to 1.2 K. Contrary to hydrogen, the Stark-effect measurements can be done in a longitudinal configuration ($\mathbf{K}_{\mathrm{laser}} || \mathbf{E}$). — [3] T. Kazimierczuk et al. Nature 514, 343 (2014)

HL 21.12 Mon 15:00 Poster B

Electrical conductivity and photoconductivity of single-crystalline In$_2$O$_3$ thin films — •Julius Rombach and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

Although the gas sensing effect of conductometric metal oxide gas sensors is known to be surface-related, contributions from the bulk and the substrate interface are unclear. Due to the presence of a surface electron accumulation layer (SEAL), electrical conductivity of In$_2$O$_3$ thin films usually consists of contributions from the bulk material, the SEAL and the substrate interface. This study aims to disentangle these sources of conductivity using MBE grown single-crystalline In$_2$O$_3$ films. By thickness variation and Mg-doping with a subsequent annealing step in Oxygen, the bulk and interface contribution to the overall conductivity was altered. The SEAL contribution was influenced by oxygen plasma treatment of the surface, which removes the SEAL, and by UV illumination during conductivity measurements. In$_2$O$_3$ shows photoconductivity in the UV range with photon energies below the fundamental absorption edge, which is believed to be a photoreduction of oxygen adatoms on the In$_2$O$_3$ surface. Hence the contribution of the SEAL to overall conductivity can be increased by UV illumination. This can help to get a better understanding of the sensing mechanism of In$_2$O$_3$-based gas sensors and to achieve higher sensitivities by specifically influencing the particular contributions to electrical conductivity.

HL 21.13 Mon 15:00 Poster B

Influence of the preparation of thin indium oxide films on the electronic surface properties — •Theresa Berthold[1], Jochen Räthel[1], Stefan Krischok[1], Marcel Himmerlich[1], Chunyu Wang[2], Volker Cimalla[2], Julius Rombach[3], Marko Perestjuk[3], and Oliver Bierwagen[3] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Germany — [2]Fraunhofer-Institut für Angewandte Festkörperphysik, Freiburg, Germany — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The electronic structure of In$_2$O$_3$ can be modified by an oxygen plasma surface treatment, to establish a surface depletion layer [1]. We analyze the influence of different preparation methods, like annealing in vacuum and oxygen environment, oxygen plasma modification as well

as indium-flash-off, on In_2O_3 surface composition and electronic properties, such as band bending, electron accumulation and work function. Thin indium oxide films grown by MBE or MOCVD are characterized using PES and the morphology is analyzed by AFM. In the initial state, an electron accumulation layer as well as hydrocarbon and hydroxide adsorbates are observed at the surface. Thermal treatments result in adsorbate removal, while the formation of surface defects can be prevented by annealing in oxygen environment. Oxygen plasma processes as well as other oxidative surface treatments induce a change in the surface composition. In all cases, the electronic surface properties are influenced and changes in band bending and work function are observed. [1] O. Bierwagen et al., Appl. Phys. Lett. 98, 172101 (2011)

HL 21.14 Mon 15:00 Poster B

Conducting mechanism in epitaxial p-type Transparent Conducting Oxide Cr_2O_3:Mg — •Leo Farrell, Karsten Fleischer, David Caffrey, Darragh Mullarkey, Emma Norton, Elisabetta Arca, and Igor Shvets — CRANN, School of Physics, Trinity College Dublin, College Green, Dublin 2, Ireland

p-type transparent conducting oxides (TCOs) are an important material class for many optoelectronic devices. However, p-type TCOs have always exhibited poorer performances than their n-type counterparts. As a result, new p-type materials remain an important area of research. Cr_2O_3 doped with Mg is a candidate p-type TCO material. In this study we improved on the electrical and optical properties of Cr_2O_3:Mg. The samples were epitaxially grown by MBE where the stoichiometry was finely tuned in order to investigate the effect on the structural, electrical and optical properties. The influence of the Mg dopants and the oxygen partial pressure were also investigated by Seebeck and resistivity measurements. Carrier transport properties are examined. The role of polaronic reduction in hole mobility for this material is also discussed. Investigating the fundamental properties in epitaxial material will allow us to add to our understanding of the role of defects in p-type TCOs, helping to improve material grown by other more industrial relevant methods.

HL 21.15 Mon 15:00 Poster B

LEEM and XPEEM studies of MgO films on Ag(100) — •Sabrina Pechmann[1], Gina Peschel[2], Hagen W Klemm[2], Thomas Schmidt[2], and Rainer H Fink[1] — [1]Physical Chemistry, Friedrich-Alexander-University Erlangen-Nuremberg, Germany — [2]Chemical Physics, Fritz Haber Institute of the Max Planck Society Berlin, Germany

Metal oxide thin films on metal supports are important for various technological applications like catalysis or the fabrication of electronic devices. Therefore, it is necessary to understand the electronic properties of the interfaces, as well as microscopic structure and morphology of the films. Especially MgO on Ag(100) serves as an attractive model system as the lattice mismatch between both bulk structures is only 3.1%, allowing epitaxial growth with just a small number of grain boundaries. Nevertheless, defects like non-stoichiometries, or vacancies influence the surface properties of the oxide layer to a large extend. Exposure to X-rays and even low-energy electrons (up to 200 eV), already leads to the formation of so-called color centers. We investigated the growth and structural properties of epitaxial MgO thin films on Ag(100) by LEEM and XPEEM as both techniques provide insight into structural and chemical sensitivity and directly visualize the influence of surface defects, e.g., step bunches. We could observe a strong influence of low-energy electrons and X-rays on the metal oxide layer, like the reversible formation of long-range ordered oxygen vacancies and even quadrangular structures. First results concerning those effects will be presented.

HL 21.16 Mon 15:00 Poster B

Impact of soft x-rays on the field effect in $SrTiO_3/LaAlO_3$ heterostructures — •Martin Zwiebler[1], Enrico Schierle[2], Emiliano Di Gennaro[3], Fabio Miletto Granozio[3], and Jochen Geck[1,4] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [3]CNR-SPIN and Dipartimento di Fisica Università "Federico II" di Napoli, Italy — [4]Dresden University of Technology, Germany

The two-dimensional electron gas (2DEG), which can be realized at the $SrTiO_3/LaAlO_3$ interface, currently receives a lot of attention. Although both constituent materials are bulk insulators, the 2DEG at the interface exhibits a high carrier mobility and can even become superconducting. Numerous spectroscopic studies aimed at clarifying the electronic properties of the $SrTiO_3/LaAlO_3$ interface. However, the connection of those results to macroscopic quantities often remained controversial. In order to directly relate spectroscopic measurements to transport properties, we combined both techniques into a single experiment. More specifically, we measured the electrical resistivity as well as Ti $L_{2,3}$ x-ray absorption and resonant x-ray reflectivity of $SrTiO_3/LaAlO_3$ field effect devices, while monitoring the electrical resistivity. In this contribution we present first results of these efforts that reveal a strong impact of the soft x-ray radiation on the 2DEG. The implications for previously published studies are also discussed.

HL 21.17 Mon 15:00 Poster B

The Electronic Structure of amorphuos SnOx thin films and SnO2 single crystals — •J. Haeberle[1], D. Gaspar[2], P. Barquinha[2], L. Pereira[2], R. Martins[2], E. Fortunato[2], S. Machulik[3], C. Janowitz[3], R. Manzke[3], and D. Schmeisser[1] — [1]Angewandte Physik/Sensorik, Brandenburgische TU Cottbus,K.-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]Department of Materials Science Faculty of Sciences and Technology,New University of Lisbon and CEMOP-UNINOVA, Campus de Caparica,2829-516 Caparica, Portugal — [3]AG Elektronische Eigenschaften und Supraleitung, Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

We compare the electronic properties of amorphous p-type SnOx thin film grown by rf magnetron sputtering with those of n-type SnO2 single crystals grown by cvt. We use resPES to study the electronic band structure. We measure the core levels, the VB PES data, partial Integrated Yield (pIY) and the XAS absorption data. From the resPES data recorded at the O1s and the Sn3d edges we derive the VB pDOS and the CB pDOS . The differences are most pronounced in the position of the VBM as for the a-SnOx films there appears a band closer to the Fermi energy. In addition for the SnOx we find in the XAS and pIY data a significant peak that appears right at the Fermi energy. This peak is absent in the single crystalline data. We attribute this to a change in the configuration of the Sn4d states to form a 4d8 configuration instead of 4d9 and 4d10 configurations which are identified in the single crystalline data.

HL 21.18 Mon 15:00 Poster B

Preparation and Characterization of Nitrogen Doped ZnMgO:Al-Thin Films — •Hannes Giese, Philipp Schurig, Limei Chen, Thomas Sander, Angelika Polity, Detlev M. Hofmann, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität, Giessen, Deutschland

ZnO has a tunable band gap with good abilities for ultraviolet optoelectronic devices. The electrical properties, especially the band gap, of ZnO can be increased by adding MgO and doping with aluminum, for example. In order to yield homojunctions of ZnO, it is necessary to produce a stable and effective p-type doping of this system. A promising way to obtain this is to dope with nitrogen because of its atomic radius and its electrical properties being comparable with oxygen. In this work, thin films were produced by RF-sputter deposition with a ceramic target of Zn(0,72)Mg(0,25)O:Al(0,03). Nitrogen was used with argon as the sputtering gas at different growth temperatures (from room temperature to 700°C) and at constant temperatures with a different nitrogen flows (from 0,02-0,2 sccm). The films were characterized by UV/Vis spectroscopy, XRD and Hall-effect measurements. The results showed a dependence of the optical, structural and electrical properties on the varied parameters. This is accompanied with different colors of the thin films and different crystal structures. Zinc nitride formation was studied as a function of nitrogen partial pressure and growth temperature. It is assumed that only at very low nitrogen flows (0,02 sccm) the doping was successful, but the results indicate that p-type doping was not achieved.

HL 21.19 Mon 15:00 Poster B

The role of oxygen ambient in the Persistent Photoconductivity of ZnO nanowires — •Florian Huber, Manfred Madel, Martin Dickel, Bruno Amann, and Klaus Thonke — Institute of Quantum Matter / Semiconductor Physics Group, Ulm University

The origin of the Persistent Photoconductivity (PPC) in zinc oxide is a widely discussed topic. The reason for the PPC is frequently attributed to intrinsic defects, especially to oxygen vacancies which are reported to act as deep traps [1]. Besides these defects, the adsorption and desorption of oxygen on the surface of the material influences the PPC strongly.

We investigated in detail especially the kinetics of the slow photo-

induced conductivity processes with respect to their photon energy, temperature, oxygen ambient and illumination time dependence. Energy barriers for the decay process after illumination are determined, and the experimental results are discussed in the frame of possible models.

[1] A. Janotti and C.G. Van de Walle, Applied Physics Letters **12**, 122102 (2005)

HL 21.20 Mon 15:00 Poster B

Impact of strain on electronic defects in (Mg,Zn)O thin films — •Florian Schmidt, Laurenz Thyen, Stefan Müller, Holger von Wenckstern, Gabriele Benndorf, Rainer Pickenhain, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig

Ternary MgZnO is an excellent material system for the fabrication of quantum well heterostructures and thus for potential application in exciton-related photonic devices.

We have investigated the impact of strain on the incorporation and the properties of extended and point defects in (Mg,Zn)O thin films by means of photoluminescence, X-ray diffraction, deep-level transient spectroscopy (DLTS) and deep-level optical spectroscopy. The recombination line Y2, previously detected in ZnO thin films grown on an Al-doped ZnO buffer layer and attributed to tensile strain [1], was exclusively found in (Mg,Zn)O samples being under tensile strain and is absent in relaxed or compressively strained thin films. Furthermore a structural defect E3' can be detected via DLTS measurements and is only incorporated in tensile strained samples. Finally it is shown that the omnipresent deep-level E3 in ZnO can only be optically recharged in relaxed ZnO samples [2].

[1] M. Brandt *et al.*, Phys. Rev. B **81**, 073306 (2010).
[2] F. Schmidt *et al.*, J. Appl. Phys. **116**, 103703 (2014).

HL 21.21 Mon 15:00 Poster B

Non-linear deformation potential in highly strained ZnO microwires — •Sherzod Khujanov, Chris Sturm, Marcel Wille, Michael Lorenz und Marius Grundmann — Institut für Experimentelle Physik II, Universität Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

Zinc oxid nano- and microwires are promising building blocks for sensor and generator applications [1]. In this work we present the investigation of the deformation potential of ZnO microwires and the ability of engineering the band gap energy via mechanical stress. The microwires (MW) were prepared by carbothermal evaporation, bent and fixed on Si substrates. Thereby we induced a uniaxial strain up to ±3.5%. The emission properties near the band edge were investigated by using cathodoluminescence. In the unstrained case the MW exhibit a sharp emission from donor bound excitons whereas in the case of an applied strain we observed a broadening and a red (blue) shift of the near band emission for tensile (compressive) strain. For strain values up to ±1.5% we observe a linear dependence between strain and observed energy shift as already reported in the literature [2]. However, for larger strain we observe that this linear relation does not hold anymore and non-linear effects have to be considered. This is supported by the fact that the magnitude of the energy shift is significantly larger for compressive strain compared to the tensile strain.

[1] Z.L. Wang MRS BULLETIN 37, 814 (2012).
[2] C.P. Dietrich et al. Appl. Phys. Lett. 98, 031105 (2011).

HL 21.22 Mon 15:00 Poster B

Effects of functionalization of ZnO nanowire Schottky diodes on their current-voltage characteristics — •Emily T. Tansey[1], Alejandra Castro-Carranza[1], Stephanie Bley[1], Olesea Volciuc[1], Tobias Voss[2], and Jürgen Gutowski[1] — [1]Institute of Solid State Physics, Universität Bremen, Bremen, Germany — [2]Institute of Semiconductor Technology, TU Braunschweig University of Technology, Braunschweig, Germany

Zinc oxide nanowires (ZnO NWs) have shown to be promising as nanoscale building blocks for optoelectronic applications due to their unique semiconductor, optical, piezoelectric, and chemical characteristics. An interesting approach to tailor the optoelectronic properties of ZnO NWs is to form hybrid junctions with other materials, e.g. polymers. It has been proposed that surface defects play a role in the tailor of the ZnO NWs properties. To gain further insight into this physical phenomenon, we explore the current-voltage characteristics of Schottky diodes formed by wet chemical-growth ZnO NW arrays and the p-type polymer Poly(3-hexylthiophene-2,5-diyl). Our results show that the thickness of the P3HT impacts the current transport mechanisms occurring at the junction.

HL 21.23 Mon 15:00 Poster B

ZnO nanowire Schottky diodes on ITO and FTO substrates: study of the junction by electrical characterization — Alejandra Castro-Carranza[1], •Jairo Cesar Nolasco[2], Emily T. Tansey[1], Stephanie Bley[1], Olesea Volciuc[1], Tobias Voss[3], and Jürgen Gutowski[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Energy and Semiconductor Research Laboratory, Carl von Ossietzky University Oldenburg, Germany — [3]Institute of Semiconductor Technology, TU Braunschweig University of Technology, Germany

Zinc oxide nanowires (ZnO NW) have been used in flexible LEDs and solar cells. As important topic for these applications is the study of the junction formed between ZnO NWs and transparent conductive oxides, e.g. fluorine doped tin oxide (FTO) and indium tin oxide (ITO), which are commonly used as front contacts. Their work functions define the nature of the junction with ZnO NWs, i.e. ohmic contacts or Schottky diodes. However, surface defect states on the ZnO NWs can influence such a junction. In the present work we explore the electrical characteristics of junctions based on wet-chemically grown vertical ZnO NW arrays on FTO and ITO by means of their current-voltage characteristics and impedance spectroscopy. We observed that a significant barrier height is formed at the junctions, corresponding to a Schottky diode, and the obtained ideality factors describe that the conduction mechanism occurring at the junctions is affected by tunneling through traps.

HL 21.24 Mon 15:00 Poster B

Simultaneous adsorption of water and molecular oxygen on non-polar ZnO($10\bar{1}0$) surface: a microscopic understanding — Delsuz Hassani, Saied Masoumi, •Ebrahim Nadimi, and Faramarz Hossein-Babaei — Faculty of Electrical Engineering, K N Toosi University of Technology, Tehran, Iran

The surface of different metallic oxides such as ZnO, SnO_2 and TiO_2 are widely used in gas sensing applications. Atomic level modeling are widely employed to explain the sensing mechanism at a microscopic level. The present work is an attempt to apply density functional theory to investigate the adsorption of water and oxygen molecules on non-polar ZnO($10\bar{1}0$) surface. The focus is on the simultaneous adsorption of two molecules which could shed more light on the oxygen sensing at different humidity levels.

HL 21.25 Mon 15:00 Poster B

Field-effect transistors based on printed amorphous zinc-tin-oxide — •Benedikt Sykora and Heinz von Seggern — Technische Universität Darmstadt Fachbereich Materialwissenschaften Fachgebiet Elektronische Materialeigenschaften Alarich-Weiss-Straße 2 64287 Darmstadt Germany Building L2|01 - Room 156 Tel.: +49 (0) 6151 16-6331 Fax: +49 (0) 6151 16-6305

Since the last two decades metal-oxides like ZnO are widely studied as semiconductors for transistor applications. The benefits of these materials are, that they can be processed out of solution, they are transparent and cost efficient. This contribution presents field-effect transistors based on a printed amorphous zinc-tin-oxide (ZTO) semiconductor. Thin films are analysed by XRD, TEM, SEM and absorption measurements. The used ethanol based precursor solution is cheap and easy to process, non-toxic and long term stable. The saturation mobility increases from 0.05 cm^2/Vs, if a single semiconducting layer is applied, to a value of 7.7 cm^2/Vs for a transistor composed of 8 layers. To the best of our knowledge this is the highest reported value for a printed ZTO transistor. The reason for this huge increase in electron mobility is presumable d an improved film coverage and increased density which could be confirmed by AFM and that is known from other oxide semiconductors (1). The devices also show large output currents, high on/off ratios and low subthreshold voltages.

(1) Walker et al. ACS Appl. Mater. Interfaces 4, 6835-6841 (2012)

HL 21.26 Mon 15:00 Poster B

Determination of the Mn-spin temperature of photo-excited n-doped $Zn_{1-x}Mn_xSe$ by magneto-luminescence and spin-flip Raman spectroscopy — •Alexander Gerhard Knapp[1], Michael Hetterich[2], and Jean Geurts[1] — [1]Universität Würzburg, Experimentelle Physik 3, Würzburg, Germany — [2]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

The wide-gap semiconductor $Zn_{1-x}Mn_xSe$, as a II-VI-based diluted magnetic semiconductor, offers the opportunity for an independent tuning of the magnetic and the electronic properties by variation of either the Mn content or the dopant concentration. The strong s,p-d exchange coupling gives rise to a giant Zeeman splitting in magneto-photoluminescence (PL). Furthermore, magneto-Raman spectroscopy (RS) shows local spin flip excitations on Mn atoms, as well as electronic spin flip excitations of donator atoms in n-type material. The spectral position of the latter reflects the spin-selective energy splitting of the conduction band due to the s-d exchange interaction. We performed polarization-selective magneto-PL and and magneto-RS on $Zn_{1-x}Mn_xSe$ (x = .05 to .06) with various n-doping levels up to 10^{18} cm^{-3}, i.e. up to the range of the Mott density, at T = 1.6 K in Voigt configuration in B-fields up to 7 T. For near-resonant optical excitation in the range of the fundamental energy gap E_0, we investigated the influence of the variation of excitation power on the Mn-spin temperature. For this purpose, the Brillouin-function fit parameters of the PL- and RS-peak positions as well as the Stokes-to-Anti-Stokes intensity ratio of the local Mn spin flip were evaluated.

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Photon-assisted field emission from a Si tip with applied AC field (10 Hz-10 MHz) — Anna Zaporozhchenko[1], Sergey Chernov[2], Larisa Odnodvorets[1], Boris Stetsenko[3], •Sergej Nepijko[2], Hans-Joachim Elmers[2], and Gerd Schönhense[2] — [1]Sumy State University, Rimsky-Korsakov Str. 2, 40007 Sumy, Ukraine — [2]Institute of Physics, University Mainz, Staudingerweg 7, 55128 Mainz, Germany — [3]Institute of Physics, National Academy of Sciences of Ukraine, pr. Nauki 46, 03028 Kiev, Ukraine

We investigated the field emission current from a p-type silicon tip with large resistivity of 4×10^3 Ω·cm for illumination with a photon energy of 1.3 eV (close to the optical gap) and tip-anode voltages of $(0.7\div5)\times10^3$ V. Variations of the emission current due to an additional AC component of 30-60 V with varying frequency in the range of 10 to 10^7 Hz were observed. We investigated the dependence of this phenomenon on the AC frequency, light intensity and temperature. The resonant-like frequency dependence of the emission current is attributed to a dielectric resonance in the semiconducting tip material. The tip behaves like a driven plasmonic resonator. The results represent an important step forward for the development of high frequency display systems based on electron field emission.

HL 21.28 Mon 15:00 Poster B

Lattice dynamics of defect systems: The test case of Si — •Marcel Giar, Andreas Rühl, and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-University, D-35392 Giessen, Germany

Our research aims at calculating the vibrational properties, in particular Raman spectra, of defect systems. In order to realize sufficiently small defect concentrations very large supercells have to be considered. As a direct first principles approach is computationally too expensive for very large systems (>1000 atoms) we resort to Molecular Dynamics (MD) simulations for calculating lattice dynamical properties of the defect systems. The required effective potentials for carrying out the MD simulations are still based on *ab initio* data, created in the scope of Force Matching. We test our approach by constructing the respective potential for Si to reproduce phonon spectra obtained from *ab initio* calculations. The dynamical matrix is obtained within the so called small displacement method, which relies on displacing single atoms and calculating the resulting forces.

HL 21.29 Mon 15:00 Poster B

Transport properties of individual photoluminescent silicon quantum dot studied by scanning tunneling microscopy — •Tuhin Shuvra Basu, Simon Diesch, and Elke Scheer — Fachbereich Physik, Universität Konstanz, Universitätsstraße 10, 78457 Konstanz, Germany.

Silicon quantum dot (Si QD) exhibit room temperature photoluminescence (PL) property due to size induced quantum confinement effects in an ensemble measurement. The ensemble measurement of the PL provides average estimation of their excitonic bandgap and is dependent on size and surface protection [1]. Thus it is important to study the band-structure and exciton dynamics of Si QD on a single particle level. It is expected that the charging energy of Si QD will be appreciably high and will exhibit pronounced single-electron tunneling (SET) effects [2]. By studying tunneling spectroscopy, the conduction and valence band states and their degeneracy can be separately probed. In this work, the electronic transport and bandgap modification of Si QD on a single particle level has been studied by scanning tunneling spectroscopy (STS). The dI/dV curves exhibit features corresponding to the excitonic bandgap. Further the STS study of the individual Si QD by changing the size and the temperature (from 300 mK to 30 K) reveals bandgap fluctuations. We discuss our results in terms of correlations between the exciton dynamics, size, and temperature.

References:
[1]X. Cheng et al., Chem. Soc. Rev. 43, 2680 (2014).
[2]B. Weber et al., Nat. Nanotech. 9, 430 (2014).

HL 21.30 Mon 15:00 Poster B

Herstellung und Untersuchung von Bor-dotierten polykristallinen CVD-Diamantschichten — •Regina Berendakova, Nicolas Wöhrl und Volker Buck — Universität Duisburg-Essen und CENIDE, Forsthausweg 2, 47057 Duisburg

Bor-dotierte polykristalline Diamantschichten wurden mittels Mikrowellen-Plasma CVD aus einem Ar-CH_4-H_2 Plasma hergestellt. Die Dotierung der Schichten erfolgte durch Zugabe eines neuartigen flüssigen Bor-Precursors Tripropylboran $B(C_3H_7)_3$. Dieser Precursor wurde zuvor noch nicht für die Dotierung von Diamantschichten verwendet. Es konnte gezeigt werden, dass eine höhere Bor-Konzentration im Plasma auch zu einer höheren Dotierung der resultierenden Diamantschichten führt. Der spezifische elektrische Widerstand der Proben wurde mittels Vier-Punkt-Messung charakterisiert und liegt im Bereich von 10^{-4}-10^{-5} Ωm bei Raumtemperatur. Es wurde ein fast exponentieller Abfall des spezifischen Widerstandes der Proben mit steigendem Bor-Signal in den OES-Spektren des Plasmas festgestellt. Des Weiteren wurde der Einfluss des Bor-Precursors auf die Schichtmorphologie untersucht. In vorangegangenen Arbeiten ohne Bor-Dotierung wurden bei ähnlichen Prozessparametern ultra-nanokristalline Diamantschichten (UNCD) hergestellt. REM-Untersuchungen ergaben, dass alle dotierten Schichten eine deutlich erkennbare kolumnare Struktur aufweisen, was die Proben als mikrokristallinen Diamant (MCD) klassifizieren lässt. Es wurde also ein Übergang vom UNCD zum MCD Wachstum durch die Zugabe des Bor-Precursors ins Plasma beobachtet und charakterisiert.

HL 21.31 Mon 15:00 Poster B

Towards stabilization of the negatively charged nitrogen-vacancy center in diamond — •Samuel Müller[1], Jochen Scheuer[1], Boris Naydenov[1], Junichi Isoya[2], and Fedor Jelezko[1] — [1]Institut für Quantenoptik, Universität Ulm, Ulm, Germany — [2]Research Center for Knowledge Communities, University of Tsukuba, Tsukuba, Japan

The nitrogen-vacancy centers in diamond (NV) are very promising solid state single quantum systems with a wide application as qubits and ultra sensitive nano-scale field sensors. The NV is constantly changing its charged state from NV0 to NV-, whereas the latter is relevant for the applications. We propose a new method of stabilizing the NV- state via doping the diamond with an electron donor (phosphorus) and continuous irradiation with infrared light. We show that the NV- spin state can be measure using an orange laser light, which usually leads to photo-ionization in standard diamond crystals. We performed single shot nuclear magnetic resonance measurements in order to determine the degree of stability in the NV- state [1,2].

[1] Neumann, Philipp, et al. "Single-shot readout of a single nuclear spin." Science 329.5991 (2010): 542-544.

[2] Waldherr, G., et al. "Dark states of single nitrogen-vacancy centers in diamond unraveled by single shot NMR." Physical review letters 106.15 (2011): 157601.

HL 21.32 Mon 15:00 Poster B

Close to surface UHV-preparation of NV centers in diamond — •Stefan Borgsdorf[1], Lina Elber[1], Andreas Kaivers[1], Aniela Scheffzyk[1], Frederico Brandao[2], Dieter Suter[2], and Ulrich Köhler[1] — [1]Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum, Germany — [2]Experimentelle Physik IIIA, Technische Universität Dortmund, Germany

Color centers in diamond, especially NV-centers, are practical single photon emitters due to RT operation and are candidates for applications in quantum computing. NV-centers close to the surface allow electrical addressing and can be used for magnetic sensors. Here we present a setup for low energy implantation of NV centers near to the surface using UHV-conditions. We survey the influence of UHV-implantation and -annealing compared to the usual HV-heating. The usual etching processes with boiling tri-acid to remove graphitic com-

ponents after the annealing process is unnecessary. In general, the all-UHV-process leads to a cleaner diamond surface and decreases the background intensity in optical characterizations of the samples.

HL 21.33 Mon 15:00 Poster B

Accelerated two dimensional NMR spectroscopy using matrix completion — •Jochen Scheuer[1], Alexander Stark[1], Matthias Kost[2], Boris Naydenov[1], Martin Plenio[2], and Fedor Jelezko[1] — [1]Institut für Quantenoptik, Albert-Einstein-Allee 11, Universität Ulm, Ulm, Germany — [2]Institut für Theoretische Physik, Albert-Einstein Allee 11, Universität Ulm, Ulm, Germany

2D nuclear magnetic resonance (NMR) spectroscopy is one of the major tools for analysing the chemical structure of molecules and proteins. Usually this technique requires quite long measurement times, which limits its application only to stable samples. Here we demonstrate a method which allows to keep the full signal to noise ratio by collecting only a fraction of the experimental data. Our method is based on two dimensional compressed sensing (matrix completion) and with using spectral value decomposition we can recover the full spectral information from randomly sampled data points[1,2]. We experimentally demonstrate the applicability of our technique by performing 2D electron spin echo modulation (ESSEM) experiments on single nitrogen vacancy (NV) centres in diamond. We show that the main peaks in the spectrum can be obtained with only up to 5 % of the total number of the data points. We believe that our results can find an application in all types of two dimensional spectroscopy, as long as the measured matrix has a low rank.

[1] M. Kost, et al., http://arxiv.org/abs/1407.6262, 2014.

[2] Cai, Jian-Feng, et al., SIAM Journal on Optimization 20.4 (2010): 1956-1982.