KFM 16: Oxide Semiconductors (joint session HL/KFM)

Time: Wednesday 9:30–12:30 Location: H33

KFM 16.1 Wed 9:30 H33

Heavily doped Zinc Oxide with plasma frequencies in the telecommunication wavelength range — •Alexander Koch[1], Hongyan Mei[2], Jura Rensberg[1], Martin Hafermann[1], Jad Salman[2], Chenghao Wan[2,5], Raymond Wambold[2], Daniel Blascke[3], Heidemarie Schmidt[3], Jürgen Saalfeld[4], Sebastian Geburt[4], Mikhail Kats[2,5,6], and Carsten Ronning[1] — [1]Institute for Solid State Physics, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Department of Electrical and Computer Engineering, University of Wisconsin Madison, Madison, Wisconsin 53706, USA — [3]Leibniz Institute of Photonic Technology, 07745 Jena, Germany — [4]Innovavent GmbH, 37077 Göttingen, Germany — [5]Department of Materials Science and Engineering, University of Wisconsin Madison, Madison, Wisconsin 53706, USA — [6]Department of Physics, University of Wisconsin Madison, Madison, Wisconsin 53706, USA

We demonstrate high doping of ZnO by a combination of Ga ion implantation using a focused ion beam (FIB) system and post-implantation laser and flash lamp annealing. While ion implantation allows for the incorporation of impurities with nearly arbitrary concentrations, the additional optical annealing processes enable dopant activation close to the solid-solubility limit of Ga in ZnO. By this means, we achieved highly-doped ZnO:Ga with free-carrier concentrations of $9.5 \cdot 10^{20}$ cm^{-3}, which results in a plasma wavelength shorter than the telecommunication wavelength of 1.55 μm. Thus, ZnO:Ga is a very promising plasmonic material for optical applications in the near-infrared spectral region.

KFM 16.2 Wed 9:45 H33

Side-by-side display of optical and resistive H_2S gas sensing properties of pristine and gold functionalized ZnO nanowires — •Angelika Kaiser[1], Tanja Mauritz[1], Joachim Bansmann[3], Ulrich Herr[1], and Klaus Thonke[2] — [1]Institute of Functional Nanosystems, University Ulm, 89081 Ulm, Germany — [2]Institute of Quantum Matter, Semiconductor Physics Group, University Ulm, 89081 Ulm, Germany — [3]Institute for Surface Chemistry and Catalysis, University Ulm, 89081 Ulm, Germany

We investigate the mechanism of hydrogen sulfide (H_2S) gas sensing in pristine and gold functionalized zinc oxide (ZnO) nanowires (NW), two potent nanomaterial systems with an enlarged surface-area-to-volume ratio for medical breath analysis in the sub-ppm regime through the "electronic nose" approach. Pristine ZnO NWs (ZnO(NM)) are grown by high-temperature chemical vapor deposition (CVD) and functionalized with gold (Au) nanoparticles by magnetron sputtering (ZnO(Au)). The sensor response is studied by photoluminescence (PL) and electrical conductivity measurements of as-grown ZnO NWs and open gate ZnO NW ChemFET structures. A systematical side-by-side comparison of PL-intensity-time measurements and current-time measurements reveal a two-step detection process between 1 ppm of H_2S and ZnO(NM)/ZnO(Au) NWs. Temperature series hints at underlying gas adsorption/desorption processes. Additional X-ray photoelectron spectroscopy (XPS) confirms the beneficial gas-sensitive affinity between Au functionalization and H_2S gas, which leads to a significant improvement of the sensitivity for H_2S detection.

KFM 16.3 Wed 10:00 H33

Growth window of α-Ga_2O_3 on m-plane sapphire by pulsed laser deposition — •C. Petersen, S. Vogt, M. Kneiss, H. von Wenckstern, and M. Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

Due to its high bandgap of 4.6-5.3 eV and high predicted breakdown field of 8 MV/cm [1], much attention is drawn to the wide bandgap semiconductor Ga_2O_3 for applications in high-power devices. However, besides the well-studied thermodynamically stable monoclinic β-phase of Ga_2O_3, the metastable α-polymorph with corundum structure is gaining scientists' interest. Since it is isostructural to Al_2O_3, miscibility over the entire composition range of α-$(Al_xGa_{1-x})_2O_3$ can be achieved [2] and the growth on cost-effective sapphire substrates becomes feasible. Thereby m-plane sapphire facilitates the growth of the corundum phase [3] and allows for thin films with electron mobilities as high as 65 cm^2(Vs)$^{-1}$ [4]. We present phase-pure α-Ga_2O_3 thin films grown on m-plane sapphire over a wide temperature range of 565 °C up to 750 °C with high cristallinity and surface roughnesses as low as 0.7 nm (RMS). We further demonstrate that for oxygen partial pressures above 0.001 mbar the formation of the monoclinical β-phase and spinel-defective γ-phase occurs and provide a corresponding phase diagram. Resulting samples were investigated employing X-ray diffraction, reciprocal space maps and atomic force microscopy. [1] Higashiwaki, Sc. Sci. Tech., 034001, 2016. [2] Hassa, pss-b, 2000394, 2020. [3] Kneiß, jmr, 4816-4831, 2021. [4] Akaiwa, pss-a, 1900632, 2020.

KFM 16.4 Wed 10:15 H33

Simulation of Switching Processes Inside Bilayer Valence Change Memory Cells by a Drift-Diffusion Model — •Nils Sommer[1], Stephan Menzel[1], and Rainer Waser[1,2] — [1]Peter Grünberg Institut 7, Forschungszentrum Jülich, Germany — [2]Institut für Werkstoffe der Elektrotechnik 2, RWTH Aachen, Germany

Valence change memory (VCM) cells are promising candidates for future nonvolatile storage devices [1]. VCM cells are characterized by their ability to switch between at least two stable resistance states by applying suitable bias voltages. A special structure of VCM cells are bilayer cells consisting of two semiconducting oxide layers, with one oxide serving as a tunnel barrier. Experiments show that a change in resistance of the cell can be caused by the exchange of oxygen between the two oxide layers [2]. However, the processes taking place are not yet well understood. We use a drift-diffusion model to simulate the movement of oxygen inside the semiconductor to gain a better understanding of the exchange process between the layers. We investigate the internal electric fields acting as a driving force on the oxygen, as well as the oxygen diffusion process that causes it to return to an equilibrium state. We show that an oxygen exchange deforms the shape of the tunnel barrier and by this changing the resistance of the cell. Further, we show that the change in resistance depends on the permittivity of the oxides.

[1] R. Waser, R. Dittmann, G. Staikov, K. Szot, Adv. Mater. 2009, 21, 2632 [2] A. Gutsche, S. Siegel, J. Zhang, S. Hambsch, R. Dittmann, Frontires in Neuroscience,2021, 15, 661261

KFM 16.5 Wed 10:30 H33

Phonons, Isotope Effects, and Point Defects in β-Ga2O3 — •Benjamin M. Janzen[1], Piero Mazzolini[2,3], Roland Gillen[4], Andreas Falkenstein[5], Vivien F. S. Peltason[1], Hans Tornatzky[1], Daniel Cierpinsky[1], Andrea Ardenghi[2], Manfred Martin[5], Janina Maultzsch[4], Roberto Fornari[2,3], Zbigniew Galazka[6], Oliver Bierwagen[2], and Markus R. Wagner[1] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V, Germany — [3]Department of Mathematical, Physical and Computer Sciences, University of Parma, Italy — [4]Chair of Experimental Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [5]Institute of Physical Chemistry, RWTH Aachen University, Germany — [6]Leibniz-Institut für Kristallzüchtung, Berlin, Germany

We present a combined experimental and theoretical study of lattice vibrations in a homoepitaxial β-Ga2O3 thin film grown by MBE with different oxygen isotopes (16O, 18O). Using polarized first- and second order micro-Raman spectroscopy, we identified all 15 first-order Raman modes of β-Ga2O3. In combination with density functional perturbation theory calculations, we identify the atomistic origins (Ga-Ga, Ga-O or O-O) of all Raman active phonon modes in β-Ga2O3 by quantifying the isotopically-induced relative frequency shifts of the individual Raman modes and investigate the presence of point defects on specific lattice sites.

KFM 16.6 Wed 10:45 H33

Epitaxial ZnO thin films and NWs — •Maximilian Kolhep[1], Margit Zacharias[1], and Jürgen Bläsing[2] — [1]Laboratory for Nanotechnology, Department of Microsystems Engineering (IMTEK), University of Freiburg, Freiburg 79110, Germany — [2]Otto-von-Guericke-University Magdeburg, Institute of Physics, Magdeburg, Germany

Due to its high piezoelectric coefficient and direct band gap of 3.37 eV, ZnO and especially ZnO nanowires are of interest for numerous future applications. We demonstrate the epitaxial growth of ZnO on Si(111) substrates using an AlN buffer layer by atomic layer deposi-

tion (ALD). ALD is a promising technique as it allows the deposition of extremely thin films with precise thickness control and excellent conformality over large areas. The crystalline quality of ZnO thin films determined by XRD increases with increasing deposition temperature and an additional post-annealing step. These thin films have a great potential as a substrate for the subsequent catalyst-free and epitaxial growth of ZnO NWs by CVD. The influence of growth parameters on the morphology of ZnO NWs will be discussed.

15 min. break

KFM 16.7 Wed 11:15 H33

Investigation of $CuBr_xI_{1-x}$ thin films and CuI bulk material — •Michael Bar[1], Evgeny Krüger[1], Steffen Blaurock[2], Stefan Merker[2], Holger von Wenckstern[1], Harald Krautscheid[2], and Marius Grundmann[1] — [1]Universität Leipzig, Felix-Bloch Institute, Germany — [2]Universität Leipzig, Institute of Inorganic Chemistry, Germany

Oxide based wide-bandgap materials with suitable transparency in the visible range are typically unipolar, such that heterostructures are needed for complementary devices. The search for a suitable p-type candidate has led to copper iodide (CuI), which unites transparency in the visible spectral range with exceptional hole mobility, therefore sharing and yet complementing typical properties of oxides. Fabrication methods include sputtering, spin coating and molecular beam epitaxy. [1,2] We present structural, electrical and optical properties of CuI bulk material, and thin films which were grown by pulsed laser deposition (PLD). Furthermore, alloyed thin films of $CuBr_xI_{1-x}$ were deposited with a segmented target PLD approach and investigated using x-ray diffraction, transmission and photoluminescence measurements. This PLD approach allows for deposition of thin films in the full composition range using only a single target without the need of sintering. [3] A systematic shift of lattice constants as well as the excitonic features can be observed as function of alloy composition.

[1] C. Yang *et al.*, Proc. Natl. Acad. Sci. USA, **113**(46), 12929, (2016).
[2] S. Inagaki *et al.*, Appl. Phys. Lett., **116**(19), 192105, (2020).
[3] H. Wenckstern *et al.*, Phys. Stat. Sol. (b), **257**(7), 1900626, (2020).

KFM 16.8 Wed 11:30 H33

A Koopman's compliant exchange correlation potential for semiconductors — •Michael Lorke[1], Peter Deak[2], and Thomas Frauenheim[2] — [1]Institute for Theoretical Physics, University of Bremen, Germany — [2]BCCMS, University of Bremen, Germany

Density functional theory is the workhorse of theoretical materials investigations. Due to the shortcoming of (semi-)local exchange correlation potentials, hybrid functionals have been established for practical calculations to describe surfaces, molecular adsorption, and defects. These functionals operate by mixing between semi-local and Hartree-Fock exchange semi-emprically. However, their parameters have to be optimized for every material separately. To treat materials with a more physics driven approach and without the need of parameter optimization is possible with many-body approaches like GW, but at an immense increase in computational costs and without the access to total energies and hence geometry optimization.

We propose a novel exchange correlation potential[1] for semiconductor materials, that is based on physical properties of the underlying microscopic screening. We demonstrate that it reproduces the low temperature band gap of several materials. Moreover it respects the required linearity condition of the total energy with the fractional occupation number, as expressed by the generalized Koopman's theorem. We also show that this novel functional can be used as a kernel in linear response TDDFT to reproduce excitonic effects in optical spectra

[1] Physical Review B 102 (23), 235168 (2020)

KFM 16.9 Wed 11:45 H33

The role of defects in polaron hopping transport in epitaxial BiVO4 for solar water splitting — •Malte Luca Weber, Viktoria Franziska Kunzelmann, and Ian Sharp — Walter Schottky Institute, TUM, Am Coulombwall 4, 85748 Garching, Germany

Use of green hydrogen as a fuel, energy storage medium, and reactant in chemical industry is one of the key strategies on the way to a sustainable economy. In this regard, solar driven water splitting using semiconductor photoelectrodes is a promising approach for sustainable production of hydrogen. Among various investigated semiconductor photoelectrodes, BiVO4 offers several desirable characteristics, including favourable band edge energetics, high carrier separation efficiency, and potential for stable operation under photoelectrochemical conditions. However, the material is characterised by very low carrier mobilities due to self-trapping formation of small polarons. Here, the effect of intentionally introduced defects on charge carrier mobility is investigated. Using a novel solution-based synthesis technique, high-quality epitaxial BiVO4 thin films were grown on YSZ (001). Post-synthetic vacuum annealing enables tuneable introduction of tuneable concentrations of oxygen vacancy defects. Optical characterisation by photothermal deflection spectroscopy clearly indicates an increase of the sub-bandgap absorption for an increasing defect concentration, leaving unaltered the bandgap. Temperature-dependent electrical conductivity measurements indicate a thermally-activated hopping behaviour, which is characterised by higher conductivities and lower hopping behaviours with increasing native point defect concentrations.

KFM 16.10 Wed 12:00 H33

Conduction channels in polycrystalline copper iodede thin films — •Tillmann Stralka — Universtität Leipzig, Felix Bloch Institute for Solid State Physics, Linnéstr. 5, 04103 Leipzig, Germany

The search for high-performance, transparent p-type conductive materials has been a major challenge for decades [1]. Copper iodide (CuI) or alloys based on CuI [2] could offer a solution, since CuI does outperform all other known p-type TCMs, concerning transmittance in the visible spectrum as well as electrical conductivity at room temperature [3]. In this contribution polycrystalline CuI thin films, grown by sputtering, are investigated. Hereby we try to understand and differentiate the contribution of grains and grain boundaries (GBs) to electrical transport. Extended structural defects such as GBs lead to a depletion of majority charge carriers in their vicinity and even a localised inversion (two dimensional electron gas) within GBs was reported [4]. To acquire morphological (grain and GBs) and electrical properties with a high spatial resolution we employ current probe atomic force microscopy and Kelvin probe force microscopy. We evaluate these measurements with a novel approach that offers the possibility to correlate topographic and electrical properties over a whole series of scans in dependence on an externally applied voltage [5], measuring temperature, probe force, plasma treatment and degradation over time.

[1] M. Grundmann et al., J.Phys.D.Apps.Phys., 49(213001), 2016 [2] T. Jun et al., Adv. Mater., 30(1706573), 2018 [3] C. Yang et al., PNAS 113(412929), 2016 [4] M. Kneiß et al., Adv. Mater. Interfaces, 5(6), 2018 [5] I. Visoly-Fisher et al., Adv. Funct. Mater., 16(649), 2016

KFM 16.11 Wed 12:15 H33

First-Principles Studies of Defects in Bismuth Vanadate — •Nicklas Österbacka[1], Francesco Ambrosio[2], and Julia Wiktor[1] — [1]Chalmers University of Technology, Gothenburg, Sweden — [2]University of Salerno, Fisciano, Italy

Bismuth vanadate, a transition-metal oxide semiconductor with a bandgap of 2.4 eV, has shown great promise as a water-splitting photocatalyst. Its practical performance remains limited due to slow hole transfer, high charge recombination rates, and low conductivity, however. An atomistic understanding of the relationship between the material's structure and its properties is key to solving these issues. To this end, we have performed first-principles calculations on the native defects of bismuth vanadate, revealing their structural complexity and highlighting the importance of taking charge localization into account for this class of materials. Additionally, we show that oxygen vacancy-induced distortions in the material complicates phase identification of synthesized samples by making powder X-ray diffraction ambiguous.