HL 40: Oxide Semiconductors: Transport and Spectroscopy

Time: Thursday 9:30–12:30 Location: POT/0251

HL 40.1 Thu 9:30 POT/0251

Unraveling metal-induced redox mechanisms on SrTiO3 via combined in-situ laser reflectometry and x-ray photoelectron spectroscopy — •Georg Hoffmann, Shi-Hui Liu, Serkan Sirt, Oliver Bierwagen, and Roman Engel-Herbert — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

SrTiO3 has long served as a key platform for emergent phenomena in perovskite oxides such as polar discontinuity driven two-dimensional electron gases (2DEGs) when interfaced with LaAlO3 [1]. Recently, increasing attention has been brought to 2-DEGs that emerge at SrTiO3 surfaces from redox-reactions induced by amorphous metal deposition on top [2]. Studying these processes, however, requires complex in-situ techniques like photoelectron spectroscopy (XPS) with long measurement cycles. Here, we introduce laser reflectometry (LR) as a complementary technique that enables monitoring of redox-reactions at oxide/metal interfaces. We show that LR in an oxide molecular beam epitaxy setup can distinguish between Al deposition on non-reactive substrates and Al oxidation, e.g. through oxygen scavenging from SrTiO3. Atomic force microscopy, Capacitance-Voltage profiling, and XPS measurements corroborate our findings. Our results demonstrate how LR can guide future investigations of redox-reactions at oxide/metal interfaces. [1] A. Ohtomo, and H. Y. Hwang., Nature 427, 423 (2004). [2] T. Rödel, et al., Adv. Mater. 28, 1976 (2016).

HL 40.2 Thu 9:45 POT/0251

Resonant Raman studies in rutile-Germaniumdioxide — •Kenneth Brandt[1,3], Moritz Meissner[1,3], Zbigniew Galazka[2], Tobias Schultz[2], Markus Wagner[1,3], and Hans Tornatzky[1,3] — [1]Paul-Drude-Institut, Berlin — [2]Leibniz-Institut für Kristallzüchtung, Berlin — [3]Technische Universität Berlin

Ultra-wide bandgap (UWBG) semiconductors are a new research area of interest, with promised applications in power electronics. Germaniumdioxide in the rutile phase (r-GeO_2) has been characterised to be such an UWBG Material with a Bandgap at about 4.5 eV. To be able to create homojunction devices, the material needs to be ambipolar dopable, which poses a challenge for β-Ga_2O_3, as p-type doping has yet to be achieved, while r-GeO_2 is predicted to be ambipolar dopable. Raman measurements show a non typical intensity relationship, in which explicitly the E_g mode does not follow the expected $I \propto \omega^4$ relation of the Raman-Scattering processes but decreases in intensity with higher excitation energies. We are performing resonant Raman studies, with excitation energies ranging from 1.2 eV provided by a tunable Ti:Sa Laser, as well as multiple additional single line Lasers with energies up to 5.1 eV, to investigate the atypical Raman response and electron-phonon coupling.

To quantise the measurements CaF_2 is used as a calibration standard and GaAs is included in the measurement series to compare with literature.

HL 40.3 Thu 10:00 POT/0251

Theoretical Description of a Photo-induced Hidden State in Bismuth Vanadate — •Philip Schwinghammer[1], Verena Streibel[1,2], Frederico Delgado[1], Franziska S. Hegner[1], Viktoria Kunzelmann[1,2], Konrad Merkel[1], Frank Ortmann[1], Ian Sharp[1,2], and David A. Egger[1] — [1]TUM School of Natural Sciences, Technical University of Munich, Germany — [2]Walter Schottky Institute, Technical University of Munich, 85748 Garching, Germany

Bismuth Vanadate has attracted attention in recent years as a promising photoactive material and complex model system. In order to understand new experimental results which show a light-sensitive structure at room temperature, we perform a detailed analysis of the chemical bonding and impact of the exchange-correlation functional. In addition to the use of hybrid functionals, spin-orbit coupling (SOC) stabilizes the experimentally observed monoclinic structure over its high-symmetry tetragonal counterpart. The physical mechanism behind the stabilization is explained through the increase of both covalent and ionic bonding as symmetry breaking causes shortening of select Bi-O bonds. These mechanisms are strongly affected by photo-induced excitation of charge carriers, as the states responsible for the monoclinic distortion are depleted. The alteration of the structure through light may then affect the photo-catalytic efficiencies of the material, as we also find significant differences in the optoelectronic properties of the monoclinic and tetragonal structures.

HL 40.4 Thu 10:15 POT/0251

E-field modulated phase change properties in highly epitaxial VO2 thin film monitored via Raman spectra and IR transmission — •Sonika Singh[1], Rajendra Singh[2], and Ankur Goswami[3] — [1]IIT Delhi, New Delhi, India — [2]IIT Delhi, New Delhi, India — [3]IIT Delhi, New Delhi, India

VO2 is a highly explored smart oxide semiconductor showing metal insulator transition (MIT) at near room temperature ~67 oC. It is observed that optoelectronic properties of highly epitaxial VO2 thin films offer several advantages as compared to polycrystalline film in terms of E-MIT and thermal switching. Here we investigate E-MIT on epitaxial VO2 deposited using PLD technique. Prior to electrical measurement, electrical contacts with 8 *m separation distance were made using Ti/Au metallization. The dual voltage sweep carried over the device demonstrated a high thermal switching ratio (around 30) between high resistive and low resistive state. Furthermore, the dual current sweep was performed on the devices reflected snapback transition signifying uncontrolled and rapid phase transition of VO2. Additionally, E-field dependent Raman spectroscopy revealed modulation of phase transition of VO2 monitored via Raman peaks and triggered via square signal of E-field. These findings suggest that epitaxial thin film of VO2 can be explored for further studies involving modulation of phase change properties via E-field that find direct applications in neuromorphic devices, THz transmissions, thermal switches.

HL 40.5 Thu 10:30 POT/0251

Spatially Resolved Phase Transition and Characterization in Gallium Oxide — Umutcan Bektas[1], Paul Chekhonin[2], Nico Klingner[1], Azat Abdullayev[3], Alexander Azarov[4], René Hübner[1], Zhandos Utegulov[3], Andrej Kuznetsov[4], and •Gregor Hlawacek[1] — [1]Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328, Dresden, Germany — [2]Resource Ecology, Helmholtz-Zentrum Dresden-Rossendorf, 01328, Dresden, Germany — [3]Department of Physics, Nazarbayev University, 010000, Astana, Kazakhstan — [4]Centre for Materials Science and Nanotechnology, University of Oslo, N-0316, Oslo, Norway

In this study, we investigate ion-irradiated β-Ga_2O_3 samples (varying ions and fluences) alongside α- and κ-Ga_2O_3 thin films. Using focused ion beam (FIB) irradiation, we locally modified the samples under controlled conditions by tuning beam current, size, spacing, scan type, and ion species. Structural changes in the irradiated regions were characterized via electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM). Our results demonstrate that ion induced transition to the γ polymorph can be achieved also through FIB irradiation, enabling the fabrication of in-plane polymorph patterns on the nanometer scale. Furthermore, time-domain thermoreflectance (TDTR) measurements further revealed the thermal conductivity of irradiated regions, highlighting opportunities to optimize heat transport in Ga_2O_3 power electronic devices. This research is supported by the tax funds on the basis of the budget passed by the Saxonian state parliament in Germany.

HL 40.6 Thu 10:45 POT/0251

Bandgap, exciton dynamics, and anisotropic thermal transport in rutile-GeO_2 — •Markus R. Wagner[1,2], Luca S. M. Choi[2], Nils Bernhard[2], Pouria Emtenani[2], Felix Nippert[2], Moritz Meissner[1], Hans Tornatzky[1], and Zbigniew Galazka[3] — [1]Paul-Drude-Institut für Festkörperelektronik — [2]Technische Universität Berlin, Institut für Physik und Astronomie — [3]Leibniz-Institut für Kristallzüchtung

Rutile germanium dioxide (r-GeO_2) is a promising ultra-wide bandgap material, predicted to support ambipolar doping and display high thermal and electronic conductivity, making it a strong candidate for power electronics. However, essential aspects of its properties, such as exciton and phonon dynamics as well as the role of defects and impurities, remain only partially explored. Here, we present our recent spectroscopic studies on r-GeO_2. High-resolution spectroscopy of free exciton ground and excited states enables us to determine exciton binding energies and the temperature dependence of the

bandgap. Polarization-resolved photoluminescence reveals pronounced differences between near-UV and visible emission bands, which we analyze regarding thermal quenching, recombination dynamics, and charge transfer through temperature- and power-dependent PL, TRPL, and PLE. Using time-domain thermoreflectance down to cryogenic temperatures, we establish the temperatur dependence of thermal conductivity and anisotropy, supported by Boltzmann transport calculations. Finally, polarization-resolved Raman spectroscopy identifies all first-order Raman-active phonons and their relative tensor elements.

15 min. break

HL 40.7 Thu 11:15 POT/0251

MESFETs based on α-$(Al_xGa_{1-x})_2O_3$ thin films — •Sebastian Köpp, Sofie Vogt, Holger von Wenckstern, and Marius Grundmann — Leipzig University, Leipzig, Germany

We present the electrical properties and key parameters of metal-semiconductor field effect transistors (MESFET) on α-$(Al_xGa_{1-x})_2O_3$. The functional thin films were grown by pulsed laser deposition. The transistors were investigated in dependence on the Al content up to x=0.1. The devices exhibit an electrical breakdown field larger than that of comparable transistors on binary α-Ga_2O_3, demonstrating the advantages of the $(Al_xGa_{1-x})_2O_3$ alloy system.
With its ultra-wide bandgap of 5.3 eV to 5.6 eV [1,2] and a high predicted breakdown field of 10 MV/cm [3], α-Ga_2O_3 is a promising material for high-power devices, as well as deep-UV photodetectors. α-Ga_2O_3, being isostructural to aluminium oxide, allows for heteroepitaxial growth on cost-efficient sapphire substrates, and also opens up the option of α-$(Al_xGa_{1-x})_2O_3$ alloys [4], with even higher dielectrical breakdown field than binary Ga_2O_3.

[1] A. Segura *et al.*, Phys. Rev. Materials 1, 024604 (2017)
[2] E. Ahmadi *et al.*, J. Appl. Phys. 126, 160901 (2019)
[3] M. Biswas and H. Nishinaka, APL Mater. 10, 060701 (2022)
[4] J. Steele *et al.*, APL Mater. 12, 041113 (2024)

HL 40.8 Thu 11:30 POT/0251

Group-III doping study of p-type oxide tin monoxide — •Nicola Gutmann, Georg Hoffmann, Aidan Campbell, and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany.

The use of transparent conducting oxides has so far been limited to n-type materials, hindering the development of transparent oxide-based pn-junctions and CMOS devices. In contrast, SnO shows natural p-type conduction with reported hole mobilities up to 21 cm^2/Vs [1] and well-performing p-type transistors demonstrated.

Adjustment of hole concentration by doping with Ga, Na, K and Y has been demonstrated [2]. Al is theoretically predicted to be an n-type dopant [3], which would enable SnO-based pn-homojunctions.

In this work, we comparatively explore doping of suboxide molecular beam epitaxy grown SnO by the group-III elements Al, Ga and In.

[1] M. Minohara et al., J. Phys. Chem. C, vol. 124, no. 2, pp. 1755-1760 (2020).
[2] S. Chae et al., APL Materials, vol. 13, no. 10, p. 101114 (2025).
[3] M. Graužinyte et al., Phys. Rev. Materials, vol. 2, no. 10, p. 104604 (2018).

HL 40.9 Thu 11:45 POT/0251

Realization of highly rectifying pn-heterojunctions and junction field-effect transistors on pulsed laser deposited α-Ga_2O_3 thin films — •Paul Bokemeyer, Clemens Petersen, Holger von Wenckstern, Marius Grundmann, and Sofie Vogt — University Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany

The wide band gap of about 5.3 eV[1] and a high expected breakdown field of up to 10 MV/cm[2], renders the corundum α-phase of Ga_2O_3 interesting for high power electronics. We present lateral p^+n-heterojunction diodes on α-Ga_2O_3:Sn grown by pulsed laser deposition (PLD) using a two step approach[3]. ZnCoO (ZCO) and NiO deposited by PLD at room temperature were used as p^+-type materials. Further, the influence of a remote oxygen plasma treatment prior to the deposition of the p-type layers on the device performance was investigated. High current rectification ratios of 8.2 (ZCO) and 7.8 (NiO) orders of magnitude at ± 3V were achieved. Additionally, both p-type materials were used as gate materials in the fabrication of α-Ga_2O_3:Zr junction-field-effect-transistors (JFETs), yielding on/off current ratios of more than 9 orders of magnitude and sub-threshold-swings down to 119 mV/dec. Furthermore, breakdown was detected at drain voltages of up to 476 V which is estimated to a field of 1.7 MV/cm [4].

[1] A. Hassa et.al., J.Phys. D: Appl. Phys. **54**, 223001 (2021)
[2] M. Biswas et al., APL Mater. **10**, 060701 (2022)
[3] S. Vogt et al., Phys. Status Solidi A, **220** 2200721 (2023)
[4] P. Bokemeyer et al.,Phys. Status Solidi RRL, 2400388 (2025)

HL 40.10 Thu 12:00 POT/0251

Defect-Induced Resistive Switching in Titanate-based Perovskites — •Parrydeep Kaur Sachdeva[1], Wahib Aggoune[1,2], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at FHI of MPG, Berlin — [2]Institut für Physik and CSMB, Humboldt-Universität zu Berlin, Berlin

Perovskites possess strong potential for exhibiting ferroelectric resistive switching (RS), a functionality recently realized yet not understood in titanate perovskites [1]. Controlled deviation from stoichiometry has revealed high RS, indicating a defect-mediated origin. Using hybrid functional DFT calculations, we show that the Ti antisite defect (Ti-interstitial with Ca-vacancy) can induce ferroelectricity in $CaTiO_3$ which is an incipient ferroelectric, stabilized in a non-polar state by strong octahedral tilts. The Ti-interstitial atom breaks this balance by its off-center displacement and induces a local polarization. This polarization is switchable between different off-center positions of the defect, with energy barriers in the range of 0.25 eV. Additionally, the Ti antisite defect gives rise to mid-gap states, with a charge density mainly localized around the Ti-interstitial atom. Switching the defect between equivalent off-center positions switches the polarization direction and alters the spatial distribution of the charge state. This can influence the material's overall response under external stimuli. These results are discussed with respect to the experimentally observed resistive switching in titanate-based perovskites [1], as reported by Leibniz-Institut für Kristallzüchtung (IKZ) Berlin.

[1] A. Baki, *et al.*, *Sci. Rep.*, **11**, 7497 (2021).

HL 40.11 Thu 12:15 POT/0251

ZnM_2O_4 (M = Co, Rh, Ir) spinels as potential p-type transparent conducting oxides — •Daniel Fritsch — Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam, Germany

ZnM_2O_4 (M = Co, Rh, Ir) spinels are under investigation as potential p-type transparent conducting oxides (TCOs) [1]. Here we extend our previous investigation of $ZnRh_2O_4$ into the whole series of ZnM_2O_4 (M = Co, Rh, Ir) spinels.

To this end, we perform *first-principles* calculations based on density functional theory employing a recently developed *self-consistent* hybrid exchange and correlation functional [2], and compare the results to more standard HSE06 hybrid functional calculations. In order to judge the results on the electronic and optical properties, additional calculations based on many-body perturbation theory, i.e. G_0W_0 calculations, have been performed and allow for a more detailed analysis of the applicability of ZnM_2O_4 (M = Co, Rh, Ir) spinels as potential p-type TCOs.

The obtained structural, electronic, and optical properties will be discussed alongside earlier experimental and theoretical investigations, and will open a pathway to potential applications of ZnM_2O_4 (M = Co, Rh, Ir) spinels.

[1] D. Fritsch, Electron. Mater. **2**, 504 (2021).
[2] D. Fritsch, B. Morgan, and A. Walsh, Nanoscale Res. Lett. **12**, 19 (2017).