HL 11: Focus Session: Functional Metal Oxides for Novel Applications and Devices

Metal oxides exhibit a myriad of fascinating physical properties that enable a large variety of potential applications such as sensors and detectors, solar energy harvesting, transparent and potentially bendable electronics, power electronics, high-electron-mobility transisitors, memristors, topological quantum computation and so on. These functionalities typically require homo- or heteroepitaxial layers of high crystallinity with bendable amorphous semiconducting oxides as an exception. This session sets a focus on growth of bulk and thin films, experimental and theoretical investigation of their physical properties as well as fabrication and characterization of demonstrator devices.

Organizers: Oliver Bierwagen (Paul-Drude-Institut für Festkörperelektronik, Berlin), Holger Eisele (TU Berlin), Jutta Schwarzkopf (Leibniz-Institut für Kristallzüchtung, Berlin) and Holger von Wenckstern (Universität Leipzig).

Time: Tuesday 13:30–16:30 Location: H4

Invited Talk HL 11.1 Tue 13:30 H4

Modulation Doping in High-Mobility Alkaline-Earth Stannates — •Bharat Jalan — University of Minnesota, Twin Cities, USA

The vast majority of work concerning a conducting oxide interface focus on the LaAlO3/SrTiO3 (LAO/STO) interfaces including some on Al2O3/STO and ReTiO3/STO (Re refers to the rare-earth elements) interfaces among others. Amazingly, all these heterostructures involve the use of STO as an active layer where electron transport occurs. Attempts to synthesize non-STO based modulation-doped heterostructure have been unsuccessful so far despite theoretical predictions. Nor has any appreciable level of control been gained over the electron density at the interface, which is critical to device applications. In this talk, we will report the first demonstration of true modulation doping in a wider bandgap perovskite oxides without the use of STO. We show that the La-doped SrSnO3/BaSnO3 system precisely fulfills the theoretical criteria for electron doping in BaSnO3 using electrons from La-doped SrSnO3, and we demonstrate how rearrangement of electrons can be used to control the insulator-to-metal transition in these heterostructure. We further show the use of angle-resolved HAXPES as a non-destructive approach to not only determine the location of electrons at the interface but also to quantify the width of electron distribution in BaSnO3. The transport results are in good agreement with the results of self-consistent solution to one-dimensional Poisson and Schrödinger equations.

Invited Talk HL 11.2 Tue 14:00 H4

Ultrathin oxides on InGaN nanowires: Hybrid nanostructure photoelectrodes and optical analysis of chemical processes — P. Neuderth[2], J. Schörmann[2], M. Coll[3], M. de la Mata[4], J. Arbiol[4], R. Marschall[5,6], and •M. Eickhoff[1,2] — [1]Inst. of Solid State Physics, Univ. of Bremen, Germany — [2]Inst. of Exp. Phys. I, JLU Giessen, Germany — [3]Inst. de Ciencia de Materials de Barcelona, Spain — [4]ICN2, Barcelona, CAT, Spain — [5]Inst. of Phys. Chem., JLU Giessen, Germany — [6]Phys. Chem. III, Univ. of Bayreuth, Germany

We demonstrate an experimental strategy for systematically assessing the influence of surface passivation layers on the photocatalytic properties of nanowire (NW) photoanodes by combining photocurrent analysis, photoluminescence spectroscopy and high resolution transmission electron microscopy. We apply this approach to separate the influence of different mechanisms on recombination and transport processes of photogenerated carriers and to compare the effect of TiO2, CeO2 and Al2O3 coatings deposited by atomic layer deposition (ALD). Due to efficient charge transfer from the InGaN NW core a stable TiO2-covered photoanode with visible light excitation is realized. As further applications we demonstrate the quantitative optical analysis of oxygen diffusion in ultrathin CeO2 and of the Li intercalation in TiO2 using hybrid nanostructures. In both cases the optical properties of the InGaN NWs are used as a probe for chemical processes in the ultrathin oxide layer that was deposited by ALD. Further potential applications of advanced hybrid nanostructures are discussed.

Invited Talk HL 11.3 Tue 14:30 H4

Doping and charge compensation mechanisms in semiconducting oxides — •Andreas Klein — Technical University of Darmstadt

Different charge compensation mechanisms are known for ionic solids. Among them are the formation of compensating defects such as electronic or ionic defects, the valence changes of atoms and the segregation of dopants. In principle, the introduction of positive charges by donor doping or reduction results either in the compensation by electrons, negatively charged intrinsic acceptors as metal vacancies, the reduction of a one of the species in the compound, or in the segregation of the dopant species. The situation is reversed for the addition of negative charges. While the different mechanisms are well-documented for different materials, predicting the prevailing compensation mechanism in a material is hardly possible. It is well known that the Fermi energy is determined by the defect concentrations but it is equivalent to describe the concentration of defects as a function of the Fermi energy. This enables a direct comparison of the different compensation mechanisms. The challenges in discriminating the different compensation mechanisms are discussed using the example of Sn-doped indium oxide.

Invited Talk HL 11.4 Tue 15:00 H4

Oxide Memristors for edge computing and secure electronics — •Heidemarie Schmidt — Leibniz-IPHT, Jena, Germany — Friedrich-Schiller-Universität Jena, Jena, Germany — Fraunhofer ENAS, Chemnitz, Germany

In the future, new hardware components will determine the power and strength of artificial intelligence and manchine learning. These components are called memristors [1]. The first memristor with unified analog data storage and information processing is the BiFeO3 (BFO) memristor. BFO is an electroforming-free, bipolar memristor and its potential has been shown in in-memory information processing [2], edge computing [3], and hardware cryptography. Another electroforming-free memristor is the unipolar memristor YMnO3 (YMO) [4]. In order to develop memristor technology and applications further, it is more than ever necessary to understand the underlying resistive switching mechanisms when a write voltage is applied. We discuss results from quasi-static test measurements on BFO [5] and from temperature dependent transport measurements on YMO [6]. [1] Leon Chua, IEEE Transactions on Circuit Theory 18, 507, 1971 [2] T. You et al., Adv. Funct. Mat. 24, 3357-3365, 2014. [3] N. Du et al., Front. Neurosci. 15, 660894, 2021. [4] H. Schmidt, 118, 140502, 2021. [5] N. Du et al., Phys. Rev. Applied 10, 054025, 2018. [6] V.R. Rayapati et al., J. Appl. Phys. 126, 074102, 2019.

Invited Talk HL 11.5 Tue 15:30 H4

Integration of 33°Y-$LiNbO_3$ films with high-frequency BAW resonators — Sondes Boujnah[1], Mihaela Ivan[2], Vincent Astié[3], Samuel Margueron[1], Mario Constanza[1], Jean-Manuel Decams[3], and •Ausrine Bartasyte[1] — [1]FEMTO-ST Institute, University of Bourgogne Franche-Comté Besançon, France — [2]SATT-Sayence, Dijon, France — [3]Annealsys, Montpellier, France

The next generation telecommunications require RF filters operating at frequencies of 6-9 GHz. $LiNbO_3$ (LN) films were identified as one of the materials with sufficient electromechanical coupling, K^2, for these applications. To attain 6-9 GHz frequencies in bulk acoustic wave (BAW) devices, LN film thickness has to be below 200 nm, which makes challenging their fabrication by popular smart-cut process. This motivates further development of integration of deposited highly-coupled LN films with BAW resonators. Several challenges have to be overcome in the case of LN direct growth on electrodes/mirrors/sacrificial layers used in BAW devices: (i) heterostructure has to be stable chemically/structurally at LN growth temperature/atmosphere, (ii) eliminate interaction between Li_2O and SiO_2, (iii) bottom electrode with

good conductivity.

The aim of this work is to optimize SMR and HBAR structures adapted to high-deposition temperatures, and chemically not interacting with LN thin films. The Bragg mirror with a reflection coefficient of 0.98 and a stopband width of 3.1 GHz, centered at 6 GHz, for the longitudinal mode was designed. Deposition parameters were optimized to fabricate the Bragg reflectors with small roughness, without defaults and good stability and Pt bottom electrode with low resistivity ($4\mu\Omega$·cm). The SMR resonator based on 125 nm thick 33°Y-LN film allows attain pure longitudinal mode with K^2 as high as 14.5 % at 5.9 GHz. 33°Y-LN films grown on seed layer/Pt bottom electrode presented single orientation, and dielectric constant close to bulk LN. After electrical poling, the pyroelectric coefficient increased from 11 $\mu C \cdot m^{-2} \cdot K^{-1}$ to the value of bulk 33°Y-LN indicating single domain state of the film. The acoustical performance of BAW devices will be presented, as well.

HL 11.6 Tue 16:00 H4

Observation and control of improper ferroelectric nano-domains in Gd2(MoO4)3 — •Ivan Ushakov[1], Theodor Holstad[1], Didier Perrodin[2], Edith Bourret[2], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, Norway — [2]Materials Science Division, Lawrence Berkeley National Laboratory, USA

Gd2(MoO4)3 is a classical example of an improper ferroelectric material and has been extensively studied with respect to its ferroic properties and ferroelectric/ferroelastic domains. Here, we revisit the ferroelectric domain structure and expand previous optical investigations to the nanoscale. By using Piezoresponse Force Microscopy (PFM), we resolve the established pattern of ferroelectric and anti-phase domains in Gd2(MoO4)3. In addition, we discover stripe-like nano-domains with a periodicity of about 50 nm. The response of the ordered nano-domains to locally applied electric fields, pressure, and temperature is presented. Our findings provide new insight into the physics of Gd2(MoO4)3 at the level of the domains and introduce novel opportunities for property engineering at the local scale.

HL 11.7 Tue 16:15 H4

Electronic Raman scattering study of Ir4+ ions in beta-Ga2O3 — •Palvan Seyidov[1], Manfred Ramsteiner[2], Zbigniew Galazka[1], and Klaus Irmscher[1] — [1]Leibniz-Institut für Kristallzüchtung, Max- Born-Str. 2, 12489 Berlin, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

Currently, beta-Ga2O3 is in the research focus as a material for power electronic devices because of its anticipated high electric break down field (~8MV/cm). For such applications, unintentional impurities in bulk crystals can lead to detrimental effects in device performance. Here we study electronic Raman scattering (ERS) of Ir4+ ions in bulk crystals grown by the Czochralski method. The optical excitation energy was varied between 1.95eV to 3.81eV by using Ar+ ion and HeCd lasers. Conventionally, Raman scattering is used to investigate vibrational modes of molecules and crystals. In contrast, inelastic light scattering due to electronic transitions can be studied by ERS. We observed an ERS feature at 5152 cm-1 (1.94 um, 0.639 eV) in room-temperature spectra from bulk beta-Ga2O3. The observed spectral feature is attributed to Ir4+ ions incorporated on Ga sites and assigned to an intra-center d-d transition within the t2g orbitals. The ERS efficiency is found to strongly depend on the photon energy used for optical excitation. The observed maximum at 2.8 eV can be explained by a resonance enhancement involving an electron transfer from Ir3+ to the conduction band at ~2.2 eV and an Ir4+ intra-center transition at ~0.6 eV.