HL 52: Focus Session: Functional Metal Oxides for Novel Applications and Devices I (joint session HL/DS)

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: Wednesday 15:00–18:15 Location: POT 81

Invited Talk HL 52.1 Wed 15:00 POT 81

Modulation Doping in High-Mobility Alkaline-Earth Stannates — •Bharat Jalan — Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455, U.S.A.

Interfaces between perovskite oxides have created tremendous excitement because of the potential for emergent phenomena and novel field-effect devices. The vast majority of these papers focus on the $LaAlO_3/SrTiO_3$ (LAO/STO) interfaces including some on Al_2O_3/STO and $ReTiO_3$/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 $SrSnO_3/BaSnO_3$ system precisely fulfills the theoretical criteria for electron doping in $BaSnO_3$ using electrons from La-doped $SrSnO_3$, 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 $BaSnO_3$. The transport results are in good agreement with the results of self-consistent solution to one-dimensional Poisson and Schrödinger equations.

HL 52.2 Wed 15:30 POT 81

Two-dimensional electron (hole) gas in $BaSnO_3/LaInO_3$ heterostructures: A first-principles study — •Wahib Aggoune, Dmitrii Nabok, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

We investigate the structural and electronic properties of heterostructures formed by the nonpolar $BaSnO_3$ (BSO) and polar $LaInO_3$ (LIO) perovskites, employing density functional theory. Focusing on the impact of thickness and surface termination of the LIO side, we analyze the electronic properties of the interface. For the stoichiometric LIO film, an internal electric field is induced due to the different terminations of its two sides. Increasing the LIO thickness, this field causes an upward shift of the valence band maximum (VBM). Reaching a thickness of 6 LIO unit cells, the VBM crosses the Fermi level, leading to partial occupation of the conduction band minimum (CBM). Consequently, a two-dimensional electron gas (2DEG) forms at the BSO side of the interface, confined within three unit cells. A high electron mobility is expected due to the *s*-character of the CBM. The corresponding hole gas (2DHG) forms at the LIO side, confined within one unit cell. As a result, this combination gives rise to the formation of a conducting interface starting from the insulating BSO and LIO components. We also present its results for interfaces with non-stoichiometric LIO. Depending on the surface termination, either a 2DEG or a 2DHG forms at the interface. In this case, the 2D charge confinement is mainly attributed to the spontaneous polarization induced at the interface.

HL 52.3 Wed 15:45 POT 81

Epitaxial growth of Lanthanum doped BaSnO3 thin films by PLD — •Reshma Ravindran, Daniel Pfützenreuter, Julian Stöver, Klaus Irmscher, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2 12489 Berlin

Barium stannate (BaSnO3) has gained a lot of attention during the last few years due to its high charge carrier mobility, which is higher than for most transparent conducting oxides and the highest reported for perovskite materials [1]. This makes BaSnO3 especially interesting for the use in electronic applications, e.g. field effect transistors. For single crystals, a mobility of 320 cm2/Vs at room temperature has been published. However, the mobility in epitaxial films is in the range of 70-100 cm2/Vs. This has initiated research efforts to improve structural and electrical properties of BaSnO3 thin films.

In our study, we report on epitaxially grown La-doped BaSnO3 (La concentration was 4 wt.-%) thin films on SrTiO3 substrates by pulsed laser deposition (PLD). We will show that PLD parameters like substrate temperature, target-to-substrate distance and laser spot size have to be carefully adjusted in order to obtain the formation of phase pure BaSnO3 thin films. Hall measurements will indicate that the charge carrier mobility is critically correlated with the structural quality of the epitaxial films analyzed by atomic force microscopy and x-ray diffraction. [1] H. J. Kim et al. Phys. Rev. B 86, 165205 (2012)

HL 52.4 Wed 16:00 POT 81

Epitaxial growth of La doped $BaSnO_3$ thin films by Plasma-assisted molecular beam epitaxy — •Georg Hoffmann[1], Martina Zupancic[2], Martin Albrecht[2], Zbigniew Galazka[2], and Oliver Bierwagen[1] — [1]Paul-Drude-Institut für Festkörperelektronik Leibniz-Institut im Forschungsverbund Berlin e.V. — [2]Leibniz-Institut für Kristallzüchtung

For oxide molecular beam epitaxy (MBE), the use of suboxides is an essential part for the growth of complex oxides, e.g. SnO for $BaSnO_3$ (BSO). However, the conventional approach of BSO growth using SnO suboxide from a SnO_2 charge ($SnO + Ba + 2O \rightarrow BaSnO_3$) requires high cell temperatures and adds a parasitic oxygen background due to the reaction $SnO_2 \rightarrow SnO + 1/2\ O_2$. Using a SnO_2 + Sn mixture as a charge can address both issues, first: the suppression of the parasitic oxygen due to the reaction $SnO_2 + Sn \rightarrow 2\ SnO$ and second: providing higher fluxes at lower temperatures.

Using this new approach, smooth BSO films were grown by plasma-assisted MBE on $SrTiO_3$ (STO) substrates. The crystal quality was analyzed in-situ by reflective high energy electron diffraction. Ex-situ, morphology and structural parameters were determined by atomic force microscopy, X-ray diffraction, and high resolution transmission electron microscopy images.

The results reveal an increased BSO growth-temperature window with decreasing SnO/Ba flux ratio. Further, the influence of the STO miscut angle, as well as the STO orientation will be discussed, and electrical properties of La doped BSO films are pointed out.

30 min. break

Invited Talk HL 52.5 Wed 16:45 POT 81

Engineering of LiNbO3 films for next generation acoustic and energy harvesting applications — •Ausrine Bartasyte, Samuel Margueron, Vincent Astié, Giacomo Clementi, Mihaea Ivan, and Merieme Oubahaz — FEMTO-ST Institute, University of Franche-Comté, Besançon, France

The next generation of high frequency wide-band RF filters or frequency-agile filters are urgently needed for the development of 5G infrastructures/networks/communications. Today, LiNbO3 and LiTaO3 single crystals are key materials in electro-optics and RF acoustic filters. This motivates further development of acoustic wave devices based on highly electromechanically coupled LiNbO3 thin films, adapted to the high-frequency applications. The challenges and the achievements in the epitaxial growth of LiNbO3 films and their integration with Si technology and to acoustic devices will be discussed in detail. The deposition techniques enabling the control of film composition/ nonstoichiometry of volatile alkali metal oxides & the methods of compositional analysis will be presented. We have demonstrated an extremely high acoustical performance compatible with filter applications for SAW devices, based on epitaxial LiNbO3 films, operating in the frequency range around 5 GHz. Moreover, it was demonstrated that the power density of 9.62 mW .cm-3 (comparable to present performance of lead-based piezoelectric harvester) can be harvested by vibrational energy transducer based on thick LiNbO3 films.

Invited Talk HL 52.6 Wed 17:15 POT 81

Oxide Memristors for unified data storage and data processing — •Heidemarie Schmidt — Leibniz-IPHT Jena — IFK, FSU Jena — Fraunhofer ENAS Chemnitz

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], neuromorphic computing [3], and hardware cryptography [4]. Another electroforming-free memristor is the unipolar memristor YMnO3 (YMO). 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. 9, 227, 2015. [4] N. Du et al., J. Appl. Phys. 115, 124501, 2014. [5] N. Du et al., Phys. Rev. Applied 10, 054025, 2018. [6] V.R. Rayapati et al., J. Appl. Phys. 124, 144102, 2018

HL 52.7 Wed 17:45 POT 81

Investigations on leakage current in epitaxial K0.5Na0.5NbO3 thin films grown by PLD — •Daniel Pfützenreuter, Julian Stöver, Klaus Irmscher, Jens Martin, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin

KxNa1-xNbO3 is a lead-free, ferro- and piezoelectric compound, which offers a high potential for memory applications and sensors in thin films form. However, KxNa1-xNbO3 thin films often suffer from a high leakage current. This is assumed to be mainly attributed to the high volatility of the alkaline components at high temperatures, but also interface effects have to be regarded. Pulsed laser deposition (PLD) represents a suitable method for the epitaxial growth of K0.5Na0.5NbO3 films. In this study the impact of strain, film thickness and bottom electrode on vertical electric behaviour of epitaxially grown K0.5Na0.5NbO3 films is investigated. For this purpose, K0.5Na0.5NbO3 films were grown on SrRuO3 and La0.67Sr0.33MnO3 covered SrTiO3 and DyScO3 substrates as well as directly on SrTiO3:Nb substrates with a film thickness between 20 and 200 nm. While for small film thicknesses Ohmic charge transport is observed in I-V-measurements, the charge transport mechanism changes to pronounced Schottky like behaviour at thicker films. This transition is investigated in more detail by comparing the measured I-V curves with calculated ones for different mechanisms of current flow. Furthermore, we find a strong correlation between the lattice strain in the films and the kind of charge transport mechanism.

HL 52.8 Wed 18:00 POT 81

Tuning the composition properties of SrTiO3 thin films grown by metal-organic vapor phase epitaxy (MOVPE) — •Aykut Baki, Julian Stöver, Toni Markurt, Carsten Richter, Klaus Irmscher, Martin Albrecht, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2 12489 Berlin

SrTiO3 represents a prototype cubic perovskite and has several of interesting physical properties as for instance a high dielectric constant at room temperature and resistive switching behavior. MOVPE is employed as deposition method since it provides film growth close to the thermodynamic equilibrium and thus stoichiometric, defect-poor thin films with smooth surfaces and interfaces. In this study, epitaxial SrTiO3 films were successfully grown on 0.5 wt.% Nb-doped SrTiO3 substrates by using the metal-organic precursors Sr(tmdh)2-tetraglyme and Ti(iso-propoxid)2(tmdh)2 solved in dry toluene. It has been shown that the phase formation of phase-pure SrTiO3 is achieved by adjusting the substrate temperature to a range of 675 °C $<$ TC $<$ 725 °C. By varying the Sr/Ti ratio in the gas phase, the cation ratio in the SrTiO3 thin films has been precisely controlled. The structural quality of the grown films has been proved by high-resolution x-ray diffraction, atomic force microscopy and transmission electron microscopy. The insulating films have been tested for their dielectric properties by a Pt/SrTiO3/SrTiO3:Nb test-structure for temperatures between 20 K and 300 K. IV-curves have shown strong forming-less resistive switching.