HL 16: Focus Session: Oxide Semiconductors for Novel Devices III

Organizers: Holger Eisele (TU Berlin) and Holger von Wenckstern (Uni Leipzig)

Time: Tuesday 9:30–13:15 Location: H34

HL 16.1 Tue 9:30 H34

Mechanical properties of HfO_{2-x} and ZrO_{2-x} suboxides — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Hafnia is a well-known high-k material that is compatible with silicon technology. Both hafnia and its crystallographic sibling, zirconia, are intensively investigated as resistive switching materials for the next generation non-volatile memory and potential neuromorphic computing applications. Zirconia-based ceramics are widely employed in industry and medicine because of their high strength and fracture toughness. Observed shape-memory effect is related to the martensitic transition from tetragonal to monoclinic phase in zirconia. A fundamental understanding of the mechanical properties and stability of these materials is, therefore, very important for their practical applications.

Recently [1,2], we reported the new suboxide phases in Hf-O and Zr-O systems, which contain ordered vacancy chains, a desired property for the resistive switching devices. Here we focus on the mechanical properties of these phases. We will report a prediction of superelastic behavior of these phases and discuss the role of ordered oxygen vacancies in the mechanical properties of hafnia and zirconia. We acknowledge the support by DFG via SFB 917 "Nanoswitches".

[1] K.Z. Rushchanskii, S. Blügel, M. Ležaić, Phys. Rev. Materials **2**, 115002 (2018); [2] K.Z. Rushchanskii, S. Blügel, M. Ležaić, Faraday Discussions (2019).

HL 16.2 Tue 9:45 H34

Protective coatings for photoelectrochemical applications — •David Silva, Oliver Bienek, and Ian Sharp — Technische Universität München, Walter Schottky Institut, Munich, Germany

Several photoactive semiconductor materials have been reported to yield promising energy conversion efficiencies in photocatalytic applications. However, the harsh chemical environments in which photoelectrochemical conversion (PEC) systems operate causes accelerated (photo) corrosion of many semiconductor light absorbers. In recent years, this issue has been mitigated via the application of conformal thin film protection layers, such as TiO_2, deposited via atomic layer deposition (ALD). However, interfacial charge transfer pathways, as well as the nature and impact of electronically active defects in highly disordered protection layers, remain poorly understood. Here, we report on optical characterization of these films using photothermal deflection spectroscopy (PDS), combined with complementary photocurrent measurements and surface photovoltage spectroscopy (SPS). Together, these measurements provide a deeper understanding of defect properties of these materials and their roles in photoelectrochemical energy conversion. Impacts of heterojunction energetics are analyzed by extending these approaches to model systems comprising TiO_2 on GaN substrates.

HL 16.3 Tue 10:00 H34

Theoretical and experimental investigation of optoelectronic properties of Ti:Nb3O7(OH) photoelectrodes — •Haseen Ullah Jan[1], Walayat Khan[1], Christina Scheu[2], and Jan Minar[1] — [1]University of West Bohemia (UWB), Pilsen, Czech Republic — [2]Max Planck Institute, Germany

Global warming and CO2 resulting from the combustion of fossil fuels adds the largest mass to the scales caused by continuous emission of greenhouse gases. Therefore, new technologies for power generation and energy storage are required. Our study focuses on the design[1], development[2], synthesis[3] and characterization[3] of novel materials for solar cells as photo-catalyst for water-splitting. Water photolysis is a renewable source for hydrogen fuel and is therefore considered as a solution for the energy crises. Recently, Nb3O7(OH) has been proposed as a promising material for this propose due to stability and suitable band gap. Our main goal to achieve is to find the possible stable position for the hydrogen atom by modifications of the structure and electronic properties of Nb3O7(OH) due to the Ti doping. Our theoretical study is based on the density functional theory using full potential linearized augmented plane wave (FP-LAPW) method. Structural properties reveals that the surface of the host material was enhanced at the loading of Ti. In addition, the optical spectra of Nb3O7(OH) and Ti:Nb3O7(OH) systems revealed that the optical band gap energy was not changed upon the addition of Ti, but the amount of photoabsorption drastically increased with increased contents of Ti.

HL 16.4 Tue 10:15 H34

Simulation of retention and endurance in memristive devices — •Max Huber[1,2], Jörg Schuster[2], and Michael Schreiber[1] — [1]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany

Memristors are promising candidates for next generation memory. For practical purposes nonvolatility and reliability of the switching process are crucial to build high performance memristive devices. These properties can be checked with retention and endurance tests.

In our contribution we demonstrate, how such tests can be performed based on state-of-the-art physical device models [1]. For this purpose, Poisson's equation as well as drift-diffusion equation and continuity equation for electrons are solved selfconsistently for a one-dimensional device model. The movement of mobile donors and Joule heating of the device are considered as well. For the retention test, the device is switched from high resistance state (HRS) to low resistance state (LRS). In the following the device is read out for many times in order to check that this procedure does not change the topical state of the device. In contrast, the endurance test is performed by repeating the cycle *HRS* → *read out* → *LRS* → *read out* many times. We show how retention and endurance depend on device parameters like Schottky barriers, average donor concentration and mobility of charges.

[1] A. Marchewka, R. Waser, and S. Menzel: Proc. of 2015 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), pp. 297-300, IEEE, 2015.

HL 16.5 Tue 10:30 H34

Investigating the Memristive Behavior of Hydrothermally Grown TiO2 Nanorod Arrays — •Carola Ebenhoch[1], Julian Kalb[1], Joohyun Lim[2], Christina Scheu[2], and Lukas Schmidt-Mende[1] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Metal oxide memristors gained great attention during the last decade in using them for nonvolatile data storage, as well as for artificial synapses. The key reason for changing the resistance state of a metal oxide material is the possibility to form conductive filaments due to oxygen vacancies. The known mechanisms for building such filaments are unipolar, bipolar and complementary switiching, which are based on the electromigration of oxygen ions by applying an electric field and thermophoresis caused by Joule heating. The investigated hydrothermally grown TiO2 nanorod arrays (NRAs) show a combination of these effects, whereas dependence of the growth temperature on the memrisitive behavior of the NRAs will be demonstrated.

HL 16.6 Tue 10:45 H34

Structural, electronic and magnetic properties of Iron doped hexagonal $BaTiO_3$: First principles investigation — •Waheed A. Adeagbo[1], Sanjeev K. Nayak[2], Hichem B. Hamed[1], Hans T. Langhammer[3], Rolf Böttcher[4], and Wolfram Hergert[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, 06120 Halle, Germany — [2]Department of Materials Science and Engineering, University of Connecticut, USA — [3]Institute of Chemistry, Martin Luther University Halle-Wittenberg, 06120 Halle, Germany — [4]Faculty of Physics and Earth Sciences, Leipzig University, Germany

DFT calculations of Fe-doped hexagonal $BaTiO_3$ resulted in three different Fe^{3+} defects incorporated at Ti sites: Two isolated defects and one associate of Fe^{3+} with a neighbouring oxygen vacancy. Substitution of Fe at Ti sites leads to a distortion of the surrounding oxygen octahedron. Fe is considered in different charge states. These charge states affect the Fe-O bonds and overall geometry near the defect and also influence the stability. The calculated formation energies, which are measure of the relative stability are in agreement with EPR exper-

iment and demonstrate that Fe in BTO must exist in oxidation state of 3+ and has to occupy a face-sharing Ti(2) site while compensated by V_O located in its first coordination sphere. Magnetic configurations of Fe pairs for all possible crystallographic nearest neighbor sites are also studied by calculations of the exchange interactions. A ferromagnetic coupling for the closest Fe pair is predicted and their formation is stabilized by V_O. Achieving ferromagnetism in this material through impurity doping is a promising direction for further research.

15 min. break

HL 16.7 Tue 11:15 H34

Molecular beam epitaxy of SnO: Investigation of growth parameters including the comparison of a Sn and a SnO source — •Melanie Budde, Georg Hoffmann, and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

Tin monoxide (SnO) is a p-type transparent semiconducting oxide (TSO) with a relatively high mobility for this class of materials. However, the SnO phase is instable and easily oxidized to SnO2 or reduced into metallic Sn.[1] On the other hand, SnO2 is a n-type TSO allowing a change in the carrier type only by controlling the oxygen stoichiometry x of SnOx. The investigations of Vogt[2] on the sub-oxide formation during the SnO2 growth also shows additional formation of SnO under metal-rich conditions. However, SnO was volatile at the growth temperature of 600 °C and desorbed from the substrate, thus not contributing to the film growth.

In this work, the desorption of SnO for growth temperatures below 600 °C are investigated using a line-of-sight quadrupole mass spectrometer to find a growth window for the formation of SnO. First, the SnO layers are grown and characterized using a SnO source. Secondly, different fluxes from a Sn cell in combination with an oxygen plasma are used. The grown layers are investigated using X-ray diffraction and energy dispersive x-ray spectroscopy.

[1] Zhang et al., J. Phys.: Condens. Matter 28 (2016). [2] Vogt and Bierwagen, Appl. Phys. Lett. 106 (2015).

HL 16.8 Tue 11:30 H34

Structural, optical and electrical properties of orthorhombic $(In_xGa_{1-x})_2O_3$ thin films — •A. Hassa, H. von Wenckstern, D. Splith, C. Sturm, M. Kneiss, C. Krömmelbein, and M. Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstraße 5, 04103 Leipzig, Germany

Gallium oxide is a wide bandgap semiconductor appearing in various polymorphs. The orthorhombic κ-phase is of increasing interest because of its predicted large polarization of 23 μC/cm^2 [1] rendering it well suited for usage e.g. in high electron mobility transistors. We present material properties of a κ-$(In_xGa_{1-x})_2O_3$ thin film grown with continuous composition spread [2] by pulsed laser deposition on (00.1) Al_2O_3. As target segments we used Ga_2O_3/In_2O_3 doped with tin to facilitate formation of the orthorhombic phase [3], which was observed for an indium content up to $x \sim 0.35$ enabling band gap engineering between 4.3 and 4.9 eV. In order to induce n-type conductivity we doped a sample consisting of $(In_{0.01}Ga_{0.99})_2O_3$ with 1.3 at.% zirconium and achieved electrically conducting thin films with room temperature conductivity of up to 0.1 S/cm. Resulting samples were investigated by means of X-ray diffraction, transmission, energy-dispersive X-ray spectroscopy, atomic force microscopy, and electrical transport measurements. Further, properties of Schottky barrier diodes are presented in dependence on the temperature.

[1] M. B. Maccioni *et al.*, Appl. Phys. Express 9, 04102 (2016).
[2] H. v. Wenckstern *et al.*, CrystEngComm 15, 10020 (2013).
[3] M. Kneiß *et al.*, APL Materials, Accepted (2018).

HL 16.9 Tue 11:45 H34

Temperature dependence of the Seebeck coefficient of epitaxial β-Ga_2O_3 thin films — •Johannes Boy[1], Martin Handwerg[1], Robin Ahrling[1], Rüdiger Mitdank[1], Günter Wagner[2], Zbigniew Galazka[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, Max-Born-Strasse 2, 12489 Berlin, Germany

In the past years, β-Ga_2O_3 crystals and thin films have proved to be promising materials for high power devices. However, one drawback is the low thermal conductivity[1,2], which enhances the energy-dissipation by Joule heating. One approach could be a direct cooling using the Peltier effect. For this purpose values of the Seebeck coefficient of β-Ga_2O_3 need to be known.

In this work, the temperature dependence of the Seebeck coefficient of homoepitaxial metal organic vapor phase grown, silicon doped β-Ga_2O_3 thin films was measured relative to aluminum. For room temperature we found the relative Seebeck coefficient of $S_{\beta\text{-}Ga_2O_3\text{-}Al} = (-300 \pm 20)$ μV/K. At high bath temperatures $T > 240$ K, the scattering is determined by electron-phonon-interaction. For lower bath temperatures between $T = 100$ K and $T = 300$ K, an increase in the magnitude of the Seebeck coefficient is explained in the frame of Strattons formula.

[1] M. Handwerg, *et al.*, Semicond. Sci. Technol. **30**, 024006 (2015).
[2] M. Handwerg, *et al.*, Semicond. Sci. Technol. **31**, 125006 (2016).

HL 16.10 Tue 12:00 H34

Realization of MESFET and inverter devices based on Mg-doped In_2O_3 — •Fabian Schöppach, Robert Karsthof, Daniel Splith, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Linnéstraße 5, 04103 Leipzig, Germany

Indium oxide (In_2O_3) has promising physical properties such as high conductivity and transparency in the visible. However In_2O_3 is not used in active devices such as diodes or transistors yet. This is due to its tendency to form an electron accumulation layer on its surface preventing the formation of a significant depletion layer.

In this work, metal-semiconductor field-effect transistors (MESFETs) and inverters are presented for the first time. These are based on thin In_2O_3 films with various Mg doping concentrations. These films are grown via high-temperature pulsed laser deposition in oxygen atmosphere. For source and drain contacts gold is deposited via inert ambient sputtering. Schottky gate diodes are fabricated in a reactive sputter process which is a requirement for obtaining rectifying contacts to In_2O_3 [1,2]. Transistors with on-off ratios of over 5 orders of magnitude are reported.

[1] H. v. Wenckstern, et al. APL Mater. 2, 046104 (2014)
[2] Th. Schultz, et al. Phys. Rev. Appl. 9, 064001 (2018)

HL 16.11 Tue 12:15 H34

Integrated Logic Circuits Based on Amorphous Zinc-Tin-Oxide Thin Films Processed at Room Temperature — •Oliver Lahr, Sofie Vogt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Semiconductor Physics Group, Leipzig, Germany

Currently there exists an increasing demand for low cost electronics and novel devices based on sustainable materials. Amorphous zinc-tin-oxide (ZTO) is a promising candidate for such technology since it consists of abundant, non-toxic elements and can be deposited at room temperature. Recently, the first metal field-effect transistors (MESFETs) as well as inverters based on amorphous ZTO channels have been reported [1,2].

We present Schottky diode FET logic (SDFL) inverters and SDFL ring oscillators based on MESFETs and junction field-effect transistors using amorphous n-type ZTO as channel material. The channels were deposited at room temperature by radio frequency long throw magnetron sputtering using a target with a 67 % SnO_2 and 33 % ZnO composition. MESFET-based inverters show high peak gain magnitudes up to 330 at an operation voltage of 3 V with uncertainty levels below 113 mV. Single stage delay times down to 1.9 μs at $V_{DD} = 10$ V are observed for ring oscillators based on our ZTO-MESFETs.

[1] Dang *et al.*, Appl. Phys. Lett., **110**, 7, 2017.
[2] Vogt *et al.*, Appl. Phys. Lett., **113**, 13, 2018.

HL 16.12 Tue 12:30 H34

IR-Vis-UV optical properties of α-Ga_2O_3 films grown by halide vapor phase epitaxy — •Pingfan Ning[1], Martin Feneberg[1], Jürgen Bläsing[1], Hoki Son[2], Dae-Woo Jeon[2], and Rüdiger Goldhahn[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg — [2]Korea Institute of Ceramic Engineering & Technology, 15-5, Chungmugong-dong, Jinju-si, Gyeongsangnam-do

Ultra wide band gap semiconductor α-Ga_2O_3 has been attracting increasing interest due to their potential advantages in UV optoelectronics, power devices, RF electronics as well as transparent electronics. However, many basic physical properties are still unclear, including optical properties, which must be investigated in detail to fully exploit their functions. We investigated the linear optical response

of metastable α-Ga_2O_3 epitaxial layers by spectroscopic ellipsometry. The α-Ga_2O_3 films are grown on (0001) α-Al_2O_3 substrates by halide vapor phase epitaxy method while the precursors GaCl and O_2 are controlled in different ways. The ordinary dielectric function has been determined by point-by-point fitting of the ellipsometry data from the infrared (300 cm^{-1}) to the ultraviolet (6.5 eV). Effects of GaCl and O_2 gas controlling on the infrared-active phonon modes, dielectric limits, and interband transitions are discussed. The infrared dielectric function is accurately described with a sum of Lorentzian oscillators and the dielectric limit. Characteristic energies, broadening factors, and amplitudes of three out of the four expected E_u infrared-active modes are determined.

HL 16.13 Tue 12:45 H34

Influence of strain on yellow excitons in cuprous oxide with different principle quantum numbers — •Patric Rommel[1], Christoph Uihlein[2], and Jörg Main[1] — [1]Institut für Theoretische Physik 1, Universität Stuttgart, Germany — [2]Experimentelle Physik 2, TU Dortmund, Germany

Recently J. Mund et al. demonstrated Second Harmonic Generation (SHG) for the yellow series in cuprous oxide [1]. Assuming perfect O_h symmetry, SHG is forbidden along certain high-symmetry axes. Perturbations can break this symmetry and forbidden transitions may become allowed. We investigate the effect of strain in the crystal structure on the yellow exciton lines of cuprous oxide. Strain in a high-symmetry direction of the crystal leads to a splitting of the exciton lines according to the related symmetry reduction [2]. For the S states of symmetry Γ_5^+, this splitting can be described using a simple 3×3 matrix model. We derive the strengths of the splitting in dependence on the main quantum number n by numerically diagonalizing the exciton Hamiltonian including an appropriate strain term.

[1] J. Mund et al., Phys. Rev. B 98, 085203 (2018)
[2] H.-R. Trebin et al., Phys. Rev. B. 23, 597 (1981)

HL 16.14 Tue 13:00 H34

Tuning functionality at the nanoscale — •Donald M. Evans[1], Theodor. S. Holstad[1], Aleksander. B. Mosberg[2], Per-Erik Vullum[2], Didirik Småbråten[1], Zewu Yan[3], Sverre Selbach[1], Antonius Van Helvoort[2], and Dennis Meier[1] — [1]Department of Materials Science and Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway. — [2]Department of Physics, Norwegian University of Science and Technology (NTNU), Trondheim, Norway. — [3]Department of Physics, ETH Zurich, 8093 Zürich, Switzerland

One of the stand out scientific achievements of the twenty first century is the ability to tune a material*s functional properties, e.g. doping silicon to become either p- or n-type. As we reach the limits of silicon technology other options to tune functional properties become interesting, particularly local changes rather than bulk changes. In this work we use an atomic force microscope (AFM) to locally apply an electric field that changes the conductive properties of a hexagonal manganite (ErMnO3). This has all the control and resolution of an AFM giving us the freedom to write any combination of shapes and sizes for nano-circuitry. We analyse these areas of enhanced conductivity with a transmission electron microscope (TEM) to find changes in crystal structure and do electron energy loss spectroscopy (EELS) to look for changes in chemical composition. These are combined with Density Functional Theory (DFT) work to establish the likely mechanism of enhanced conductivity.