DS 32: Focussed Session: Oxide Semiconductors for Novel Devices II

Wide band gap semiconducting oxides such as the group-III sesquioxides find potential application in e.g. UV- or deep UV-sensors, transparent photovoltaic devices, power electronics or quantum well infrared photo detectors. This session sets a focus on growth of binary bulk material and thin films, the physical properties of these and their surface, properties of heterostructures and interfaces and the fabrication and performance of demonstrator devices.

Organizers: Oliver Bierwagen (PDI Berlin) and Holger von Wenckstern (U Leipzig)

Time: Wednesday 14:45–17:45 Location: CHE 89

Topical Talk DS 32.1 Wed 14:45 CHE 89

Defect induced magnetic or optical properties in gallium-based oxides — •Laurent Binet and Didier Gourier — Chimie-ParisTech, Paris, France

Gallium based oxides such as Ga2O3 and ZnGa2O4 are wide-gap transparent conducting oxides, which have been receiving a growing interest. Indeed, their electrical, optical and magnetic properties can be tuned by intrinsic defects or doping.

In Ga2O3, the magnetic interaction between the delocalized electron spins released by intrinsic shallow donors and the gallium nuclear spins results in an original memory effect, the so-called bistable conduction electron spin Resonance, which is based on a bistable dynamic nuclear polarization. This effect appears in the magnetic resonance of the conduction electrons as the possibility of switching between two different resonance states by acting on the external magnetic field, the microwave power or the temperature.

In ZnGa2O4, which shares some common features with Ga2O3, intrinsic defects are able to store a fraction of the excitation energy of Cr3+ dopants, which is responsible of a long persistent luminescence of Cr3+ in the red-near infrared. This unprecedented property can be applied to in vivo optical imaging of tumours.

DS 32.2 Wed 15:15 CHE 89

Photo- and electroluminescence of chromium doped β-Ga_2O_3 — •Andreas Fiedler, Zbigniew Galazka, and Klaus Irmscher — Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin, Germany

Chromium doped β-Ga_2O_3 single crystals were grown by the Czochralski method. The Cr doping produces a greenish coloration of the crystal, which results from two broad absorption bands centered at wavelengths of about 450 nm and 600 nm, respectively. Similar absorption bands are well know from Al_2O_3:Cr (ruby) and assigned to Cr^{3+} on Al site. This suggest that in the β-Ga_2O_3:Cr crystals Cr prefers Ga site occupation in the Cr^{3+} oxidation state. In analogy to ruby, we also see the characteristic red photoluminescence (PL) line due to an intra-center transition of Cr^{3+}. The PL line of ruby at 694.3 nm is shifted to 695.6 nm in β-Ga_2O_3:Cr due to the different ligand field. The PL was characterized between 4.2 K and 300 K. With increasing temperature an increasing broadening of the PL peak occurs. The excited state has a lifetime of 160 μs at room temperature, which makes it possible to generate a population inversion. In contrast to ruby, our β-Ga_2O_3 is semiconducting, hence an electroluminescence can be generated by electron impact excitation, which shows two transitions at 695.1 nm and at 696.2 nm. The beat frequency of these transitions is 0.7 THz, which is in the so called terahertz gap. This may be used for a terahertz laser, which opens a new field of applications for β-Ga_2O_3 beside the power devices and the photo detectors.

Topical Talk DS 32.3 Wed 15:30 CHE 89

Vacancy defects and electrical compensation in gallium oxide — •Filip Tuomisto — Aalto University, Espoo, Finland

Ga_2O_3 has recently generated significant interest and high quality growth (both thin-film and bulk) has been achieved with several techniques. Its distinctive feature compared to other transparent semiconducting oxides is the high transparency all the way to UV thanks to a wide 4.9 eV band gap. Hence this material has potential applications in future UV devices and high power electronics. n-type doping is achieved with Sn and Si, and highly resistive material can be produced by doping with Fe and Mg. p-type doping is yet to be achieved. Ga vacancies have been shown to act as efficient compensating centers in n-type material. In order use Ga_2O_3 as a semiconductor in electronics, detailed understanding and control of defects and doping are required. In this work, we analyze the formation mechanisms of Ga vacancies with positron annihilation spectroscopy in Ga_2O_3 thin films. We show that the choice of substrate, growth conditions and n-type dopant all have a dramatic effect on the efficiency of Ga vacancy formation and hence on the electrical properties of thin-film Ga_2O_3.

DS 32.4 Wed 16:00 CHE 89

Localized defect states and charge trapping in Al_2O_3 films prepared by atomic layer deposition — •Karsten Henkel, Malgorzata Kot, and Dieter Schmeisser — BTU Cottbus-Senftenberg, Angewandte Physik-Sensorik, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany

The evaluation of the electronic structure and intrinsic defect mechanisms in Al_2O_3 thin films is essential for their effective use in applications with desired functionality such as surface passivation schemes for solar cells [1]. We present a comparative study of different Al_2O_3 films grown by atomic layer deposition (ALD) [2]. The layers were deposited on different substrates using the same aluminum precursor (TMA, trimethylalumium) and employing different process parameters (thermal-ALD, plasma-enhanced-ALD, substrate temperature). These films were characterized by resonant photoelectron spectroscopy and by electrical measurements (capacitance-voltage). For all films investigated intrinsic defect states within the electronic band gap were observed including excitonic, polaronic, and charge-transfer defect states, where their relative abundance is subject of the choice of ALD parameters and of the used substrate. The spectroscopic assigned in-gap defect states are related with electronic charges as determined in the electrical measurements. [1] G. Dingemans and W.M.M. Kessels, J. Vac. Sci. Technol. A 30, 040802 (2012). [2] K. Henkel, M. Kot, D. Schmeißer, J. Vac. Sci. Technol. A 35, (2017), accepted.

15 min. break.

Topical Talk DS 32.5 Wed 16:30 CHE 89

Integration of Oxide Semiconductors with Traditional Semiconductors - A New Twist — •Scott Chambers — Pacific Northwest National Laboratory, Richland, Washington, USA

Over the past two decades, a significant amount of research has been carried out on the integration of oxides with Si and various III-V semiconductors, most notably GaAs. In much of this work, the emphasis has been on the development of new gate dielectrics. However, other efforts have looked into the discovery and utilization of novel functional oxides as more active components in devices. In contrast, Ge has received relatively little attention. Yet, Ge has many highly desirable properties, including high electron and hole mobilities and a small bandgap. The latter is of particular interest for visible light harvesting applications, such as water splitting.

In this talk, I will present our recent work on the MBE growth and properties of SrZrxTi1-xO3 (SZTO) on p-Ge(001), a system with considerable potential as a photocathode for the hydrogen evolution reaction associated with water splitting. As-grown SZTO is typically n-type due to the formation of oxygen vacancies resulting from the low O2 partial pressure required to prevent oxidation of the Ge substrate during MBE growth. I will present our investigation of band alignment at the n-SZTO/p-Ge heterojunction via high-energy-resolution x-ray photoemission spectroscopy (XPS), along with preliminary results on water chemistry with the SZTO surface by means of ambient-pressure XPS and in situ photoelectrochemistry.

DS 32.6 Wed 17:00 CHE 89

Growth-control of the ordered double-perovskite stucture in $(Pr_{0.5}Ba_{0.5})CoO_{3-\delta}$ thin films — •Felix Gunkel[1], Clemens Hausner[2], David N. Müller[2], Lei Jin[2,3], Chunlin Jia[2,3], Daniel Bick[1], Theo Schneller[1], Ilia Valov[2], and Regina Dittmann[2] — [1]Institute of Electronic Materials (IWE2), RWTH Aachen University — [2]Peter Grünberg Institut, Forschungszentrum Jülich GmbH —

[3]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Jülich

The complex oxide compound $(Pr_{0.5}Ba_{0.5})CoO_{3-\delta}$ (PBCO) is considered as an efficient catalytic oxide for oxygen evolution half-reaction (OER) taking place during water splitting operation. We discuss structural and electrical properties of epitaxial PBCO thin films serving a model systems for exploring atomistic processes during OER. PBCO thin films are synthesized in a disordered and in an ordered double-perovskite crystal structure by controlling the growth temperature during pulsed laser deposition. The thin films show defined surface morphology and crystal orientation. During the growth process, the transition from disordered to ordered phase can be monitored directly by means of electron diffraction (RHEED). The epitaxial thin films show catalytic activity comparable to their porous counter parts fabricated by chemical routes, making them ideal model templates for systematic studies. The ability to control the ordered double-perovskite phase of PBCO bears the potential to force the formation of structural oxygen vacancies within the lattice with atomic precision and to tailor active sites for OER on the nanoscale.

DS 32.7 Wed 17:15 CHE 89

Influence of annealing on the conductivity and transparency of niobium doped titanium dioxide electrodes prepared by sol-gel and their function in organic solar cells — •Peter Fischer[1], Roland Rösch[2], Shahidul Alam[2], Ulrich Schubert[2], Harald Hoppe[2], and Edda Rädlein[1] — [1]TU Ilmenau, Inst. für Werkstofftechnik, Gustav-Kirchhoff-Str. 6, 98693 Ilmenau, Germany — [2]Friedrich-Schiller-Universität Jena, Center for Energy and Environmental Chemistry Jena, Philosophenweg 7a, 07743 Jena, Germany

In this work the conductivity and transmittance of niobium doped titanium dioxide (TNO) layers produced by sol-gel technique are investigated. The samples were coated by spin-coating. The thickness of the TNO was adjusted with different spin speeds. A pre-baking of the films on a hot plate at 80°C for one hour was performed. Further, the samples were heated in a rapid thermal processing furnace under different gas atmospheres, temperatures and time. The conductivity of the samples was measured using a four-point set-up and the transparency through a UV-VIS spectrophotometer. The best heating procedure was when the sample is annealed in an N2/H2 atmosphere to 1000°C for 10 minutes. In this case, a good sheet resistance of 181 Ω/Sq. was reached, which enables the use of the TNO processed with sol-gel as an electrode in optical devices. Finally, organic solar cells were manufactured using TNO as the electrode.

DS 32.8 Wed 17:30 CHE 89

Characterization of Unipolar Zinc-Tin-Oxide Devices — •Sofie Bitter, Peter Schlupp, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Exp. Physik II, Germany

Amorphous zinc-tin-oxide (ZTO) consists of naturally abundant, nontoxic elements only and can be deposited at room temperature with a tunable electron density between $10^{16}\,cm^{-3}$ and $10^{19}\,cm^{-3}$ and a mobility as high as $10\,cm^2/Vs$ [1,2]. Therefore, ZTO is a suitable material for low-cost, flexible, transparent transistors and thus low-cost and bendable electronic applications.

We present metal semiconductor field effect transistors (MESFETs) using amorphous ZTO as *n*-type channel. Room temperature long throw magnetron sputtering from a target with a composition of 67% SnO_2 and 33% ZnO was used to deposit the ZTO channel [3]. On/Off ratios of 10^5 are achieved for reactive sputtered Pt gate contacts. The stability of the MESFETs under positive and negative bias stress is investigated. Further, an aging of unipolar devices based on ZTO is reported, which increases the on/off ratio of the devices.

[1] Bitter et al., ACS Comb. Sci., **18**, 4, 2015.
[2] Jayaraj et al., J. Vac. Sci. & Technol. B, **26**, 2, 2008.
[3] Frenzel et al., Physica Status Solidi (a), **212**, 7, 2015.