**HL 67: Focus Session (Posters): Crystalline n-type semiconducting oxides - SnO₂, Ga₂O₃, and In₃O₅ for novel devices**

**Properties of tin oxides prepared by Ion-Beam-Sputtering** — **Martin Becker, Robert Hamann, Angelika Polity, Davar Farid, and Bruno K. Meyer** — Liebig-Universität Gießen, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany

The success of n-type oxide semiconductors and its application in oxide-based electronic devices has motivated the interest in p-type oxide based semiconductors. Therefore synthesis of tin monoxide (SnO) recently has received increasing attention. Another phase of this binary system, SnO₂, is of great technological interest in manifold applications, such as transparent electrodes, heat-reflecting filters and gas sensing.

The preparation of tin oxide thin films has been performed by many different procedures such as sol/gel, epitaxial procedures or methods working under vacuum conditions like sputtering techniques. Radio-Frequency-Ion-Thrusters, as designed for propulsion applications, are also qualified for thin film deposition and surface etching if utilized as ion source.

Tin oxide thin films were grown by ion-beam sputtering using a 3 inch metallic tin target. Different aspects of growth and properties of the tin oxide phases were investigated in relation to growth parameters such as substrate temperature or flux of oxygen. Structural, optical and electrical properties of the films will be discussed.

**Ab-initio investigation of various tin oxides** — **Bianca Effert and Christian Heiliger** — Physikalisches Institut, Justus Liebig University Giessen, D-35392 Giessen, Germany

Tin forms a stable dioxide and monoxide which are of great interest for applications ranging from optoelectronics to electrochemistry. Tin dioxide (SnO₂) is a wide-bandgap n-type semiconductor, and it is the only oxide of tin that has been investigated in some depth experimentally and theoretically so far. Tin monoxide (SnO) is usually regarded as a semimetal or a small-bandgap p-type semiconductor. It is less well examined than the dioxide and disproportionate to Sn and SnO₂ at elevated temperatures. During this disproportionation reaction, oxides of intermediate stoichiometries such as Sn₅O₈ or Sn₅O₆ are often reported, and some experimental values for possible lattice parameters are available. The preferred stoichiometry and the exact crystal structure, however, remain unknown, and the electronic structure of these oxides is also not known yet. In the present work, we gain new theoretical insight into some of these open questions using density functional theory (DFT). We present calculations for the electronic structure of SnO₂ as well as possible crystal structures of the intermediate oxides. The stabilities of the candidate structures will be compared to those of SnO and SnO₂ in order to suggest whether one of these metastable structures might be grown experimentally.

**Structural properties and defect-induced conduction mechanism in spinel-type ferrites** — **Kerstin Brachwitz, Michael Lorenz, and Marcus Gründmann** — Linnéstraße 5, 04103 Leipzig, Germany

Zinc ferrite (ZFO), cobalt ferrite (CoF₀), and nickel ferrite (NiF₀) are promising candidates for application in magnetic tunnel junctions (MTJs) for both, as conducting electrode and as insulating barrier. In this respect we have investigated such spinel-type ferrite thin films grown by pulsed laser deposition (PLD). We have varied the growth temperature (Tg) by controlling the heater power in a range from 400°C to 600°C. The thin films were grown on (100)-oriented strontium titanate (STO) substrates at p(O₂) = 5 x 10⁻₂ mbar. The out-of-plane orientation of the thin films was found to be (100) and the in-plane epitaxial relation to the substrate was confirmed by ϕ-scan. 2θ-XRD scans reveal an increasing out-of-plane lattice constant with decreasing substrate temperature for all investigated ferrites. The film thickness of about 200–400 nm and the large lattice mismatch between ferrite film and STO substrate (8.8%) lead to relaxed film growth. The electrical conductivity of the thin films can be tuned btw. 10⁻⁴ and 10² S/m by different substrate temperatures during growth. It increases with decreasing substrate temperature. The conduction mechanism is not only affected by electron hopping between Fe²⁺ and Fe³⁺, but also defects like oxygen vacancies and structural disorder have great influence. The conductivity is thermally activated and a model with two activation energies fits the temperature dependent conductivity.

**ZnFe₂O₄ dielectric function** — **Raimo Böttgen, Kerstin Brachwitz, Rüdiger Schmidt-Grund, Michael Lorenz, and Marcus Gründmann** — Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig

We present a detailed investigation of the dielectric function (DF) of spinel ZnFe₂O₄ (ZFO) thin films on a-plane sapphire. The films were grown by pulsed laser deposition at various temperatures and oxygen partial pressures. The optical measurements were carried out using spectroscopic ellipsometry in the spectral range from 0.5 eV to 9.5 eV. The ZFO DF model dielectric functions (Gauss and critical-point-functions) were used to allow the derivation of transition energies and unravel the effect of the different growth conditions (i.e. temperature, substrate, oxygen pressure). The observed transitions are related to transitions allowed by ligand field theory. The dominant transitions were observed at ±3.5 eV and ±6 eV and identified as Fe³⁺ to Fe²⁺ transitions. ZFO has a special position within the spinel ferrites because Zn and its ions have a filled 3d shell. Thus no on site d-d transitions and no transitions from the O2p to the Zn3d band are possible. This results in a high transparency (compared to other ferrites) and reduces the number of observed transitions. While the oxygen partial pressure has a neglectable effect on the optical properties, the growth temperature induces a distinct shift in the transition energies was found. Also a notable shift of the absorption edge is observed. This change can be correlated to a change in the lattice constant as observed using wide-angle X-ray diffraction.

**CVD of Epitaxial SnO₂ Films grown on c-cut and r-cut Sapphire by SnI₂/O₂ Precursor** — **Yinmei Lu, Gunther Haas, Melanie Pinisch, Philipp Hering, Martin Becker, Johannes Bieber, and Bruno Meyer** — Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Thin films of SnO₂ have been successfully deposited by CVD using SnI₂/O₂ (CVD) and O₂ only. The electrical conductivity is not affected by oxygen partial pressures and substrates temperatures. The electrical conductivity of the thin films can be tuned btw. 10⁻⁴ and 10² S/m by different substrate temperatures during growth. The electrical conductivity of the thin films can be tuned btw. 10⁻⁴ and 10² S/m by different substrate temperatures during growth. It increases with decreasing substrate temperature. The conduction mechanism is not only affected by electron hopping between Fe²⁺ and Fe³⁺, but also defects like oxygen vacancies and structural disorder have great influence. The conductivity is thermally activated and a model with two activation energies fits the temperature dependent conductivity.

**Low Rate Deep Level Transient Spectroscopy: A new method for detecting deep levels in wide gap semiconductors** — **Rainer Pickelmann, Florian Schmidt, Ottwin Breitenstein, Herrmann von Wengen, and Marius Grundmann**

1. Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig
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Deep level transient spectroscopy (DLTS) has been widely applied to study defect states within the entire bandgap of various semiconductors. The method typically uses time windows in the kHz regime which is not sufficient to study defect states in the entire bandgap of wide bandgap materials such as ZnO. In these materials the emission rates of deep defects are too low to be detected by standard DLTS. Optical DLTS (ODLTS) fails because the photon flux of conventional light sources is too small in order to shift the optical emission rates towards the kHz regime. In this contribution we propose a method (LR-DLTS) allowing the measurement of capacitance transients in the MHz range maintaining high sensitivity. The method is applied to ZnO and first results will be presented demonstrating that LR-DLTS allows to construct experimental Arrhenius-plots of defects exceeding the emission rate span of conventional ones more than three orders of magnitude. On this basis we easily separated signals from the close-lying defects E₃ and E₃' in ZnO. Furthermore several defects states within the vicinity of the valence band and close to mid gap in ZnO were detected by LR-ODLTS and will be discussed.

**Deep level transient spectroscopy of Zinc Oxide** — **Marius Grundmann** — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany

Deep level transient spectroscopy (DLTS) has been widely applied to study defect states within the entire bandgap of various semiconductors. The method typically uses time windows in the kHz regime which is not sufficient to study defect states in the entire bandgap of wide bandgap materials such as ZnO. In these materials the emission rates of deep defects are too low to be detected by standard DLTS. Optical DLTS (ODLTS) fails because the photon flux of conventional light sources is too small in order to shift the optical emission rates towards the kHz regime. In this contribution we propose a method (LR-DLTS) allowing the measurement of capacitance transients in the MHz range maintaining high sensitivity. The method is applied to ZnO and first results will be presented demonstrating that LR-DLTS allows to construct experimental Arrhenius-plots of defects exceeding the emission rate span of conventional ones more than three orders of magnitude. On this basis we easily separated signals from the close-lying defects E₃ and E₃' in ZnO. Furthermore several defects states within the vicinity of the valence band and close to mid gap in ZnO were detected by LR-ODLTS and will be discussed.
and the dependence of electronic properties on oxygen partial pressures were investigated with scanning electronic microscope/atomic force microscope (SEM/AFM) and Hall measurements, respectively. The absolute average transmittance of the films in the visible and infrared range exceeds 90%. The band gap of the obtained SnO2 films is about 4.2 eV. Optical properties were investigated using low temperature photoluminescence (PL) measurements.

HL 67.7 Wed 16:00 Poster A
Investigation of the Rutile Structure on the Semiconductor Oxides SnO2 Doped with Fe by the Perturbed Gamma-Gamma Angular Correlation Spectroscopy — **Juliana Marques Ramos**1, Thiago Martucci2, Artur Wilson Carbonari2, and Reiner Vianden3 — 1Helmholtz-Institut für Strahlen- und Kernphysik — 2Instituto de Pesquisas Energéticas e Nucleares

In the present work the perturbed gamma-gamma angular correlation (PAC) spectroscopy was used to measure hyperfine interactions in the rutile structure of semiconducting SnO2 [1] thin films doped with Fe. The motivation for this study is that both oxides are candidates for diluted magnetic semiconductor in the emerging area of spintronics [2]. The thin films were deposited by sputtering on Si (100) substrate with an applied magnetic field of 500 G. The thicknesses were 100 nm. The implantation of 111In(111Cd) was made into the films at the Bonn Isotope Separator (BONIS) at the University of Bonn. The thermal treatment for the samples was done for 10 minutes at 873 K in vacuum for TiO2 and in air for the SnO2. PAC results are compared with ab-initio first principles calculations [3] and show a weak magnetic interaction for the rutile site, what confirms the results of our previous [4] work for thin films as well.


**HL 67.8 Wed 16:00 Poster A**
Electronic properties of Si-doped (Ga,In)2O3 PLD thin films — **Marcus Purfürst**1, **Stefan Müller**1, **Zhipeng Zhang**3, **Holger von Wencckstern**1, and **Marius Grundmann** — Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany

The wide bandgap oxide semiconductor β-Ga2O3 (Eg = 4.9 eV at RT) is a promising material for the realization of solar-blind photodetector applications like flame detection or missile warning systems. In order to tune the onset of the photo response as desired we investigated in a first step the incorporation of In into the Ga2O3 matrix and the change of the bandgap in dependence on the incorporated In content. The Si-doped (Ga,In)2O3 thin films were grown by pulsed laser deposition on c-plane sapphire substrates. Thin films grown at 730°C from a Ga2O3 target containing, for example, 1wt.% SiO2 and 2wt.% In2O3 are single crystalline with (-2 0 1)-orientation for oxygen growth pressures (pO2) up to 2×10⁻³ mbar. For higher pO2 polycrystalline thin films are obtained. According to the Hall measurements the conductivity shows a maximum of 635/S/m at a growth pressure of 2×10⁻³ mbar. The absorption edge decreases with increasing pO2 from 4.8eV to 4.65eV in the investigated pressure range. Compared to binary β-Ga2O3 thin films, In2O3 leads to an increased conductivity and a reduction of the optical band gap.

**HL 67.9 Wed 16:00 Poster A**
Fabrication and characterization of thin β-Ga2O3 samples — **Sukjana Dasah1**, **Christine Beclow1**, **Saskia F. Fischer1**, **Zhigang Galazka2**, and **Martin Albrecht2** — 1Novel Materials, Humboldt Universität zu Berlin, D-12489 Berlin — 2Leibniz Institute for Crystal Growth, D-12489 Berlin

The understanding of transport phenomena in transparent semiconductor oxides is the current subject of great excitement. Among the transparent semi conducting oxides β-Ga2O3 is very much interesting because of its transparency from deep ultraviolet region to infrared region. It has widest energy gap of 4.9 eV [1]. Here we report preparation and characterization of the thin β-Ga2O3 samples. β-Ga2O3 single crystals are grown by Czochralski technique [2]. Thin films are prepared via exfoliation technique. The samples are characterized using confocal microscopy, atomic force microscopy and scanning electron microscopy. Transport measurements will be discussed.


**HL 67.10 Wed 16:00 Poster A**
The Seebeck coefficient of In2O3 - Inferences on causes of unintentional conductivity and electron effective mass — **Natalie Preissler**1, **Oliver Bierwagen1,2**, **Ashok T. Ramu2**, and **James S. Speck** — 1Paul-Drude-Institut, Berlin, Germany — 2University of California, Santa Barbara, USA

If synthesized with high quality and purity, In2O3 along with SnO2 and Ga2O3 can become true wide band gap semiconductors in their own right, allowing new applications such as transparent electronics or power electronics. A long standing issue with these oxides is the source of unintentional n-type conductivity, and the more recent suspicion that the In2O3 surface dominate the thin film conductivity. Furthermore, literature values on the electron effective mass show a large spread. In this contribution we measured and modeled the room temperature Seebeck coefficient of high-quality, plasma-assisted molecular-beam-epitaxy-grown In2O3 for a wide range of electron concentrations, including the previously unexplored non-degenerate regime. We then use Hall and Seebeck measurements to (1) confirm the bulk nature (and not the surface) of the unintentionally doped electron system in In2O3, and (2) estimate the electron effective mass.