HL 23: Oxide Semiconductors I

Oxide Semiconductors except for ZnO

Time: Tuesday 9:30–13:00 Location: H13

HL 23.1 Tue 9:30 H13

Method of choice for the fabrication of Schottky contacts for unipolar devices on heteroepitaxial Ga_2O_3 — •Daniel Splith, Stefan Müller, Florian Schmidt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

Ga_2O_3 is a promising material for a new generation of high-power devices. For the fabrication of devices like unipolar diodes or metal-semiconductor field-effect-transistors (MESFETs), the optimization of the fabrication of Schottky contacts (SCs) is crucial.

In this contribution we compare different methods for the fabrication of Pt-Schottky contacts on heteroepitaxial Ga_2O_3 thin films: While the rectification of SCs fabricated by standard dc-sputtering remains poor, contacts fabricated by thermal evaporation and long-throw (LT) sputtering show rectification ratios above 6 orders of magnitude and ideality factors of about 1.3 for the best contacts. Using a reactive atmosphere during the sputtering process additionally increases the barrier height from about 1 eV to values of 1.4 eV for the best contacts. Contacts comparable to those fabricated with LT sputtering can be achieved in a standard sputtering chamber by positioning the sample out of the axis of the plasma, thereby reducing the kinetic energy of the impinging particles.

We used the latter method to fabricate circular MESFETs [1] on heteroepitaxial Ga_2O_3 thin films. Although the channel resistances are high, on/off ratios of up to 5 orders of magnitude were achieved.

[1] M. Higashiwaki *et al.*, Appl. Phys. Lett. 100.1, 013504 (2012)

HL 23.2 Tue 9:45 H13

Cu deficient, nanocrystalline $CuCrO_2$ — Leo Farrell, Emma Norton, Christopher Smith, David Caffrey, Igor Shvets, and •Karsten Fleischer — School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College, University of Dublin, Dublin 2, Ireland

The delafossite structured $CuCrO_2$ system is well known as one of the best performing p-type transparent conducting oxides. In this paper the details of a low temperature facile growth method for highly copper deficient Cu_xCrO_2 by spray pyrolysis is described. The dependence of the growth on the precursors, the temperature and oxygen partial pressure are examined. The decomposition routes are critical to obtain the best performing films. The thermopower and electrical measurements indicate p-type films with conductivity ranging from 1-12 Scm^{-1} depending on the growth conditions. This p-type conductivity is retained despite the nanocrystallinity and Copper deficiency of the films ($x \approx 0.4$). The figure of merit of these films can be as high as 350 μS, which is the best performing p-type TCO by solution methods to date. The optical properties are also investigated using ellipsometry and UV-Vis spectrophotometry.

HL 23.3 Tue 10:00 H13

Nitrogen incorporation in SnO2 thin films grown by chemical vapor deposition — •Jie Jiang, Yinmei Lu, Benedikt Kramm, Fabian Michel, Christian T. Reindl, Max Kracht, Bruno K. Meyer, Detlev M. Hofmann, and Martin Eickhoff — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Gießen, Germany

As a transparent conducting oxide film, SnO2 have great technological potential for the application in opto-electronic devices, due to its large band gap of 3.6 eV, and high carrier mobility of about 250 cm2/Vs at room temperature. Nitrogen is proposed to be an excellent anion dopant in SnO2 owing to its suitable electronegativity and ion size, high solubility limit, and non-toxicity. Here we study the characteristics of SnO2 films with high concentrations of incorporated nitrogen. We deposited SnO2-xNx thin films on c-sapphire substrates via chemical vapor deposition (CVD), using SnI2 powder and O2 and NH3 gas as source materials. The crystal structure, electrical properties and optical properties of the films were measured and investigated. The N atomic concentration in SnO2-xNx film increases from 0 to 7.9 at.% (XPS) without phase separation with increasing NH3 flow rate during the deposition. The substitutional lattice location in this concentration range was confirmed. The carrier concentration increases from 4.1E18 to 3.9E19 cm-3 and the absorption edge shifts from 4.26 to 4.08 eV. The effect of annealing on the structural, optical and electrical properties is also analyzed.

HL 23.4 Tue 10:15 H13

Doped and Undoped β-Ga_2O_3 Structures Prepared by Ultrasonic Nebulization and Spray Pyrolysis — •Constance Schmidt, Axel Fechner, and Dietrich R. T. Zahn — TU Chemnitz, Insitut für Physik, Reichenhainerstr. 70, 09126 Chemnitz

With its wide band gap of around 4.9 eV, β-Ga_2O_3 is a promising semiconductor for many applications like optoelectronic devices. Besides the established techniques for the preparation of β-Ga2O3 layers,for instance chemical vapor deposition, electron beam deposition, molecular beam epitaxy, and pulsed laser deposition, low cost techniques such as ultrasonic nebulization and spray pyrolysis are also of great interest. With the latter we obtained different types of microstructures of β-Ga_2O_3 (from 3D structures to thin films) on silicon substrates.

For the preparation of β-Ga_2O_3 a solution of $Ga(NO_3)_3$ in water, or in a water/ethanol mixture was employed. Rare earths, like Er^+, Sm^+ and Gd^+, were used as dopants. The different β-Ga_2O_3 microstructures were confirmed by SEM, and investigated with XRD, Raman spectroscopy, and microscopic ellipsometry. In all cases β-Ga_2O_3 was clearly identified. Since the structures have dimensions in the micrometer range, Raman spectroscopy (325 nm, 514.7 nm) was used to investigate individual β-Ga_2O_3 structures and determine their composition and other effects like strain in detail.

The experimental results demonstate that even with the low cost techniques it is possible to produce high quality doped and undoped β-Ga_2O_3 thin films and other structures, which are interesting for potential applications.

HL 23.5 Tue 10:30 H13

Temperature-dependent anisotropic thermal properties of β-Ga_2O_3 bulk-crystals — •Martin Handwerg[1,2], Rüdiger Mitdank[1], Zbigniew Galazka[3], and and Saskia F. Fischer[1] — [1]AG Neue Materialien, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany — [3]Leibniz Institute for Crystal Growth, 12489 Berlin, Germany

Transparent semiconducting oxides like Ga_2O_3 are important materials for high power electronics and optoelectronics. Here, we investigate the crystallographic anisotropy of the thermal conductivity and the thermal diffusivity for a β-Ga_2O_3 single crystal. The thermal conductivity, thermal diffusivity and specific heat capacity is measured by applying multiple electrical AC-heating methods on Czochralski-grown[1] β-Ga_2O_3 bulk crystals. At room temperature the thermal conductivity along the [100]-direction in Mg-doped electrical insulating and undoped semiconducting β-Ga_2O_3 is confirmed as 13 ± 1 $Wm^{-1}K^{-1}$[2]. Additionally a value for the [001]-direction of 15 ± 1 $Wm^{-1}K^{-1}$[3] is detected. The observed function $\lambda(T)$ is in accord with phonon-phonon-Umklapp scattering and the Debye-model for 50 K $< T <$ 300 K. Here a detailed discussion of the phonon-phonon-Umklapp scattering for $T < \theta_D$ is carried out.

[1] Z. Galazka *et al.* J. Cryst. Growth **404**, 184 (2014)
[2] M. Handwerg *et al.* Semcond. Sci. Technol. **30**, 024006 (2015)
[3] M. Handwerg *et al.* arXiv 1506.05294 (2015)

HL 23.6 Tue 10:45 H13

Influence of thermal and oxidative treatments on the electronic surface properties of In_2O_3 films — •Theresa Berthold[1], Thomas Stauden[1], Stefan Krischok[1], Marcel Himmerlich[1], Markus Mischo[2], Volker Cimalla[2], Julius Rombach[3], and Oliver Bierwagen[3] — [1]Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau — [2]Fraunhofer-Institut für Angewandte Festkörperphysik, Freiburg — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin

In_2O_3 is widely used as sensitive gas sensor material. As grown films typically exhibit a high surface electron concentration, which can be modified by an oxygen plasma treatment [1]. In this study, the surface composition and electronic properties of undoped and Mg-doped

In_2O_3 films grown by MBE or MOCVD are characterized by photoelectron spectroscopy to investigate the underlying mechanisms. We analyze the influence of different surface preparation methods, like thermal annealing in vacuum or O_2, oxygen plasma treatment as well as exposure to O_3, on formation of adsorbates, oxygen vacancies and defects as well as on variation in band bending, electron concentration and electric dipoles at the In_2O_3 surface. Oxygen plasma and other oxidative surface treatments induce attachment of negative O adsorbates forming an effective negative dipole at the surface that increases the barrier for electron emission and induces depletion of the surface electron layer via charge transfer, which can be reversed by adsorbate desorption. [1] O. Bierwagen, et al., Appl. Phys. Lett. 98, 172101 (2011)

30 min. Coffee Break

HL 23.7 Tue 11:30 H13

Influence of incoherent twin boundaries on the electrical properties of homoepitaxial β-Ga_2O_3 layers grown by metal organic vapor phase epitaxy — •Andreas Fiedler, Klaus Irmscher, Robert Schewski, Martin Albrecht, Michele Baldini, and Günter Wagner — Leibniz-Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin, Germany

Doped β-Ga_2O_3 layers have been grown homoepitaxially on (100) orientated substrates by metal organic vapor phase epitaxy (MOVPE) using either the shallow donor impurity Sn or Si. Conductivity and Hall effect measurements at room temperature show n-type conductivity. However, the measured electron concentrations between $5\times10^{17}\,\mathrm{cm}^{-3}$ and $2\times10^{19}\,\mathrm{cm}^{-3}$ indicate a strong electrical compensation and the electron mobilities of up to $30\,\mathrm{cm}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$ unexpectedly decline for low carrier densities. A possible explanation for this behavior comes from a structural analysis by transmission electron microscopy (TEM). It reveals that the layers contain a high density of planar defects consisting of twin lamellas and stacking faults. The lateral twin boundaries are incoherent and contain dangling bonds that trap charge carriers. This leads to charge accumulation and hinders lateral charge carrier transport. This behavior is in analogy to that of dislocation walls treated in [1]. Based on this model, we explain the observed steep decline in electron mobility at low carrier concentrations. Furthermore, the strong compensation of the donor dopants can, at least partly, be ascribed to the acceptor effect of the incoherent twin boundaries.
[1] Farvacque *et al.*, *Physical Review B* **63** 115202 (2001).

HL 23.8 Tue 11:45 H13

Influence of cation stoichiometry on performance of unipolar and bipolar zinc-tin-oxide diodes — •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 an electron density and a mobility as high as $10^{19}\,\mathrm{cm}^{-3}$ and $10\,\mathrm{cm}^2/\mathrm{Vs}$, respectively [1]. Therefore, ZTO is a suitable material for low-cost, transparent transistors and thus low-cost, transparent electronic applications.

We present our results on the influence of the Zn/Sn ratio on the electrical properties of thin films grown by pulsed laser deposition on glass substrates using a continuous composition spread method (CCS) [2]. Furthermore we discuss the performance of diodes fabricated thereon. Opposite to previous reports on only a limited number of discrete Zn/Sn ratios [3], we obtained a comprehensive data set for almost the entire composition range. Using energy dispersive X-ray analysis the spatial dependence of the Zn/Sn ratio was mapped. Charge carrier concentration and resistivity were determined in dependence on the composition. Further, the properties of Schottky diodes and all-amorphous *pn*-heterojunctions using $ZnCo_2O_4$ as *p*-type electrode will be discussed in dependence on the thin film stoichiometry.

[1] Jayaraj et al., J. Vac. Sci. & Technol. B, **26**, 2, 2008
[2] von Wenckstern et al., CrystEngComm, **15**, 10020, 2013
[3] Görrn et al., Applied Physics Letters, **91**, 193504, 2007

HL 23.9 Tue 12:00 H13

Dielectric and Raman tensor of monoclinic Ga_2O_3 — •Chris Sturm[1], Christian Kranert[1], Jürgen Furthmüller[2], Friedhelm Bechstedt[2], Rüdiger Schmidt-Grund[1], and Marius Grundmann[1] — [1]Institut für Experimentelle Physik II, Universität Leipzig, Linnéstr. 5, 04103 Leipzig, Germany — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Ga_2O_3 is a promising material for deep UV applications due to its band-gap energy of about 4.8 eV. At ambient conditions it crystalizes in a monoclinic structure and the dielectric function is a tensor consisting of 4 independent elements. The magnitude and dispersion of these elements were not known previously. We determined the full dielectric tensor in the spectral range of $0.5-8.5$ eV by using generalized spectroscopic ellipsometry. The obtained DF is in excellent agreement with that obtained by many-body perturbation theory including quasiparticle and excitonic effects. This analysis yield that the off-diagonal element cannot be neglected in the entire investigated spectral range. Although this element seems to be negligible small in the transparent spectral range ($|\varepsilon_{xz}|\leq 0.02$), it causes a rotation of the dielectric axis of about 20°. Using this DF we applied a new formalism for Raman scattering in anisotropic crystals to model the dependency of the Raman intensities on the scattering geometry for most phonon modes and determined the Raman tensor elements for these modes.
[1] C. Sturm *et al.*, APL Mater. **3**, 106106 (2015).

HL 23.10 Tue 12:15 H13

An *ab initio* study of defect complexes in Fe- and Gd-doped MgO co-doped with Li — •Sergey V. Levchenko, Sebastian Alarcon Villaseca, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, DE

Li/Fe- and Li/Gd-co-doped MgO have recently attracted attention due to their potential applications in catalysis and dosimetry [1,2]. In this work, we calculate formation energies of defect complexes in these materials using DFT with the hybrid PBE0 functional, and estimate their relative concentrations at realistic temperatures and oxygen pressures using the *ab initio* atomistic thermodynamics. We find that the Fe_{Mg}-Li_{Mg} defect pairs are bound weaker than Gd_{Mg}-Li_{Mg} pairs, and the dissociated Fe_{Mg}-Li_{Mg} pairs are favored at elevated temperatures due to the increased configurational entropy. This explains why experimental EPR spectra of Gd^{3+} showed apparent changes upon Li-doping of Gd-MgO, while no changes have been detected in Li/Fe-MgO samples [3]. This qualitative result is found to be insensitive to the fraction of the exact exchange α in the hybrid functional for $0<\alpha<0.5$. – [1] U. Simon *et al.*, Catal. Comm. 18, 132 (2012); [2] L.C. Oliveira, B.A. Doull, E.G. Yukihara, J. Luminescence 137, 282 (2013); [3] U. Simon, S. Arndt, T. Otremba, S. Alarcon Villaseca, S.V. Levchenko, M. Wollgarten, J.D. Epping, A. Kwasniewski, A. Berthold, F. Schmidt, O. Gorke, M. Scheffler, R. Schomacker, K.P. Dinse, in preparation.

HL 23.11 Tue 12:30 H13

Electronic band structure and infrared lattice dynamics of single-crystal nickel oxide (NiO) — •Stefan Zollner, Cayla M. Nelson, Travis I. Willett-Gies, Ayana Ghosh, and Lina S. Abdallah — New Mexico State University, Las Cruces, NM, USA

Using spectroscopic ellipsometry, we determined the dielectric function of bulk NiO from 25 meV to 6 eV to study its lattice dynamics and electronic structure. In the visible and UV, NiO looks remarkably similar to Si: Both materials are transparent in the near-infrared. A slow rise of the absorption throughout the visible is followed by a sharp peak at 3.4 eV (Si) and 3.8 eV (NiO). In Si, this peak is caused by transitions from the highest valence band to the lowest conduction band along the (111) direction of the BZ. In NiO, it is associated with the charge-transfer (Hubbard) gap. In both materials, the peaks broaden and redshift with increasing temperature, due to electron phonon interactions. Many recent band structure calculations for NiO focus on the charge-transfer absorption peak (3.8 eV) and ignore the absorption below the main peak. Our data show a direct band gap of NiO at 0.85 eV, which we attribute to interband transitions from the Ni+O valence band to the Ni(4s) conduction band at the zone center. We also find strong TO phonon absorption in infrared ellipsometry spectra, which is modified by two-phonon absorption.

HL 23.12 Tue 12:45 H13

Lattice dynamics of EuO: an evidence for giant spin-phonon coupling — •Ramu Pradip[1,2], Przemysław Piekarz[3], Alexei Bosak[4], Dániel Géza Merkel[4], Olga Waller[1,2], Anja Seiler[1,2], Alexander I. Chumakov[4], Rudolf Rüffer[4], Andrzej M. Oleś[5,6], Krzysztof Parlinski[3], Michael Krisch[4], Tilo Baumbach[1,2,7], and Svetoslav Stankov[2,1] — [1]Laboratory for Applications of Synchrotron Radiation, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Institute for Photon Science and Synchrotron Radiation, KIT, Eggenstein-Leopoldshafen, Germany — [3]Institute of Nuclear Physics, Polish Academy of Sci-

ences, Kraków, Poland — [4]European Synchrotron Radiation Facility, Grenoble, France — [5]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [6]Marian Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland — [7]ANKA, KIT, Eggenstein-Leopoldshafen, Germany

Europium monoxide is a semiconducting ferromagnet recently proposed as a spin-filter in the emerging field of spintronics. Using inelastic x-ray scattering and nuclear inelastic scattering combined with ab initio calculations we determined the lattice dynamics of EuO. The results revealed a giant momentum and temperature dependent spin-phonon coupling above and well below the Curie temperature.
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