HL 4: Focus Session: Oxide Semiconductors for Novel Devices I (joint session HL/DS)

The class of semiconducting oxides materials is currently investigated in terms of promising applications in devices, including low temperature processed amorphous thin films for bendable electronics and display technology as well as highly crystalline materials such as the wide band group-III sesquioxides. Possible devices applications are UV and DUV photo sensors, power electronics and even memristors. This session sets a focus on physical properties of semiconductor oxide materials, their growth methods and heterostructures for demonstrator devices.

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

Time: Monday 9:30–12:45 Location: H34

Invited Talk HL 4.1 Mon 9:30 H34
The role of suboxide kinetics and thermodynamics for the catalysis and facet formation during the molecular beam epitaxy of oxides — •Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Leibniz Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5–7, 10117 Berlin, Germany.

Based on its wide band gap of E_g=4.7 eV Ga_2O_3 is a promising oxide semiconductor for novel applications such as power electronics and UV detection. Band-gap engineering by alloying with In_2O_3 (E_g=2.7 eV) allows tuning the detection wavelength and enable heterostructure devices. Thin film growth of these oxides by molecular beam epitaxy (MBE) enables the high material quality (purity and crystallinity) required for novel applications. This contribution shows how the intermediate formation and desorption kinetics of Ga_2O and In_2O limits the MBE growth rate of Ga_2O_3 (and of In_2O_3 to a less extent).[1] Nevertheless, the stronger Ga-O than In-O bonds thermodynamically leads to a favorable incorporation of Ga into the alloy $(In_xGa_{1-x})_2O_3$.[2] The collaborative effect of these kinetics and thermodynamics is shown to lift the growth rate limitation of Ga_2O_3 in the presence of an additional In-flux by metal-exchange catalysis.[3,4] Finally, the impact of the metal-to-oxygen flux ratio on the anisotropy of surface free energy is shown to control the formation of surface facets on both oxides.[4,5] [1] Vogt et al., Phys. Rev. Mater. **2**, 120401(R) (2018). [2] Vogt et al., APL Mater. **4**, 086112 (2016). [3] Vogt et al., Phys. Rev. Lett. **119**, 196001 (2017). [4] Mazzolini et al., APL Mater. **7**, 022511 (2019). [5] Bierwagen et al., J. Phys.: Condens. Matter **28**, 224006 (2016).

Invited Talk HL 4.2 Mon 10:00 H34
Is There a Perspective of p-type Doping in Gallium Oxide? — •David Rogers[1], Ferechteh Teherani[1], Philippe Bove[1], Eric Sandana[1], Ryan McClintock[2], and Manijeh Razeghi[2] — [1]Nanovation, 8 Route de Chevreuse, 78117 Chateaufort, Francenh — [2]Center for Quantum Devices, Department of Electrical Engineering and Computer Science, Northwestern University, Evanston, IL60208, US

Recently, there has been a surge in interest for the ultra wide bandgap semiconductor Ga2O3. Key drivers for this are that bulk β-Ga2O3 wafers have become commercially available and that a variety of film growth methods have been shown to give n-type doping control. A major drawback associated with Ga2O3, however, has been lack of a method for fabricating p-type material. Indeed, it is generally proposed that p-type doping is unlikely to be obtained because of a combination of factors including the relatively low energy level of the valence band, the lack of an identified shallow acceptor, the relatively high effective masses of holes at the top of the valence band, the propensity for self-trapping of holes and the comparatively low formation energy of the oxygen vacancy donor (which favors compensation of acceptors). Recently, however, Chikoidze et al. [1] and Razeghi et al. [2] independently presented direct evidence of majority p-type conduction Ga2O3. The former concerned nominally undoped layers grown by PLD and the latter concerned Si doped layers grown by MOCVD. In this talk we will give an overview of these results. [1] Chikoidze et al. Materials Today Physics 3 (2017) [2] Razeghi et al., Photonics West, Feb (2018)

Invited Talk HL 4.3 Mon 10:30 H34
Highly rectifying contacts on Ga_2O_3, In_2O_3 and $(In,Ga)_2O_3$ thin films — •Daniel Splith — Felix-Bloch-Institut für Festkörperphysik, Universität Leipzig, Germany

Oxide semiconductors like gallium oxide or indium oxide are promising materials for a new generation of transparent electronic devices. Additionally, alloying both materials allows band-gap engineering, enabling e. g. the fabrication of wave-length selective photodetectors. In order to realize devices like diodes, field-effect transistors and photodetectors, the fabrication of rectifying contacts is essential. Further, such contacts also enable the investigation of the materials by means of space charge region based methods like thermal admittance spectroscopy.

In this contribution the properties of Schottky contacts and pn-heterojunctions on heteroepitaxial Ga_2O_3 and In_2O_3 thin films grown by pulsed laser deposition are discussed. Additionally, the properties of such rectifying contacts on $(In,Ga)_2O_3$ thin films having a lateral composition gradient are presented. In order to improve the rectification of the contacts, different vertical layouts were investigated. Further, a comprehensive model, taking into account thermionic emission, thermionic field emission and charging currents as well as non-idealities like barrier height inhomogeneities, current spreading and variations of the net-doping density in growth direction, was employed in order to understand the measured characteristics.

15 min. break

Invited Talk HL 4.4 Mon 11:15 H34
Understanding the impact of vibrations and defects on the optical properties of phosphors — •P. Erhart[1], C. Linderälv[1], D Åberg[2], Y.-C. Lin[1], M Bettinelli[3], N. C. George[4], S. F. Parker[5], and M. Karlsson[1] — [1]Chalmers University of Technology, Sweden — [2]LLNL, USA — [3]University of Verona, Italy — [4]UCSB, USA — [5]ISIS Facility, UK

Activator ions such as Ce are used to control the luminescent properties of phosphors, which are core components in white-light-emitting diodes. Their optical signatures are temperature dependent as they are sensitive to changes in the local environment due to atomic vibrations. Using a combination of experiment and first-principles calculations, we have recently provided a complete phonon assignment for the oxide garnet $Y_3Al_5O_{12}$ (YAG). An increase in temperature causes larger tetragonal distortion of the CeO_8 moieties and an increase of the crystal-field splitting, which gives rise to a redshift of the emitted light. The lattice thermal expansion on the other hand reduces the tetragonality and induces a blue-shift. The non-linear shift of the color of the emitted light with increasing temperature can then be explained as a competition between these two processes. Thermal quenching of the emission due to non-radiative processes limits the efficiency of these devices. In this context, we have investigated the potential contribution of oxygen vacancies. It is found that these defects exhibit very strong and localized electron-phonon coupling, providing an efficient non-radiative recombination channel.

Invited Talk HL 4.5 Mon 11:45 H34
atomically resolved termination engineering of electronic states at oxide semiconductors — •Ya-Ping Chiu — Department of Physics, National Taiwan University, Taipei, Taiwan

Termination engineering at oxide semiconductors has become highly attractive for next-generation electronic and spintronic devices due to a delicate interplay of different correlated processes including orbital, charge, and magnetic ordering as well as lattice degrees of freedom at the interfaces. Therefore, to achieve a detailed physical understanding of such exotic phenomena at oxide interfaces becomes important. Only with such detailed high resolution experimental data, will it be possible to explore the relevance of the different physical models. In our studies, cross-sectional scanning tunneling microscopy and spectroscopy is employed to provide direct experimental insight into the origin and the natural evolution of the electronic properties with atomic precision across the heterointerfaces. In this talk, topics to be discussed include ferromagnetic/superconducting and multiferroic/ferromagnetic heterointerfaces. This study highlights the importance of a direct atomically resolved access to electronic interface states, which is useful

in understanding the intriguing interface properties in oxide semiconductors and providing a lot of insights for these communities. [1-3] Selected references: 1.*ACS nano, 12 (2), 1089 (2018). 2. Phys. Rev. Lett., 109, 246807 (2012). 3. Adv. Mater., 23, 1530 (2011).

Invited Talk HL 4.6 Mon 12:15 H34

Nanoscale Control of Native Point Defects and Doping in Oxide Semiconductors — •Leonard Brillson — The Ohio State University, Columbus, OH, USA

Nanoscale optical and electrostatic techniques can directly measure the movement of native point defects inside oxide semiconductors and how they control space charge regions, tunneling, and contact rectification. Depth-resolved cathodoluminescence spectroscopy (DRCLS) with hyperspectral imaging measures 3-dimensional defect redistribution on a nanoscale for ZnO, Ga2O3, SrTiO3, and BaSrTiO3, revealing how intrinsic and applied electric fields drive defect movement. Defects at metal-ZnO diodes change carrier densities, tunneling, and trap-assisted hopping, altering Zn- vs. O-polar Schottky barriers. Nanoscale 3D measurement and imaging reveal electrically-active defects that extend deep inside wires, altering depletion widths, conducting channel volumes, and metal-ZnO nano-contact rectification. Electron and ion beams alter defect distributions to create rectifying, ohmic, or blocking contacts with the same metal on the same nanowire, demonstrating the interplay between the nature of native point defects, the intrinsic doping, and the physical dimensions of the nanostructure itself in determining the electronic properties of the oxide interface. DRCLS also enabled us to correlate the dominant luminescence features of Ga2O3 with the most thermodynamically stable O vacancy, Ga vacancy, and Ga vacancy-hydrogen defect states in the band gap predicted theoretically. As with ZnO, the combined depth-resolved detection and processing of Ga2O3 suggests new avenues for defect and doping control.