DS 9: Thin Film Properties III: Oxides

Time: Tuesday 14:00–15:15 Location: REC/C213

DS 9.1 Tue 14:00 REC/C213

Analysis of the MgF_2 || VO_2 Interface in Applications as Smart Windows by Secondary Ion Mass Spectrometry (SIMS) — •Yan Ravil Wollenweber-Bienerth, Peter J. Klar, Anja Henss, and Martin Becker — Institute of Experimental Physics I and Center for Materials Research, Heinrich-Buff-Ring 16, Justus-Liebig-Universität Giessen, D-35392 Giessen, Germany

Smart Windows are special fenestration devices whose transmittance switches as a function of the ambient temperature. Vanadium dioxide (VO_2) is by far the most studied material for such applications. Usually, high substrate temperatures are needed to obtain VO_2 thin films. This results in detrimental diffusion of alkaline ions from the substrate into the thermochromic layer. Buffer layers between the substrate and the VO_2 may prove a suitable option for reducing this effect. Additionally, these help to increase visible transmittance and, in case of rutile materials, yield a reduction of the VO_2 growth temperature. Magnesium fluoride (MgF_2) is one viable candidate thanks to its excellent optical properties and chemical resistance. Simulations, however, show a significant influence of the interfaces between the layers on various properties. By controlling interface morphology, an improvement of the layer properties can be anticipated.

Here, we utilize SIMS depth-profiling to analyze multi-layer stacks of VO_2 and MgF_2 grown by ion-beam sputter deposition (IBSD). The stacks werde deposited on quartz glass substrates with MgF_2 serving as buffer layer. We show that this type of buffer layer improves the layer properties.

DS 9.2 Tue 14:15 REC/C213

Modification of crystal structure of TiO_2 thin films for artificial photosynthesis — •Lauri Palmolahti — University of Würzburg, Würzburg, Germany — Tampere University, Tampere, Finland

Progressing climate change has created a need for carbon-neutral energy production methods, such as artificial photosynthesis. The corrosive nature of artificial photosynthesis requires the use of coatings to protect otherwise unstable photocatalytic materials. The crystallite structure and size significantly affect the protective properties and chemical stability of the thin film. In this work, the effect of defect composition in amorphous TiO_2 thin films on vacuum annealing induced crystallization was studied. The chemical stability and protective properties of these crystallized films were then examined under conditions similar to those in artificial photosynthesis. The defect composition of the amorphous phase, such as Ti^{3+}, O^{1-}, and precursor traces, was tuned by changing the deposition parameters. The results showed that amorphous TiO_2 thin films without Ti^{3+} defects crystallized into microcrystalline anatase, whereas a moderate number of these defects led to the formation of nanocrystalline rutile. An excessive number of defects resulted in a mixed amorphous–nanocrystalline rutile phase. Impedance spectroscopy and stability tests revealed that microcrystalline anatase was prone to grain boundary corrosion, whereas nanocrystalline rutile was chemically stable and retained its protective properties for extended periods of time, making it a suitable choice for protective coatings in artificial photosynthesis.

DS 9.3 Tue 14:30 REC/C213

Investigation of epitaxial ITO layers on YSZ as a transparent conductive back contact for photoelectrochemical applications — •Margaretha Huber[1], Sergej Levashov[1], Tsedenia Zewdie[1,2], Ian D. Sharp[1,2], and Johanna Eichhorn[1] — [1]TUM School of Natural Sciences — [2]Walter Schottky Institut

Photoelectrochemical (PEC) water splitting is a promising route toward sustainable, high-energy-density solar fuels for carbon-neutral energy storage. Transparent conducting oxides such as indium tin oxide (ITO) often serve as back contacts due to their high electrical conductivity, electrochemical stability in the oxygen evolution reaction, and favorable band alignment. ITO grown on cubic oxide substrates such as yttria-stabilized zirconia (YSZ) can act as an epitaxial template with low lattice mismatch, enabling fully epitaxial oxide heterostructures with well-defined interfaces and reduced defect densities. Here, we investigate epitaxial ITO (100) thin films on YSZ grown by e-beam evaporation through a systematic variation of deposition rate, substrate temperature, and post-deposition annealing atmosphere, thereby tuning crystallinity, lattice parameters, carrier transport, and surface morphology. The correlation between structural quality and stoichiometry, and their impact on electrical properties, is investigated using X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and atomic force microscopy (AFM). These ITO/YSZ templates are evaluated using $BiVO_4$ as a model photoanode to enable efficient charge extraction and provide design guidelines for epitaxial oxide heterostructures for PEC water splitting.

DS 9.4 Tue 14:45 REC/C213

Room-temperature H_2 gas sensing in ultra-thin SnO_2 films grown via atomic layer deposition — •Rudi Tschammer[1], Dominic Guttmann[1], Carlo Tiebe[2], Karsten Henkel[1], Carlos Morales[1], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany

Transitioning to an energy system based entirely on renewable energy sources requires long-term energy storage utilizing energy vectors such as hydrogen (H_2). Given its high diffusivity, broad explosive range, and low ignition energy, the adoption of H_2 requires safety systems along the hydrogen value chain. Therefore, there is a need for sensitive, specific and selective conductometric H_2 sensors operating at room temperature (RT) and compatible with complementary metal-oxide semiconductor (CMOS) technology. Earlier work by our group investigated ultra-thin cerium oxide films grown by atomic layer deposition (ALD) and demonstrated H_2 sensing at RT. This performance was due to the abundant defects present in the films. Building on these results, we present a comprehensive investigation of ALD-grown tin oxide (SnO_2), a widely researched metal oxide for H_2 gas sensing. Using *in-situ* X-ray photoelectron spectroscopy (XPS), we observe a distinct dependence of defect concentration on film thickness and oxidant. *Ex-situ* H_2/air gas sensing measurements and near-ambient pressure XPS further link film properties and sensing behavior. These findings pave the way for novel RT H_2 gas sensors based on ALD technology.

DS 9.5 Tue 15:00 REC/C213

Composition and band gap of aluminum alloyed beta-gallium oxide determined by XPS — •Lukas Schewe[1], Jana Rehm[2], Ming-Chao Kao[3], Vedran Vonk[3], Zbigniew Galazka[2], Saud Bin Anooz[2], Andreas Popp[2], and Jan Ingo Flege[1] — [1]Fachgebiet Angewandte Physik und Halbleiterspektroskopie, BTU Cottbus-Senftenberg — [2]Leibnitz-Institut für Kristallzüchtung, Berlin — [3]CXNS-Center for X-ray and Nano Science, DESY, Hamburg

Beta-phase gallium oxide has a band gap of 4.85 eV, suggesting strong potential for high-power electronics applications. Its properties can be enhanced by increasing the band gap via aluminum alloying. Here, we discuss the structural, electronic, and surface properties of β-$(Al_xGa_{1-x})_2O_3$ bulk crystals and thin films grown by metal-organic vapor-phase epitaxy (MOVPE) with Al contents of up to 40 %. Their Al content was determined by X-ray photoelectron spectroscopy (XPS) and compared with values obtained from X-ray diffraction (XRD) and inductively coupled plasma optical emission spectroscopy (ICP-OES). Additionally, potential doping gradients towards the bulk have been investigated by acquiring spectra at different take-off angles and by XPS depth profiling, revealing different aluminum concentrations in the bulk and at the surface. Furthermore, we establish a correlation between Al content and electronic band gap, i. e., with changes in the optoelectronic properties, which were determined by a combination of XPS electron-loss spectra and optical absorbance measurements. Finally, Auger spectroscopy and XRD analysis confirm the excellent chemical and structural quality of β-$(Al_xGa_{1-x})_2O_3$ thin films.