O 74: Poster Session VI: Oxide and insulator surfaces: Structure, epitaxy and growth II

Time: Wednesday 13:30–15:30 Location: P

O 74.1 Wed 13:30 P

Reduction of the α-Fe$_2$O$_3$(1$\bar{1}$02) surface to Fe$_3$O$_4$ — •Erik Rheinfrank[1], Giada Franceschi[1], Igor Sokolović[1], Jesús Redondo[2], Pavel Procházka[3], Nishant Kumar[3], Ondřej Man[3], Jan Michalička[3], Jan Čechal[3], Michael Schmid[1], Gareth S. Parkinson[1], Ulrike Diebold[1], and Michele Riva[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic — [3]CEITEC, Brno, Czech Republic

Iron oxides list among the most abundant compounds in Earth's crust and are involved in many natural processes as well as in a wide range of applications. To understand their fundamental surface-chemical properties it is crucial to reproducibly prepare atomically well-defined surfaces in a controlled environment. Here we report on the local reduction of the α-Fe$_2$O$_3$(1$\bar{1}$02) surface by two processes. First, by annealing in ultra high vacuum (UHV) at 450 °C and subsequent sputtering and annealing in low 10^{-6} mbar O$_2$ at 450 °C, and second, by annealing in UHV at 600 °C. Atomic force microscopy (AFM) and x-ray photoelectron spectroscopy (XPS) reveal that both routes lead to the formation of boulder-like magnetite inclusions. Once they are created, the preferential removal of oxygen by sputtering enhances their formation instead of removing them. A pristine hematite surface can be recovered by exposure to higher oxygen pressures (1 mbar) at $\sim$ 850°C. The nature of these Fe$_3$O$_4$ inclusions was studied by low-energy electron microscopy (LEEM) and low-energy electron diffraction (LEED).

O 74.2 Wed 13:30 P

Fe$_3$O$_4$ (001) near-surface diffusion observed by nuclear resonant scattering (NRS) — •Steffen Tober[1,2], Jan-Christian Schober[1,2], Esko Erik Beck[1,2], Guilherme Dalla Lana Semione[1,2], Simon Chung[1,2], Kai Schlage[1], Olaf Leupold[1], Ilya Sergeev[1], René Steinbrügge[1], Hans-Christian Wille[1], Heshmat Noei[1], Vedran Vonk[1], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-Synchrotron, Hamburg — [2]Universität Hamburg, Fachbereich Physik

Elevated temperature cation transport processes influence the structure and stoichiometry in the near surface region of magnetite (Fe$_3$O$_4$) (001) which is of crucial importance for the performance of magnetite-based catalysts and devices [1,2]. Near surface transport was studied by stepwise annealing of a homoepitaxially grown ^{57}Fe$_3$O$_4$ layer on a (001) oriented Fe$_3$O$_4$ single crystal, monitored by nuclear resonant reflectivity (NRR) and time spectra (TS) after each step. Site selective depth profiles obtained from simultaneous fitting of NRR and TS indicate transport from 470 K on. Diffusion constants estimated from the ^{57}Fe depth profiles were in good agreement with previous results [4], while the site-selectivity of NRS revealed notable differences in the transport of oct- and tet coordinated cations enabling a more precise description of the diffusion process.

[1] Arndt et al. Chem. Comm. 1, 92 (2019) [2] Arndt et al. Surf. Sci. 653, 76 (2016) [3] Andreeva et al., Mosc. Univ. Phys. Bull. 63, 132 (2008) [4] Tober et al., Phys Rev Research. 2, 023406 (2020)

O 74.3 Wed 13:30 P

Strongly Strained VO$_2$ Thin Film Growth — •Simon Fischer[1], Jan Ingo Flege[2], Michael Foerster[3], Lucia Aballe[3], Jens Falta[1], and Jon-Olaf Krisponeit[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus, Germany — [3]ALBA Synchrotron Light Facility, Barcelona, Spain

The semiconductor-metal transition temperature of VO$_2$ strongly shifts as a result of strain applied along the rutile *c* axis, making it interesting for various switching applications, as smart coatings and as sensors. In the past, this has been demonstrated, for instance, through the application of epitaxial strain on TiO$_2$ substrates.

We extend this tailoring approach by utilizing the much larger lattice mismatch of 8.78 % occurring in the VO$_2$/RuO$_2$ system for orientations where the *c* axis lies in-plane. Depositing vanadium oxide by atomic oxygen-supported reactive MBE on an oxidized Ru(0001) template, we have grown VO$_2$ thin films on single domain RuO$_2$ islands with distinct orientations. Locally resolved electron spectroscopy was used to ascertain the correct stoichiometry of the grown VO$_2$ films on all template island types. Low energy electron diffraction reveals the VO$_2$ films to grow indeed fully strained on RuO$_2$(110) but fully relaxed on RuO$_2$(100).

Hence, the presented template allows for simultaneous access to a remarkable strain window ranging from bulk-like structures to regions of massive tensile strain.

O 74.4 Wed 13:30 P

XPS and UPS investigation of an ALD prepared Al$_2$O$_3$/ZnO heterojunction — •Christoph Janowitz[1], Ali Mahmoodinezhad[1], Franziska Naumann[2], Paul Plate[2], Karsten Henkel[1], and Jan Ingo Flege[1] — [1]Brandenburg University of Technology Cottbus-Senftenberg, K.-Zuse-Str. 1, 03046 Cottbus, Germany — [2]SENTECH Instruments GmbH, Schwarzschildstraße 2, 12489 Berlin, Germany

The band alignment of two large band gap oxides was studied by a combination of XPS and UPS using consecutive sputter steps to unravel the electronic structure and elemental composition of each layer and the interface region. An Al$_2$O$_3$/ZnO heterointerface (10 nm Al$_2$O$_3$ on 59 nm ZnO) was grown on top of a Si single crystal substrate by consecutive thermal and plasma-assisted atomic layer deposition (ALD) respectively. The valence band maximum of Al$_2$O$_3$ was found to be 1.1 eV below that of ZnO, the conduction band minimum 2.3 eV above, resulting in a type-I staggered heterojunction. A reduction of ZnO to elemental Zn in the interface region was detected by the apparent shoulder of the Zn 2p and 2s core levels and by the Zn LMM Auger. This suggests an ALD interface formation mechanism different from previous models identified for other heterointerfaces.

O 74.5 Wed 13:30 P

Functional ultra-thin oxide films deposited by atomic layer deposition on structured substrates — •Carlos Morales[1], Ali Mahmoodinezhad[1], Andreas Markus Schubert[2], Christian Wenger[2], Karsten Henkel[1], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Konrad-Zuse-Strasse 1, D-03046 Cottbus, Germany — [2]IHP - Leibniz-Institut für innovative Mikroelektronik, IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

In the last decades, atomic layer deposition (ALD) has gained prominence in the materials and surface science communities owing to its high potential for integration as a scalable process in microelectronics. ALD's largest strengths are its well-controlled layer-by-layer deposition and growth conformity on 3D structures. Yet, the ALD technique is also well known to lead to amorphous and defective, non-stoichiometric thin films, resulting in modified materials properties that may even preferentially be used in certain applications. To study these issues, we have developed an in-situ ALD reactor attached to an X-ray photoelectron spectroscopy (XPS) system, capable of switching between both pump and flow-type operation. This novel tool allows to cover the entire range of compounds and recipes used in ALD, thus clarifying the role of such defects at different deposition stages, growth conditions and film/substrate interfaces. To exemplify these sorts of studies, we show the deposition of Al2O3 5-10 nm films on nanostructured Si, and their use as substrates for functional CeOx ALD deposits.

O 74.6 Wed 13:30 P

Phase diagrams of Co$_3$O$_4$ and Mn$_3$O$_4$ surfaces under different experimental conditions — •Maria Fernanda Juarez[1], Hui Yin[1,2], and Axel Gross[1] — [1]Ulm University, Ulm, Germany — [2]South China University of Technology, Guangzhou, P. R. China

In spite of the many advantageous features of the zinc-air batteries (ZABs), one of the basic problems for its uses is the slow kinetics of oxygen evolution and reduction reactions (OER and ORR) [1]. In recent years many effort has devoted to solve this problem by finding new electrocatalysts that promote both reactions or by changing the experimental conditions and thence the reaction mechanism[2].

Presently, Mn and Co oxides are among the most active electrochemical catalysts. By doping or by introducing oxygen vacancies, the electronic configuration of the metal ions can be modified, changing their interaction with the adsorbed species and leading to modifications in the catalytic activity.

It is the objective of this work to determine the proper surface structure of Mn$_3$O$_4$ and Co$_3$O$_4$ (111) surfaces under the experimental conditions of operating ZABs: oxidating or reducting environments and non-alkaline electrolytes. Using the concept of the computational hydrogen electrode [3], we will obtain the equilibrium structures as a function of potential and OH^- concentration. As hydroxyls are strongly interacting with water, the presence of water will be taken into account.

[1] D. Yang *et al.* Elect. Energy Rev. (2019) 2:395.
[2] Sun *et al.* Science (2021) 371:46.
[3] Norskøv *et al.* J. Phys. Chem. B (2004) 108:17886.

O 74.7 Wed 13:30 P

High temperature reduction and reoxidation of cerium oxide on Cu(111) — •Linus Pleines[1], Lars Buss[1,2], Tevfik Onur Menteş[3], Francesca Genuzio[3], Andrea Locatelli[3], Jan Ingo Flege[2], and Jens Falta[1,4] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [3]ELLETRA Synchrotron Light Source, Basovizza, Italy — [4]MAPEX Center for Materials and Processes, Bremen, Germany

Cerium oxide is of great interest due to its technological importance in various electronic, optical and catalytic applications. The inverse model catalyst cerium oxide on Cu(111) shows a high activity for the production of methanol. Oxygen vacancies, e.g. in form of reduced ceria, are necessary for the production of methanol from CO_2 and H_2. The reduction of ceria may be achieved by exposure to H_2 at elevated temperatures. We studied the interaction of H_2 and CO_2 with cerium oxide islands on a Cu(111) substrate with low-energy electron microscopy (LEEM) and x-ray absorption spectroscopy (XAS). From earlier studies, the orientation of the cerium oxide is known to be decisive for the catalytic activity. In our experiments, the impact of both orientations are directly compared via growth of (100) and (111) cerium oxide islands side by side. At temperatures around 550 °C, exposure to H_2 leads to partial reduction and exposure to CO_2 leads to complete reoxidation of the cerium oxide. The (100) and (111) orientations show different reduction and reoxidation behaviors.

O 74.8 Wed 13:30 P

Low-temperature atomic layer deposition of indium oxide thin films using trimethylindium and oxygen plasma — •Ali Mahmoodinezhad[1], Carlos Morales[1], Franziska Naumann[2], Paul Plate[2], Robert Meyer[2], Christoph Janowitz[1], Karsten Henkel[1], Małgorzata Kot[1], and Jan Ingo Flege[1] — [1]Brandenburg University of Technology Cottbus-Senftenberg, K.-Zuse-Str. 1, 03046 Cottbus, Germany — [2]SENTECH Instruments GmbH, Schwarzschildstraße 2, 12489 Berlin, Germany

Indium oxide thin films were deposited on Si (100) by plasma-enhanced atomic layer deposition (PEALD) using trimethylindium (TMIn) and oxygen plasma (O2) in a low-temperature range of 80 to 200 °C. The In_2O_3 layers were characterized by in-situ spectroscopic ellipsometry (SE), ex-situ X-ray photoelectron spectroscopy (XPS) and electrical measurements. The SE data show a growth rate of 0.56 Å/cycle within the ALD window (100 to 150 °C) with a thickness inhomogeneity of $\leq$ 1.2%. In addition, the highest refractive index is 2.07 (at 632.8 nm) for the layer grown at 150 °C, and the films exhibit indirect and direct band gaps of 2.8±0.1 eV and 3.3±0.2 eV, respectively. XPS characterization indicates no carbon incorporation and a temperature-dependent off-stoichiometry of the layers. The chemical analysis of the In 3d and O 1s core levels confirms the formation of In-O bonds and suggests the additional presence of hydroxyl groups and defects. With increasing temperature, the contribution of OH groups and defects decreases whereas that of In-O bonds increases. Notably, higher growth temperatures result in an indium rich phase within the layers.