

O 39: Oxide and Insulator Surfaces: Structure, Epitaxy and Growth II

Time: Tuesday 14:00–16:00

Location: WIL C107

O 39.1 Tue 14:00 WIL C107

NEXAFS and EXAFS structure determination within quasicrystalline barium titanate on Pt(111) — ●ALIREZA BAYAT¹, STEFAN FÖRSTER¹, EVA-MARIA ZOLLNER¹, WOLF WIDDRA^{1,2}, PAULA HUTH³, REINHARD DENECKE³, ANGELIKA CHASSE¹, and KARL-MICHAEL SCHINDLER¹ — ¹Institut für Physik, Martin-Luther-Universität, Halle-Wittenberg, D-06120 Halle, Germany — ²Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle, Germany — ³Wilhelm-Ostwald-Institut, Universität Leipzig, D-04103 Leipzig, Germany

The discovery of an aperiodic barium titanate derived quasicrystalline film on a periodic platinum substrate opened a new field in science and technology [1]. The key point of understanding the physical properties and potential future applications is to determine its geometric structure. EXAFS modulations at the Ti *K*-edge of the BaTiO₃-derived quasicrystal on Pt(111) were recorded and FEFF6 calculations were performed. With respect to the first layer Pt atoms the analysis reveals the Ti in a near 3-fold hollow position with distances in the range of 2.3 - 2.4 Å. The short distances indicate bonding between Ti and Pt and emphasize their relevance for understanding the structure. Furthermore, pre-edge features of the NEXAFS spectrum at the Ti *K*-edge indicate a coordination of Ti by less than 4 O. In line with this, the chemical shift of Ti 2*p* photoemission lines proves that Ti ions exist only in the 3⁺ oxidation state.

[1] S. Förster et al., *Nature*, **502** (2013) 215-218.

O 39.2 Tue 14:15 WIL C107

Epitaxy of ultrathin nickel ferrite films on MgO(001) — ●TABEA NORDMANN, JARI RODEWALD, and JOACHIM WOLLSCHLÄGER — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Nickel ferrite (NiFe₂O₄) crystallizing in the inverse spinel structure is an interesting material for the use in magnetic devices due to its high magnetic permeability, its high Curie temperature of 865 K and its semiconducting property.

Studies on the growth of nickel ferrite by several deposition techniques have already been performed, but the deposition by reactive molecular beam epitaxy (RMBE) has just been studied rarely.

Hence, in this work ultrathin epitaxial films with different Ni/Fe ratios are deposited on MgO(001) via co-evaporation of nickel and iron in an oxygen atmosphere by using RMBE. The surface structure of the films is characterized by low-energy electron diffraction (LEED), while x-ray photoelectron spectroscopy (XPS) is executed to determine the film composition and the oxidation state of iron. Furthermore, x-ray diffraction (XRD) is performed in order to investigate the crystalline quality and the out-of-plane lattice constant of the films. Last, x-ray reflectivity (XRR) is measured to examine the film thickness.

The surfaces of all films with Ni/(Fe+Ni) contents between 7% and 60% are well ordered and the XRD results indicate a single crystalline layer. The XPS results reinforce the formation of nickel ferrite films with Ni contents of about 33% where iron only exists in the Fe³⁺ oxidation state.

O 39.3 Tue 14:30 WIL C107

Influence of Surface Structure on Solid-State Electrochemistry: Oxygen Exchange on SrTiO₃(110) Surfaces — ●MICHELE RIVA¹, MARKUS KUBICEK², XIANFENG HAO^{3,4}, STEFAN GERHOLD¹, GIADA FRANCESCHI¹, MICHAEL SCHMID¹, HERBERT HUTTER², JUERGEN FLEIG², CESARE FRANCHINI³, BILGE YILDIZ^{1,5}, and ULRIKE DIEBOLD¹ — ¹IAP, TU Wien — ²CTA, TU Wien, — ³CMS, Universität Wien — ⁴Dep. Chem. Eng., Yanshan Univ., China — ⁵Lab for Electrochemical Interfaces, MIT, USA

In solid-state electrochemistry, the efficiency for oxygen incorporation of perovskite oxides is interpreted in terms of the availability of surface oxygen vacancies, or the ease of electron transfer. Intriguingly, none of the standard models considers the role of the surface atomic structure. In the present contribution we show that the latter plays a crucial role in affecting oxygen exchange on SrTiO₃. Using a host of surface science techniques (STM, LEED, XPS, etc.) we find that the SrTiO₃(110)-(*n* × 1) and (2 × *m*) surface structures are remarkably stable under realistic conditions for oxygen-exchange reactions. We use two different ion-based spectroscopy techniques to quantify ¹⁸O

exchange and find that the reactivity of these two structures differs by a factor of three. From DFT calculations and electron spectroscopic measurements we rule out that this difference is due to oxygen vacancies or differences in work function or surface potential. Instead our results reveal that the structure itself can determine the extent of the interaction with molecular oxygen, governing the surface reactivity to oxygen exchange reactions of perovskite oxides.

O 39.4 Tue 14:45 WIL C107

Scanned probe surface structure analysis of silicas - then and today — ●GEORG HERMANN SIMON¹, BURKHARD KELL¹, KRISTEN BURSON^{1,2}, MARKUS HEYDE¹, and HANS-JOACHIM FREUND¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — ²Current address: Department of Physics, Hamilton College, 198 College Hill Road, Clinton, NY 13323, USA

Silica and silicate surfaces play an important role in nature and materials applications. They offer a wealth of structures from crystalline quartz [1] via nanoporous zeolite crystals to amorphous silicate glass [2,3]. However, achieving atomic-scale surface science results for these materials has been challenging due to the structural complexity, charging problems common to bulk insulators, and the necessity for well-controlled sample preparations. Ultrathin silica films enable atomic-scale structural characterization and aid the study of bulk quartz and glass surfaces. Such silica films have been shown to exist in crystalline and amorphous modifications [4] which are stable in ultrahigh vacuum, air, and water [5]. Here we present an atomic scale study of ultrathin silica films and bulk silica samples in vacuum and liquid performed using scanning probe microscopy.

[1] F. Bart et al.; *Surf. Sci.* 311 (1994) L671.

[2] Raberg et al.; *J. Non-Cryst. Solids* 351 (2005) 1089.

[3] J.-F. Poggemann et al.; *J. Non-Cryst. Solids* 326-327 (2003) 15.

[4] Lichtenstein et al.; *Angew. Chem. Int. Ed.* 51 (2012) 404.

[5] Burson et al.; *Appl. Phys. Lett.* 108 (2016) 201602.

O 39.5 Tue 15:00 WIL C107

The (O12) surfaces of hematite and their interactions with water - a DFT study — ●MAGDALENA BICHLER¹, FLORIAN KRAUSHOFER², ZDENEK JAKUB², GARETH PARKINSON², and PETER BLAHA¹ — ¹Institute of Materials Chemistry, TU Wien — ²Institute of Applied Physics, TU Wien

Hematite (α-Fe₂O₃) is a promising material for electrochemical water splitting with a suitable bandgap (2.2 eV) and valence band edge position. Moreover, the material is cheap, stable in water and harmless in terms of ecology. Nevertheless, it shows poor electrochemical performance, which might be improved by morphology and surface modifications.

We focus on the (012) surface of hematite (R-cut). Two different types are known. On the one hand, the (1x1) bulk terminated, stoichiometric surface exists, but at low O₂ pressure, a (2x1) reconstruction with missing oxygen atoms is formed. [1]

We carried out ab initio calculations by using the WIEN2k code. [2] In addition, STM, AFM and LEED experiments were done. Based on our DFT calculations, we present a new model of the (2x1) reconstruction, which is energetically more stable than the one that has been proposed so far [3] and agrees with experiment. Furthermore, the surfaces' interactions with water were investigated in both experiment and theory.

[1] M. A. Henderson et al., *Surf. Sci.* 1998, 417, 66-81

[2] <http://www.wien2k.at>

[3] M. A. Henderson, *Surf. Sci.* 2010, 604, 1197-1201

O 39.6 Tue 15:15 WIL C107

Morphology, structure, topological defects, and electronic effects of epitaxial SnTe topological crystalline insulator films — OMUR E. DAGDEVIREN¹, CHAO ZHOU¹, KE ZOU¹, ●GEORG H. SIMON^{1,2}, STEPHEN D. ALBRIGHT¹, MAYRA D. MORALES-ACOSTA¹, XIAODONG ZHU¹, FREDERICK J. WALKER¹, CHARLES H. AHN¹, UDO D. SCHWARZ¹, and ERIC I. ALTMAN¹ — ¹Center for Research on Interface Structures and Phenomena (CRISP), Yale University, New Haven, CT 06520, USA — ²Current Address: Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany

SnTe has been researched in the past as an ingredient in phase change

materials and in the context of infrared detection and thermoelectrics [1]. Moreover, it gained renewed attention for properties of a topological crystalline insulator (TCI), which have been predicted [2,3] and experimentally confirmed for SnTe(100) and (111) surfaces [4]. However, its enormous lattice constant should lead to large misfit epitaxy on most substrates. The resulting defects may or may not be detrimental or even beneficial for TCI properties and their applications. Here we present a surface science characterization of thick, ex situ grown, SnTe(001) films on insulating SrTiO₃(001) [5]. STM and electron diffraction data show morphology and surface structure in detail. Furthermore the growth and post-processing related defect structure as well as surface standing waves are revealed. [1] Zhang et al.: PNAS 110 (2013) 13261. [2] Fu: PRL 106 (2011) 106802. [3] Hsieh et al.: Nat. Comm. 3 (2012) 982. [4] Tanaka et al.: Nat. Phys. 8 (2012) 800. [5] Dagdeviren et al.; Adv. Mater. Interfaces, in press.

O 39.7 Tue 15:30 WIL C107

Plasma-assisted growth of VO₂ on TiO₂(110) and study of its chemical and structural properties — •SIMON FISCHER, JON-OLAF KRISPONEIT, JAN INGO FLEGE, and JENS FALTA — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

With VO₂ exhibiting a temperature-induced metal-insulator transition, thin film growth of this material is of interest for various applications such as switching devices and sensors. The transition is accompanied by a structural change from a monoclinic insulating phase, in which vanadium atoms are dimerized, to a rutile metallic phase. Since a multitude of different vanadium oxides can form, VO₂ growth by molecular beam epitaxy poses challenges in selecting a viable oxidation source and adjusting growth temperature as well as metal-oxygen ratio.

In this study, we have deposited vanadium on TiO₂(110) samples continuously and subjected the sample cyclically to different doses of atomic oxygen from a plasma source. Between growth cycles film thick-

ness as well as vanadium oxidation state was determined from x-ray photoelectron spectroscopy analysis. While atomic oxygen is critical in ensuring VO₂ stoichiometry, apparently high doses of atomic oxygen lead to the formation of a V₂O₅ capping. This observation is supported by ex-situ transport measurements. Furthermore, we discuss different surface reconstructions revealed by low-energy electron diffraction in terms of surface oxygen concentration.

O 39.8 Tue 15:45 WIL C107

Transport along grain boundaries through alumina investigated by atom probe tomography — •TORBEN BOLL^{1,2}, KINGA A. UNOCIC³, BRUCE A. PINT³, and KRYSZYNA STILLER² — ¹Institut für Angewandte Materialien, Karlsruhe Institut für Technologie, 76344 Eggenstein Leopoldshafen — ²Department of Physics, Chalmers University of Technology, SE-412 96 Göteborg, Sweden — ³Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge TN, 37831, USA

It is generally agreed upon that transport through growing alumina scales occurs predominantly due to inward oxygen diffusion along grain boundaries (GBs). However, it is also accepted that there exists some amount of concurrent outward aluminum diffusion along the GBs. Moreover, the effect of alloying elements on oxidation behavior and how they affect diffusional fluxes still remains uncertain.

For this study different Ni-Al alloys with additions of Hf, Y and Zr were investigated. The materials were subjected to an initial exposure in O₂ at 1100°C. The initial exposure was continued again at 1100°C for 5h after a smoothing of the surface. After this double exposure SEM a growth of ridges above the GBs, as an indication for outward diffusion were observed. Scanning transmission electron tomography energy dispersive X-Ray spectroscopy investigations were complemented with atom probe tomography, which gave quantitative information about the concentration of the different elements at the GBs. This helped to calculate the Gibbsian excesses and to discuss the influence of different dopants.