O 89: Oxide and Insulator Surfaces: Structure, Epitaxy and Growth I

Time: Thursday 10:30–13:00 Location: MA 041

O 89.1 Thu 10:30 MA 041

High resolution imaging of ultrathin ZnO layers epitaxially grown on Ag(111) using scanning tunneling hydrogen microscopy — •Shuyi Liu[1], Akitoshi Shiotari[2], Delroy Baugh[3], Martin Wolf[1], and Takashi Kumagai[1] — [1]Department of Physical Chemistry, Fritz-Haber Institute of the Max-Planck Society, Germany. — [2]Department of Advanced Materials Science, Japan. — [3]Department of Chemistry & Biochemistry, University of California, USA.

Ultra-high resolution imaging with a molecular STM/AFM junction has attracted increasing attention as a fascinating tool to resolve submolecular structures of adsorbates [1]. Termirow et al. found that molecular hydrogen in an STM junction can enhance the image contrast of planar organic molecules and proposed the idea of scanning tunneling hydrogen microscopy (STHM)[2]. However, the conductivity and mechanical property of the hydrogen junction are imperfectly understood. We apply STHM to image ultrathin ZnO layers epitaxially grown on Ag(111) and the atomic resolution can be obtained in a reproducible manner. We performed the gap distance-dependent conductance measurement and force spectroscopy using STM/AFM, revealing that the junction consists of multiple hydrogen molecules and the enhanced resolution can be achieved at a specific tip-surface distance. A simplified model with two hydrogen molecules in the junction reproduced the distance dependent conductance, force curve and enhanced imaging of ZnO. [1]P. Jelínek J. Phys.: Condens. Matter 29 343002 (2017). [2]R. Temirov et al. New J. Phys. 10, 053012 (2008).

O 89.2 Thu 10:45 MA 041

VO_2 growth on TiO_2(110) using atomic oxygen — •Simon Fischer, Jens Falta, Jan Ingo Flege, and Jon-Olaf Krisponeit — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

VO_2 thin film growth is of interest for switching devices and sensorics because it exhibits a temperature-induced metal-insulator transition. This is accompanied by a structural change between a monoclinic insulating phase and a rutile metallic phase, allowing for tuning the transition temperature by choice of the substrate: TiO_2(110) as a substrate applies in-plane tensile strain to the rutile *c*-axis and thus increases the transition temperature, favoring the monoclinic phase.

VO_2 growth is challenging in terms of achieving the correct stoichiometry, which is why we used an activated oxygen source. We examined the deposition of 5 to 10 nm of VO_2 on TiO_2(110) in-situ using LEEM and LEED. Additionally, from XPS measurements we determined the stoichiometry by analyzing the chemical shift of the $V2p_{3/2}$ peak and we estimated the film thickness from the attenuation of the substrate peak. High doses of atomic oxygen enable the formation of V_2O_5 domains of random azimuthal orientation, while lower doses lead to oxygen vacancies that impair transition characteristics as observed in ex-situ measurements.

Financial support from the DFG is acknowledged.

O 89.3 Thu 11:00 MA 041

Pulsed laser deposition of In_2O_3 thin films on YSZ(111) — •Michele Riva[1], Giada Franceschi[1], Jakob Hofinger[1], Margareta Wagner[1,2], and Ulrike Diebold[1] — [1]IAP, TU Wien — [2]FAU Erlangen-Nürnberg

In_2O_3 is a wide band-gap, transparent conductive oxide whose applications include optoelectronics, gas sensing, and catalytic fuel production. In all these applications In_2O_3 surfaces and their nanoscale properties play a key role, and atomic-scale investigations to unravel such properties require suitable single-crystalline model systems. However, In_2O_3 single crystals are not commercially available, and synthetically grown ones are usually very small. While this is not critical for scanning probe techniques, area-averaging techniques such as TPD and XPS require larger samples. To this purpose, we have grown well-ordered and atomically flat In_2O_3(111) thin films - with a thickness of a few hundred nanometers - onto YSZ(111) substrates by PLD. Their structure, chemical composition and morphology were characterized by RHEED, LEED, XRD, XPS, AFM, and STM. By optimizing the growth parameters, we could obtain In_2O_3(111) films exhibiting properties comparable to the best single crystals available, exhibiting atomically-flat terraces a few hundred nanometers wide, separated by monoatomic steps. The films behave like In_2O_3 single crystals, down to the atomic scale, and thus allow the combination of atomic-scale surface-science analysis and the investigation of, e.g., the electronic structure and the reactivity of their surfaces via area averaging spectroscopic techniques.

O 89.4 Thu 11:15 MA 041

The stability of ultra-thin ZrO_2 films on a metallic substrate: a challenge for DFT? — Wernfried Mayr-Schmölzer, Jakub Planer, Tobias Hruby, Florian Mittendorfer, and •Josef Redinger — Institute of Applied Physics and Center for Computational Materials Science, TU Vienna, Wiedner Hauptstrasse 8-10/134, 1040 Vienna, Austria

At first DFT calculations for bulk ZrO_2 are performed to assess the accuracy of semi-local, vdW corrected and hybrid functionals as compared to a many-body approach, ACFDT-RPA. Whereas all the functionals reproduce the experimental order of stabilities of known phases, the relative stability of two additionally found meta-stable phases with comparable energies depends on the functional used. For ultra-thin films on metals as grown both on Pt(111) [1] and Rh(111) [2], we investigate the structural stabilities of a suggested tri-layer O-Zr-O film on both substrates. The DFT calculations show that such O-Zr-O trilayers are quite strained on both metals, but they behave differently on Pt or Rh. Obviously, for Rh the tensile stress can be compensated by O-Rh bonds at the interface while this is not working for Pt. For Pt the stress leads to a heavily corrugated O-Zr-O layer not witnessed in experiment. Even the recently developed most advanced SCAN meta-GGA functional, which matches well with our ACFDT-RPA benchmark for bulk ZrO_2, does not cure the problem.

[1] M. Antlanger, et. al., PRB86, 035451 (2012)

[2] P. Lackner and M. Schmid, TU Vienna, work in progress (2017)

O 89.5 Thu 11:30 MA 041

Relaxation effects in VO_2/TiO_2(001) films — •Jon-Olaf Krisponeit[1], Simon Fischer[1], Sven Esser[2,3], Vasily Moshnyaga[3], Jan Ingo Flege[1], and Jens Falta[1] — [1]Institut für Festkörperphysik, Universität Bremen, 28359 Bremen, Germany — [2]Experimentalphysik VI, Universität Augsburg, 86159 Augsburg, Germany — [3]1. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

Bulk vanadium dioxide (VO_2) exhibits a metal-insulator transition at 340 K. On TiO_2(001) substrates, the tensile in-plane stress can be utilized for a reduction of T_{MI} to room temperature due to the compression of the out-of-plane rutile c-axis of VO_2.

Aiming for such epitaxial VO_2/TiO_2(001) films under high coherent strain, potential relaxation effects annihilating stress and/or modifying surfaces and interfaces should be taken into account. Films were prepared by reactive molecular beam epitaxy and metal-organic aerosol deposition. Structural and morphological properties were analyzed by low-energy electron microscopy and diffraction as well as scanning probe microscopy. We discuss three distinct relaxation effects: (i) surface facetting, (ii) the formation of a misfit dislocation network, and (iii) topographic buckling and even crack patterns for thick films.

Support by the Institutional Strategy of the University of Bremen funded by the German Excellence Initiative is acknowledged.

O 89.6 Thu 11:45 MA 041

Strain and ordering effects of ultrathin epitaxial ferrite films on $SrTiO_3$(001) — •Jari Rodewald, Tabea Nordmann, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Ultrathin epitaxial ferrite films as $NiFe_2O_4$ or $CoFe_2O_4$ are in the focus of spintronics since both materials are insulating and ferrimagnetic. Thus, they are well-suited to be used as spin filters due to spin dependent tunneling barrier. Here, the homogeneity of the films is essential to form tunneling barriers. Furthermore, the cation ordering on the different sublattices of the inverse spinel structure determines the magnetic properties of the ferrite films which is crucial for the performance as a spin filter. Therefore, the formation of ferrite films has to be carefully controlled if high quality devices are aimed for.

Hence, in this work ultrathin ferrite films of different thicknesses are prepared via reactive molecular beam epitaxy (RMBE) on

$SrTiO_3$(001). In order to investigate structural strain and ordering effects in the films, synchrotron radiation grazing incidence x-ray diffraction (SR-GIXRD) experiments are performed. The chemical composition and structural ordering at the surface are investigated by x-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED), respectively. Magnetic properties are characterized via superconducting quantum interference device (SQUID) magnetometry.

O 89.7 Thu 12:00 MA 041

A structure analysis of the $BaTiO_3$-derived oxide quasicrystal in physical and internal space — •Sebastian Schenk[1], Stefan Förster[1], René Hammer[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

Recently the formation of $BaTiO_3$-derived and $SrTiO_3$-derived 2-dimensional oxide quasicrystals (OQC) with 12-fold symmetry have been discovered on Pt(111) substrates [1,2]. Both OQCs exhibit a Niizeki-Gähler tiling which is composed by quadratic, triangular, and rhombic elements of equal side length. This tiling can be derived mathematically from cutting a periodic hyperhexagonal structure in the four-dimensional space and project it onto two dimensions, the so-called physical space. Here, we present a detailed analysis of the tiling characteristics as derived from atomically-resolved STM images which represent the physical space dimension. Not only the tiling frequency, but also their orientational distribution is determined to unravel the impact of the underlying periodic substrate to the OQC tiling. Additional information is gained from lifting the atomic coordinates into the four-dimensional hyperspace for a subsequent study of the internal space projection.
[1] S. Förster et al., Nature **502**, 215 (2013)
[2] S. Schenk et al., J. Phys.: Condens. Matter **29**, 134002 (2017)

O 89.8 Thu 12:15 MA 041

In-situ investigations of pulsed-laser-deposited Sr-doped lanthanum manganite thin films — •Giada Franceschi, Michele Riva, Michael Schmid, and Ulrike Diebold — Inst. Appl. Phys., TU Wien, Wiedner Haupstrasse 8-10, 1040 Wien, Austria

Sr-doped lanthanum manganite ($La_{0.8}Sr_{0.2}MnO_3$, or LSM) is a widely used material as a cathode in solid oxide fuel cells, and atomic-scale understanding of the reactions occurring at its surface is interesting from both fundamental and application-driven points of view. Atomic-scale investigations require a well-defined and well-ordered system, but LSM single-crystals are not available commercially. In the present contribution, I will show our efforts towards the establishment of a model system for LSM, in the form of a thin, pulsed-laser-deposited film onto $SrTiO_3$(110) substrates.

Combination of pulsed laser deposition with in situ surface sensitive techniques (STM, LEED, XPS, LEIS) allows to controllably tune the surface composition, and establish a relation with its structure.

O 89.9 Thu 12:30 MA 041

Formation of Transition-Metal-Oxide Chains on Ir(110) — •Tilman Kisslinger[1], Robert Jacob[1], Josef Redinger[2], M. Alexander Schneider[1], and Lutz Hammer[1] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen–Nürnberg, D–91058 Erlangen, Germany — [2]Institut für Angewandte Physik & CMS, TU Wien

Evaporation of 0.5 ML of the 3d transition metals (TM's) Co, Ni and Fe at 100 K onto the unreconstructed Ir(110)–(1×1) surface and oxidation at 920 K leads to the formation of large domains of monatomic chains that are separated by two surface lattice parameters in [001] direction as revealed by STM. For all TM = Co, Ni, Fe similar LEED I(V)–spectra are found indicating the same surface structure. This structure was quantitatively determined for the case of TM = Co (R_P = 0.117) revealing CoO_2 stoichiometry. The TM sits at hollow sites of the first Ir layer and is surrounded by four oxygen atoms being threefold coordinated towards two 3d–TM and one Ir atom. All structural parameters are in close agreement to independently conducted DFT calculations. The structural motif of this system is rather similar to the one found on Ir(100) [1]. However, on Ir(110) the TMO_2 chains do not induce a missing–row reconstruction and thus adsorption sites for possible reaction partners are blocked. This modifies e.g. their reactivity and manifests itself in the higher temperature of 420 K necessary for hydrogen–reduction of the phase on Ir(110), compared to 330 K on Ir(100) [2].
[1]: Ferstl *et al.*, Phys. Rev. Lett. **117**, 4 (2016)
[2]: Ferstl *et al.*, Phys. Rev. B **96**, 085407 (2017)

O 89.10 Thu 12:45 MA 041

A mesoscopic view on ultra-thin germania films on Ru(0001) — •Alexander Fuhrich[1], Thomas Schmidt[1], Dietrich Menzel[1,2], and Hans-Joachim Freund[1] — [1]Department of Chemical Physics, Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany — [2]Physik-Department E20, Technische Universität München, Garching, Germany

The silica bi-layer system on Ru(0001) has been intensely studied by different techniques [1,2]. However, the modification of these ultrathin films by using germanium instead of silicon offers many interesting opportunities for catalysis and the understanding of the growth of ultra-thin semiconductor oxides on metal single crystals. Using spectromicroscopy (LEEM, LEED, XPEEM and XPS), we studied the growth and structures of ultra-thin germania supported on Ru(0001). The growth of germanium and germania on Ru(0001) was observed in real-time and in-situ at mesoscopic scale. The morphology and structure of the Germania films will be discussed in dependence on preparation parameters . The presence of oxygen reduces the diffusion of germanium on Ru(0001). Though deposited in UHV, germanium is partially oxidized by oxygen pre-covered on the Ru surface. The fully oxidized Germania film exhibits a 2x2 structure on Ru(0001) and, up to now, no evidence was found for a vitreous germania phase on Ru(0001) like it is the case for silica.

References 1. H.W. Klemm, G. Peschel, E. Madej, A. Fuhrich, M. Timm, D. Menzel, Th. Schmidt, H.-J. Freund, Surf. Sci. 646, 45-51 (2016) 2. S. Shaikhutdinov, H.-J. Freund, Adv. Mater 25, 49-67 (2013)