O 51: Oxides and insulators: Epitaxy and growth

Time: Wednesday 16:45–19:15 Location: HE 101

O 51.1 Wed 16:45 HE 101

The wurtzite termination of epitaxial CoO(111) films - implications for electronic structure and growth — •Lutz Hammer[1], Pascal Ferstl[1], Matthias Gubo[1], Markus Ostler[2], Thomas Seyller[2], M. Alexander Schneider[1], and Klaus Heinz[1] — [1]Ls. f. Festkörperphysik, Univ. Erlangen-Nürnberg — [2]Ls. f. Techn. Physik, Univ. Erlangen-Nürnberg

Cobalt monoxide films are found to grow on Ir(100) in the polar [111] direction, whereby the outermost subsurface Co layer exhibits a stacking fault altering the local structure from rocksalt- to wurtzite-type [1]. This structural switch renders the surface metallic which is proved both by photoelectron and scanning tunneling spectroscopy (as well as indicated by DFT calculations from the literature [2]). The metallic surface layer allows for the compensation of the film's dipole moment. In contrast, non-polar CoO(100) films, which can be grown on the same substrate via chemical modification of the interface, remain insulating also at the very surface. The latter films are bulk-like terminated and thus can be grown layer by layer, while this is prohibited by the structural switch in case of the (111) oriented films, which can only be produced via re-crystallisation of initially amorphous films.

[1] W. Meyer et al., PRL 101 (2008) 016103; [2] T. Archer et al., PRB 78 (2008) 014431.

O 51.2 Wed 17:00 HE 101

Tuning the growth orientation of epitaxial films by the interface chemistry — •Florian Mittendorfer[1], Josef Redinger[1], Matthias Gubo[2], Christina Ebensperger[2], Wolfgang Meyer[2], Lutz Hammer[2], and Klaus Heinz[2] — [1]TU Vienna, Austria — [2]Univ. Erlangen-Nürnberg, Germany

The support of epitaxial films frequently determines their crystallographic orientation, which is of crucial importance for their electronic and catalytic properties. We have investigated the growth of CoO films on Ir(100) with density functional theory (DFT) calculations, using the Vienna Ab-initio Simulations Package (VASP), in combination with scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) experiments.

The measurements show that the oxide film grows in the (111) orientation on the bare substrate, but the orientation switches to (100) by introducing a single layer of metallic Co between the oxide and substrate. On the basis of the DFT calculations, we find that these different growth modes are triggered by an oxide precursor structure, which is only stable on the Co/Ir(100) surface. The calculations demonstrate that the stabilization of the precursor is not driven by the surface stress, but rather by the chemical modification of the interface. Therefore, this approach offers a new way to change the film orientation without changing the substrate.

O 51.3 Wed 17:15 HE 101

Oxide growth on zinc in different atmospheres — •Ying Chen[1,2], Juan Zuo[3], Paul Schneider[1], and Andreas Erbe[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237, Düsseldorf, Germany — [2]Center for Electrochemical Sciences, Ruhr-Universität Bochum, Bochum, Germany — [3]Department of Mechanical Engineering, Xiamen University of Technology, Xiamen, China

The oxide layer formed on Zn surface in oxidising and non-oxidising humid and dry atmospheres was investigated by spectroscopic ellipsometry (SE) and X-ray photoelectron spectroscopy (XPS). XPS sputter profiles, analysis of the Auger LMM peaks, as well as SE analysis provide strong evidence for the presence of metallic Zn inside the oxide layer [1]. The growth kinetics of the oxide films were measured in a specially designed optical cell. By controlling the growth conditions, such as gas atmosphere (air, argon, oxygen) and humidity, the growth of the oxide layer was studied by in-situ SE measurements over 72 h. It was found that a two-stage growth process of the film is present. Overall growth rate increases in the increasing of the concentration of oxygen in the atmosphere, with a further effect of the presence of humidity. Furthermore, changes in the absorption coefficient indicate changes in electronic structure of the films in the initial phase of the growth, but much faster than the first phase of the thickness increase [2]. REFERENCE: [1] J. Zuo, A. Erbe, Phys. Chem. Chem. Phys., 12 (2010) 11467-11476. [2] Y. Chen, P. Schneider, A. Erbe, Phys. Stat. Solidi C, submitted.

O 51.4 Wed 17:30 HE 101

LEEM/LEED investigation of Fe3O4 thin film growth on a Pt(111) substrate — •Thomas Schmidt, Alessandro Sala, Helder Marchetto, Hagen Klemm, Francesca Genuzio, Shamil Shaikhutdinov, and Hans-Joachim Freund — Fritz-Haber-Institut, Abt. CP, 14195 Berlin

The formation of the Fe3O4 film has been observed in-situ and in real-time by LEEM and LEED, with preparation conditions that differs respect to the established recipe [1]. It has been revealed that an oxidation temperature of 1000 K leads to a dewetting of the magnetite film and the formation of FeO domains upon the step bunches of the Pt(111) surface. A new recipe has been tested for the formation of the thin film: by using a closed magnetite film formed with the canonical recipe as a template, the deposition of Fe at high temperature (above 850 K) and in an O2 atmosphere allows the formation of a more flat and regular thin film, that shows also particular surface structures. By changing in real-time the deposition and oxidation conditions, the film shows different surface structures and reconstructions, detected both in LEEM and LEED. The characterization of these surface phases is discussed. [1] W. Weiss and M. Ritter, Phys. Rev. B 59, 5201 (1999)

O 51.5 Wed 17:45 HE 101

Growth and characterization of hexagonal boron nitride on Cu(111) — •Sushobhan Joshi[1], Willi Auwärter[1], Felix Bischoff[1], David Ecija[1], Saranyan Vijayaraghavan[1], Hermann Sachdev[2], and Johannes V. Barth[1] — [1]Physik Department E20, Technische Universität München, James-Franck Str. 1, D-85748 Garching, Germany — [2]Max Planck Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz, Germany

Monolayer systems as hexagonal boron nitride (h-BN) or graphene can be epitaxially grown on various metal supports and recently attract considerable interest. Here we present a scanning tunneling microscopy (STM) and spectroscopy (STS) study characterizing hexagonal boron nitride (sub)monolayers grown on a Cu(111) surface by thermal decomposition of a borazine precursor. While no h-BN related contrast is observed in topographic images recorded at low bias, Moire patterns emerge at a voltage of about 4 V. Independent on the preparation procedure, we observe the coexistence of such patterns exhibiting different periodicities and orientations. This evidences the formation of various h-BN domains on the surface and thus points to a weak interaction of the h-BN sheet with the underlying Cu(111) lattice. Electronically, the h-BN/Cu(111) system is characterized by an interface state emerging from the Cu(111) surface state. Additionally, ST spectra recorded in the field emission regime indicate a spatially modulated workfunction on h-BN that is reduced in comparison to bare Cu(111). Such local variations of the surface electronic structure influence the formation of molecular assemblies as outlined for the case of porphines.

O 51.6 Wed 18:00 HE 101

In-situ XRD and XRR investigations of the oxidation process in ultra thin praseodymia films on Si(111) — •Henrik Wilkens[1], Sebastian Gevers[1], Marvin H. Zoellner[2], Thomas Schroeder[2], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — [2]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

Due to its high dielectric constant and lattice constant between Ge and Si, praseodymia is an interesting buffer material for system on chip solutions (SOC). To build these praseodymia based systems, a detailed analysis of the various oxidation states and reaction kinetics in thin films is necessary.

Therefore, time-resolved in-situ x-ray diffraction (XRD) and x-ray reflection (XRR) measurements with an in-house built pressure cell were performed at the synchrotron beamlines W1 and P08 at HASYLAB, DESY. The oxidation and reduction process in oxygen atmosphere were studied over a wide pressure range from $1 \cdot 10^{-6}$ mbar to 1 bar and temperatures up to 500° C.

As a first result additional oxidation states in the region between cub-Pr_2O_3 and cub-Pr_6O_{11} were found, which haven't been observed in thin films up to now. Furthermore, the oxygen partial pressure seems to have larger impact on the reached oxidation state than the temperature.

O 51.7 Wed 18:15 HE 101

STM and LEED investigation of a quasicrystalline thin film phase of $BaTiO_3$ on Pt(111) — •Stefan Förster[1], Klaus Meinel[1], Karl-Michael Schindler[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

$BaTiO_3$ is the most studied ferroelectric perowskite which has an easily accessible ferroelectric to paraelectric phase transition at about 400 K. It can be grown epitaxially on Pt(100) and Pt(111) due to its small lattice mismatch of only 2% relative to the substrate. Upon annealing in an oxygen atmosphere well-ordered $BaTiO_3$(100) and $BaTiO_3$(111) thin film phases have been reported [1]. However, here we report on a surprising thin film phase upon annealing in UHV. For 4 ML $BaTiO_3$ on Pt(111), annealing at 1250 K leads to the formation of large three-dimensional islands of bulk-like $BaTiO_3$. Between these islands, the Pt terraces are covered by a remaining $BaTiO_3$ wetting layer.

By means of low-energy electron diffraction (LEED) and scanning tunnelling microscopy (STM) the structure of this wetting layer has been identified to be a 2D quasicrystalline phase of $BaTiO_3$. In LEED this structure shows bright and sharp spots with dodecagonal symmetry. STM reveals that the surface structure is composed by an arrangement of quadratic and triangular building blocks which can explain the 2D quasicrystalline lattice with dodecagonal symmetry.

[1] S. Förster, M. Huth, K.-M. Schindler, and W. Widdra, *J. Chem. Phys. 135*, 104701 **2011**.

O 51.8 Wed 18:30 HE 101

Atomic-scale optimization of homoepitaxial growth of $SrTiO_3$(110) thin film — •Zhiming Wang[1,2], Lin Gu[2], Yuan Yao[2], Jiandong Guo[2], Michael Schmid[1], and Ulrike Diebold[1] — [1]Institut für Angewandte Physik, Technische Universität Wien, Wien 1040, Austria — [2]Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Oxide multilayers display a rich diversity of properties that are different from their constituent materials. To understand the underlying physical mechanisms, it is essential to construct the oxide heterostructures with atomic-scale precision. We study homoepitaxial growth of $SrTiO_3$(110) with oxide molecular beam epitaxy and use scanning tunneling microscopy and transmission electron microscopy for characterization of the films. The $SrTiO_3$(110) surface exhibits a series of reconstructions, (n×1) and (m×8) (with n=4-6, m=2,6), which can be changed reversibly by deposition of Ti or Sr, These reconstructions are clearly observed by high energy electron diffraction at thin film growth temperature. This was used to optimize the Sr to Ti flux ratio in real time. We realized layer-by-layer growth of thin films with a deviation of cation stoichiometry of $< 0.5\%$ revealed by energy dispersive spectroscopy. The surface is always reconstructed and the buried layers transform into stochiometric $SrTiO_3$ during growth. Films prefer to grow along [1$\bar{1}$0] on (n×1) (n=4-6) surfaces, and along [001] on the (2×8) surface. This leads to the formation of nanoscale trenches on surfaces with mixed terminations. This work was supported by the Austrian Science Fund (FWF project F45).

O 51.9 Wed 18:45 HE 101

Morphology and optical properties of Cr-doped MgO films — •Fernando Stavale, Niklas Nilius, and Hans-Joachim Freund — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

MgO thin films doped with varying amounts of Cr have been analyzed from a structural, morphological and optical point of view, using cathodo- and photo-luminescence spectroscopy performed in an STM setup. Whereas at low Cr concentration, the MgO rocksalt structure is maintained, transition to a spinel-like magnesium chromate occurs at higher doping level. Depending on the Cr concentration, several zero-phonon and phonon-mediated emission lines are detected at around 700 nm in the optical spectra, originating from transition within the d-state manifold of the Cr ions. Their wavelength position and intensity provides insight into the local environment of the Cr centers. The development of the phonon sidebands, on the other hand, is governed by the excitation scheme, and the bands become particularly strong for an electronic stimulation of the system. The role of the Stark effect on the band positions is quantified by comparing photo- and cathodo-luminescence spectra performed at different tip-electric fields.

O 51.10 Wed 19:00 HE 101

Density Functional Theory study of ZrO_2 bulk phases and Pt_3Zr-ZrO_2 interfaces — •Wernfried Mayr-Schmölzer, Florian Mittendorfer, and Josef Redinger — IAP and Center of Computational Materials Science, TU Vienna

Zirconium dioxide is a material with many interesting properties, which make it useful for example as a solid electrolyte in solid-oxide fuel-cells or as an oxygen gas sensor.

We present results of DFT calculations with the Vienna Ab-initio Simulation Package of four ZrO_2 bulk modifications and Pt_3Zr-ZrO_2 interfaces using different functionals, namely LDA, PBE, PBEsol and hybrid functionals (HSE). The ZrO_2 phases we studied were the monoclinic $P2_1/c$, the tetragonal $P4_2/nmc$, the cubic $Fm\bar{3}m$ and the orthorhombic $Pnma$ phase. For each functional a structural relaxation of the bulk crystal was done and compared to both earlier calculations and experiments.

To determine the correct interface between a Pt_3Zr substrate and a thin film of zirconium oxide we first had to identify the stacking order of the Pt_3Zr surface termination. A Pt_3Zr crystal forms a hexagonal lattice with an ABAC stacking order. It is known from experiments that steps on the surface are two layers high, but using STM it is not possible to measure whether there is an A-A or a B-C step. Using DFT calculations we were able to identify the termination layer of the crystal. These results were then used to study the interface between a Pt_3Zr substrate and a thin film of zirconium oxide.