

O 59: Oxides and Insulators: Clean Surfaces

Time: Thursday 15:45–18:45

Location: H41

O 59.1 Thu 15:45 H41

Structure of the $(\sqrt{67} \times \sqrt{67})R12.2^\circ$ surface oxide on $\text{Ni}_3\text{Al}(111)$ — ●MICHAEL SCHMID¹, GEORG KRESSE², EVELYN NAPETSCHNIG¹, and PETER VARGA¹ — ¹Institut für Allgemeine Physik, TU Wien, Österreich — ²Institut für Materialphysik, Universität Wien, Österreich

With a unit cell size of 4.16 nm, the surface oxide on $\text{Ni}_3\text{Al}(111)$ is one of the largest well-defined inorganic surface structures known today [1]. We have studied this oxide by high-resolution scanning tunneling microscopy (STM) and obtained atomic resolution of the topmost oxygen layer. This information, together with the building rules of the surface oxide on $\text{NiAl}(110)$ [2] allowed us to build a raw model of the surface oxide, which was refined by density functional theory calculations. Although the structure is oxygen deficient, there are very few sites where the bonding environment of the individual atoms deviates from the rules found on $\text{NiAl}(110)$. The most intriguing structural feature is a regular array of “holes” in the oxide, which explains the excellent properties of the structure as a template for growth of ordered arrays of clusters [3].

[1] S. Degen et al., Surf. Sci. 576, L57 (2005).

[2] G. Kresse et al., Science 308, 1440 (2005).

[3] G. Hamm et al., Nanotechnology 17, 1943 (2006).

O 59.2 Thu 16:00 H41

Disorder and Complexity in the Surface Structure of Alumina on $\text{Ni}_3\text{Al}(111)$ — ●SEBASTIAN GRITSCHNEDER¹, HOLGER SCHNIEDER¹, CONRAD BECKER², KLAUS WANDEL², and MICHAEL REICHLING¹ — ¹Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — ²Inst. für Phys. u. Theo. Chemie, Universität Bonn, Wegelerstraße 12, 53115 Bonn, Germany

An alumina surface with several outstanding properties is that of a thin film grown on the (111) surface of a Ni_3Al substrate. The dominant phase of this oxide film has early been identified as an excellent template for the controlled growth of nanostructures. Templating on the alumina film is facilitated by a dot and a network super-structure that can readily be prepared but have not been understood at the atomic scale. By dynamic force microscopy, we reveal that this phase is build up from a hexagonal lattice of 0.29 nm periodicity, that is commensurate to the aluminum sub-lattice of the substrate. The complex interaction between oxide film and substrate leads to the formation of the two super-structures. By comparison of highly resolved images of the dominant phase with images of another phase of the oxide film, we reveal that their basic structural elements are identical, and therefore we speculate that different substrate conditions are responsible for the adoption of either of the phases.

O 59.3 Thu 16:15 H41

Self-Assembled Sub-Surface Oxygen Vacancy Arrays on Reduced $\text{CeO}_2(111)$ — ●STEFAN TORBRÜGGE¹, MICHAEL REICHLING¹, SEIZO MORITA², and OSCAR CUSTANCE² — ¹Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany — ²Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita, Osaka, Japan

In this contribution, we present atomic resolution dynamic scanning force microscopy (SFM) measurements of the reduced $\text{CeO}_2(111)$ surface performed at 80 K. We have been able to clearly recognize surface and sub-surface oxygen vacancies and to corroborate the topographic heights predicted by previous theoretical calculations [1,2]. A detailed structural analysis of these two types of oxygen vacancies, as well as other surface defects, is presented. We found that some terraces of the prepared $\text{CeO}_2(111)$ surface are dominated by sub-surface oxygen vacancies. By the combined analysis of two complementary SFM signals, namely topography and dissipation, we are able to clearly locate each sub-surface oxygen vacancy. Our findings suggest that sub-surface oxygen vacancies do not cluster together but tend to self-assemble in ordered arrays leading to a (2x2) locally reconstructed surface. Thus, we present experimental evidences that single sub-surface vacancies, ordered in arrays at high concentration, are energetically more favorable than sub-surface vacancy clusters.

[1] F. Esch et al., Science 309, 752 (2005)

[2] S. Fabris et al., J. Phys. Chem. B 109, 22860 (2005)

O 59.4 Thu 16:30 H41

Stability, atomic and electronic structure of reduced $\text{Fe}_3\text{O}_4(111)$ surfaces — ●MARKUS PAUL¹, MICHAEL SING¹, DAVID SCHRUPP², RALPH CLAESSEN¹, and VICTOR BRABERS³ — ¹Lehrstuhl für Experimentelle Physik IV, Universität Würzburg, Germany — ²Lehrstuhl für Experimentalphysik II, Universität Augsburg, Germany — ³Department of Physics, Eindhoven University of Technology, The Netherlands

Polar faces of ionic materials present a challenge for the determination of the atomic structure. Underlying difficulties are the relative stability and variability of such surfaces which can cause a poor reproducibility in the experiment or the coexistence of different structures on the same surface. In this work Magnetite(111) single crystal surfaces have been studied by STM, LEED and XPS under different *in situ* preparation conditions and stoichiometries, accordingly. The coexistence of several surface structures has been detected confirming only small differences in their relative stabilities. An unusual superstructure has been found for a reduced Fe_{1-x}O -like surface layer. It is explained as originating from elastic strain formation due to lateral mismatch between Fe_3O_4 substrate and Fe_{1-x}O -like overlayer.

O 59.5 Thu 16:45 H41

Stabilization of thin ZnO films by surface depolarization — ●CHRISTIAN TUSCHE, HOLGER L. MEYERHEIM, and JÜRGEN KIRSCHNER — MPI für Mikrostrukturphysik Halle, D-06120 Halle, Germany

Heterostructures of the oxide semiconductor ZnO attracted interest for application in ultra violet laser diodes and spintronic devices. Theoretical predictions rely on detailed information on the film and interface structures. Scanning tunneling microscopy (STM) and surface x-ray diffraction (SXRD) was used to study morphology and structure of ultra thin ZnO films on $\text{Ag}(111)$.

ZnO films, 0.3 to 5 monolayers (ML) in thickness, were grown by pulsed laser deposition in 10^{-7} mbar O_2 atmosphere on $\text{Ag}(111)$ at 300 K, followed by annealing at 680 K. SXRD indicates that the film is (0001) oriented, and the hexagonal lattice vectors are aligned parallel with the $\text{Ag}(111)$ surface. While single crystal (0001) or (000 $\bar{1}$) surfaces are polar, and extended flat regions (> 10 nm) are not stable, the 2 ML thick ZnO films form a flat double-layer over the whole surface.

Stabilization is achieved by a transition of the Wurtzite- towards a graphite like structure with reduced polarity, i. e., O ions move to the plane of Zn ions: SXRD shows an in-plane expansion of the ZnO lattice by 1.6% compared to bulk (3.30 Å vs. 3.25 Å), corresponding to a 7/8 coincidence with the Ag substrate (Ag: 2.89 Å). In parallel, Zn-O bonds (bulk: 1.97 Å) within the hexagonal plane shorten to 1.92 Å and intra-plane Zn-O bonds expand to 2.20 Å. The ions change their four-fold coordination (Wurtzite structure) to a three-fold one.

O 59.6 Thu 17:00 H41

Identification of reactive oxygen sites at surfaces of MoO_3 by polarization-resolved NEXAFS spectra: theoretical studies — ●MATTEO CAVALLERI and KLAUS HERMANN — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

The identification of reactive oxygen sites at metal oxide surfaces and the characterization of their physical properties is of great importance for an understanding of the catalytic activity of such materials and, thus, for a rational design of more efficient and selective catalysts. Here we evaluate Near-Edge X-Ray Absorption Fine Structure (NEXAFS) spectra, based on density functional theory and appropriate surface clusters, to study and discriminate non-equivalent oxygen centers present at surfaces of catalytically relevant molybdenum oxides. For the (010) surface of bulk MoO_3 this technique is able to unambiguously distinguish between singly coordinated molybdenyl oxygen covering the topmost molybdenum layers and other oxygen centers of similar local environment, differing only by their spatial orientation in the crystal. Theoretical predictions are also successfully used to identify and interpret characteristic features in the NEXAFS spectrum that arise from defects and oxygen vacancies¹. Upon comparison between measured and computed NEXAFS spectra for different photon polarization directions it is also possible to validate proposed structures of thin MoO_3 films at the $\text{Au}(111)$ surface.

¹ M. Cavalleri, K. Hermann, S. Guimond, Y. Romanyshyn, H. Kuhlbenck and H.-J. Freund, submitted to Cat. Today (2006)

O 59.7 Thu 17:15 H41

Lattice Dynamics of RuO₂: Bulk and (110) Surface — •KLAUS-PETER BOHNEN¹, ROLF HEID¹, and OMAR DE LA PENA SEAMAN² — ¹Forschungszentrum Karlsruhe, Institut für Festkörperphysik — ²Department of Applied Physics, CINVESTAV-Mérida, Yucatán, Mexico

Although RuO₂ has been studied as a prototype catalyst for CO oxidation no careful study of the lattice dynamics for this material has been presented so far. Using modern ab-initio methods we obtain the phonon dispersion and the generalized density of states (GDOS). Inelastic neutron scattering experiments allow for an experimental determination of the GDOS. In contrast to what is known from structural studies, we find that the local density approximation gives a much better description of the phonon spectrum than the generalized gradient corrected form. This is also consistent with Raman measurements. Besides the bulk we have also studied the lattice dynamics for the (110) surface. Unfortunately, no complete experimental phonon study of this surface has been carried out so far, however, our results are consistent with the available experimental information. These calculations allow for the first time for the determination of the bulk and surface part of the phononic contribution to the free energy, a quantity which is essential for the determination of thermodynamic properties.

O 59.8 Thu 17:30 H41

Tensor LEED study of the dynamics of the NaCl(100) surface — •JOCHEN VOGT — Chemisches Institut der Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

A wealth of theoretical studies dealt with the dynamics of the NaCl(100) surface, e.g. in relation to its melting behaviour, friction, or the simulation of image contrast in atomic force microscopy. Accurate experimental information on the temperature dependent vibrational amplitudes of ions in different layers is missing so far, although it could serve as a critical test for the various potential models applied to this prototype material. This contribution reports LEED experiments at various temperatures between 25 K and 300 K, in which beam intensities were recorded as a function of electron energy. The experimental I(E) data were analyzed using the tensor LEED approach. At all investigated temperatures the NaCl(100) surface exhibits the same relaxation, characterized by a static inward shift of the topmost Na⁺ ion of 0.09±0.03Å. The dynamics of the topmost layer is significantly higher than those of the second layer, where the measured amplitudes are close to literature bulk values. Above 100 K, Na⁺ and Cl⁻ ions in the topmost layer have nearly the same amplitudes, while the amplitudes of the cations in the second layer are larger than those of the anions. In this temperature range the mean square amplitudes of the ions at the surface are in good agreement with previously reported lattice dynamics studies.

O 59.9 Thu 17:45 H41

Photon Mapping of MgO thin Films with an STM — •HADJ-MOHAMED BENIA, NIKLAS NILIUS, and HANS-JOACHIM FREUND — Fritz-Haber-Institut der MPG, Berlin

The light emission from an STM junction consisting of an MgO thin film on Mo(001) and an Au tip is analysed with respect to its spatial distribution for various excitation conditions. The spectral characteristic of the light is compatible with an emission mechanism mediated by tip-induced plasmons that are excited by inelastic tunnel processes involving field emission resonances in the tip-sample gap. For MgO islands of distinct topographic height, the local emission yield can be tuned by changing the sample bias. This interrelation reflects the dependence of field emission resonances on the MgO work function, which in turn is a function of the number of MgO layers covering the Mo support.

O 59.10 Thu 18:00 H41

Structural and electronic properties of bulk earth alkali oxides and their surfaces — •BJÖRN BAUMEIER, PETER KRÜGER, and

JOHANNES POLLMANN — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Earth alkali oxides play a vital role in a number of technological applications, most prominently as supports in catalysis.

While structural properties of BeO, MgO, CaO, SrO and BaO are quite well described within the local density approximation of density functional theory, the calculated electronic structure suffers from well-known shortcomings, most noticeably the significant underestimate of the band gap and conduction band energies. We present results of DFT calculations using self-interaction-corrected (SIC) pseudopotentials for the aforementioned earth alkali oxides. Bulk electronic properties are in very good agreement with experimental data and – where available – with results of considerably more elaborate quasiparticle calculations. To investigate the properties of nonpolar low-index surfaces of these oxides we apply the very same SIC pseudopotentials and find that the SIC effect on the surface is comparable to that on the bulk electronic structure. The surface bandstructure of MgO(001) resulting within the SIC approach is practically identical to the one resulting from GWA calculations, while the required computational effort in SIC remains at the LDA level. We infer from this good agreement for MgO(001) that our calculations for the other earth alkali oxide surfaces are of similar quality. These results constitute a solid quantitative basis for further studies, e.g., for investigations of optical spectra or adsorbate systems.

O 59.11 Thu 18:15 H41

Imaging the muscovite mica surface by means of high resolution dynamic scanning force microscopy — •FRANK OSTENDORF, CARSTEN SCHMITZ, SABINE HIRTH, and MICHAEL REICHLING — Fachbereich Physik, Barbarastrasse 7, 49076 Osnabrück

Muscovite mica is a widespread substrate for many applications, for instance in biology and material science. Mica is famous for its large atomically flat terraces after cleavage and its atomic scale structure has been studied by dynamic force microscopy performed in a liquid environment [1]. We investigated air and UHV cleaved mica surfaces in detail by a dynamic force microscope operated in the non-contact mode under ultra-high vacuum conditions. We adapted several appropriated recipes for air cleaved mica preparation techniques from the literature and varied two major parameters, namely degassing temperature and degassing period. It has been found that none of the recipes leads to a true atomically flat and clean surface, even after degassing the sample for several hours at temperatures above 500 Kelvin. On regularly shaped flat nanostructures found on the surface, two different types of atomic scale patterns were observed.

[1] Fukuma T. et al. Appl. Phys. Lett. 87 (2005) 034101

O 59.12 Thu 18:30 H41

Band mapping the ZnO(11 $\bar{2}$ 0) surface by angle-resolved photoelectron spectroscopy — •STEFAN ANDRES, CHRISTIAN PETTENKOFER, WOLFGANG BREMSTELLER, and JOACHIM WIDER — Hahn-Meitner-Institut GmbH, Berlin, Deutschland

Zinc oxide (ZnO) is a transparent, piezoelectric semiconductor. Its large band gap of about 3.4eV and high exciton binding energy of about 60meV render ZnO an interesting material for optoelectronic devices in the UV-regime. Furthermore the piezoelectric properties can be utilized in SAW-devices.

Recent studies have shown that the ZnO(11 $\bar{2}$ 0) surface is a promising candidate for such devices.

We present angle resolved photoemission data from an in-situ cleaved, (11 $\bar{2}$ 0) oriented ZnO single crystal as well as from epitaxially grown thin ZnO(11 $\bar{2}$ 0) films. The spectra were recorded at the TGM7 beamline at BESSYII synchrotron light facility in Berlin.

It is shown, that the surface electronic structure of both the epitaxially thin films and the single crystal coincide with each other. The band dispersion along k_{\perp} and k_{\parallel} is discussed in accordance with theoretical band structure calculations.

For the $\bar{\Gamma} - \bar{X}'$ direction a new band, centered at \bar{X}' is observed which is tentatively assigned to a surface-Umklapp process.