

O 43: Clean surfaces III

Time: Wednesday 10:30–13:00

Location: MA 043

O 43.1 Wed 10:30 MA 043

STM and STS study of SrRuO₃(001) thin films on SrTiO₃(001) — ●MARTIN TRAUTMANN¹, DIETRICH HESSE², IONELA VREJOIU², and WOLF WIDDRA^{1,2} — ¹Institut für Physik, Martin-Luther-Universität Halle-Wittenberg — ²MPI für Mikrostrukturphysik, Halle/S.

For applications in oxide-based electronic devices such as ferroelectric heterostructures and non-volatile ferroelectric random access memories the electrode material plays an important role. In this context SrRuO₃ has drawn significant attention due to its high conductivity and low lattice misfit with many functional perovskites. In this study a 40 nm thick PLD grown film of orthorhombic SrRuO₃ on SrTiO₃(001) has been characterized by LEED, AFM, STM and STS. Upon heating to 400°C in 10⁻⁵ mbar of oxygen the film exhibits a well-ordered pseudocubic SrRuO₃(001)-(1x1) LEED pattern. The observed surface morphology as determined by STM is characterized by small vacancy islands as has been reported also earlier [1]. Annealing to higher temperatures in an increased O₂ atmosphere leads to a rearrangement of the vacancy islands in the high symmetry directions. STS on this SrRuO₃(001) surface is dominated by a well-resolved unoccupied density-of-states feature at 2.5 eV above E_F which is assigned to an unoccupied Ru 4d state on the basis of DFT calculations [2].

[1] H. N. Lee, H. M. Christen, M. F. Chisholm, C. M. Rouleau, and D. H. Lowndes, Appl. Phys. Lett. **84**, 4107 (2004)

[2] J. M. Rondinelli, N. M. Caffrey, S. Sanvito, and N. A. Spaldin, Phys. Rev. B **78**, 155107 (2008)

O 43.2 Wed 10:45 MA 043

Ultrathin zirconia films on Pt₃Zr — MORITZ ANTLANGER, JIŘÍ PAVELEC, PETER VARGA, ULRIKE DIEBOLD, and ●MICHAEL SCHMID — TU Wien, Austria

Zirconium dioxide (ZrO₂) has numerous applications, from high-performance ceramics for engineering and dentistry to gas sensors and solid-oxide fuel cells (SOFC). Its performance in sensors and SOFCs is based on its high bandgap (≈ 6 eV), which implies a low electronic conductivity even at high temperatures where it becomes an ionic conductor. This excludes many charged-particle techniques such as scanning tunneling microscopy (STM) for the study of bulk ZrO₂. We have therefore produced ultrathin zirconia films by oxidation of a Pt₃Zr alloy single crystal and determined their surface structure and properties by STM. The ultrathin film consists of a single O-Zr-O trilayer, exhibits a bandgap, and is remarkably stable. The interface structure between the ultrathin oxide and the substrate is analyzed from STM measurements and shows a reconstructed Pt layer. The surface is oxygen-terminated and almost defect-free, yet the surface diffusivity of Pd on the ZrO₂ film is much lower than on oxygen-terminated alumina surfaces.

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O 43.3 Wed 11:00 MA 043

Electronic structure and formation energies of neutral and charged O vacancies at MgO (100) and (111) surfaces: Exchange-correlation effects — ●NORINA A. RICHTER, SERGEY V. LEVCHENKO, and MATTHIAS SCHEFFLER — Fritz Haber Institute of the Max Planck Society, 14195 Berlin, Germany

Surface O vacancies (F-centers) can strongly influence catalytic properties of MgO and metal clusters supported on MgO, but the experimental determination of their concentration at catalytic conditions is difficult. We employ density-functional theory and the *ab initio* atomistic thermodynamics approach to determine concentration and charge states of F-centers at (111) and flat and stepped (100) surfaces of MgO at realistic (*T*, *p*) conditions. Slab models and the virtual-crystal approximation [1] are used to model charged defects at surfaces. We find a strong dependence of F⁺ and F²⁺ formation energy on the exchange-correlation (XC) functional. Varying the amount of screening and fraction of exact exchange within the HSE functional, we find a linear correlation between defect formation energies and calculated valence-band width of the host material, in line with recent results for bulk systems [2]. Using this correlation and extrapolating to experimental band width, we conclude that only F²⁺ centers can be present in significant concentrations at the (100) terraces at realis-

tic conditions. — [1] L. Vegard, Z. Phys. **5**, 17 (1921); M. Scheffler, Physica **146B**, 176 (1987); [2] R. Ramprasad, H. Zhu, P. Rinke, and M. Scheffler, *subm. to Phys. Rev. Lett.*

O 43.4 Wed 11:15 MA 043

Structure and polarity of step edges on (111) surfaces of fluorite type crystals — ●HANS HERMANN PIEPER¹, MICHAEL REICHLING¹, and CLEMENS BARTH² — ¹Universität Osnabrück, Germany — ²CINaM-CNRS, Marseille, France

The morphology and polarity of step edges found on CaF₂ and CeO₂ (111) is investigated by non-contact atomic force microscopy (NC-AFM) and Kelvin probe force microscopy (KPFM). The macroscopic shape of step edges strongly depends on sample preparation, however both materials exhibit type I and II facets at the nanoscale.

While type I steps are neutral, KPFM reveals a positive local charge at type II steps. Different models for the origin and the compensation of the charge are suggested. On CaF₂ the positive charge is compensated by subsurface fluorine ions on interstitial sites while for CeO₂ oxygen is released leaving behind Ce³⁺ sites located on step edges.

O 43.5 Wed 11:30 MA 043

Fe-rich terminations and the role of subsurface charge order at the Fe₃O₄(001) surface — ●ZBYNEK NOVOTNY, GARETH S. PARKINSON, ZOLTAN EDES, MICHAEL SCHMID, and ULRIKE DIEBOLD — Institute of Applied Physics, TU Wien, Vienna, Austria

Magnetite, Fe₃O₄, crystallizes in the inverse spinel structure with an fcc oxygen sublattice and Fe cations in tetrahedral (A) and octahedral (B) sites. The (001) surface exhibits undulating rows of Fe(B) atoms with two unoccupied Fe(A) bulk continuation sites in the 'narrow' and 'wide' regions of the unit cell, related to Fe²⁺/Fe³⁺ subsurface charge ordering [1,2]. We present a route to produce a reduced, well-ordered Fe₃O₄(001) surface by evaporating Fe on the distorted Fe(B) surface at room temperature. STM shows that this surface contains Fe(A) monomers and Fe clusters. Mild annealing of the sample leads to a surface containing Fe(A) monomers and, with increasing Fe coverage, dimers of 5-fold coordinated Fe. Both surfaces contain Fe adatoms located at the 'narrow' position within the unit cell, indicating a strong preference for sites located above Fe²⁺ cations in the subsurface layer.

This material is based upon work supported as part of the Center for Atomic-Level Catalyst Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number #DE-SC0001058.

[1] R. Pentcheva et al., Phys. Rev. Lett. **94**, 126101 (2005).

[2] Z. Łodziana, Phys. Rev. Lett. **99**, 206402 (2007).

O 43.6 Wed 11:45 MA 043

2D Scanning Force Spectroscopy on Organic Layer Crystals — ●MATTHIAS SCHULZENDORF¹, GREGOR FESSLER¹, SHIGEKI KAWAI¹, THILO GLATZEL¹, SHI-XIA LIU², and SILVIO DECURTINS² — ¹Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — ²Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, 3012 Bern, Switzerland

Bis(benzylammonium)bis(oxalato)cuprate(II) is a layered organic bulk crystal. Previous work on this crystal compound indicated that the crystal exhibits a friction anisotropy depending on the molecular structure. To further study the dependence of surface features and molecular composition the crystal was probed by non contact scanning probe microscopy in ultra high vacuum at room temperature. By means of molecular tracking, multiple series of 2D force maps were performed along the [100] crystal axis. The background of a second minimum in the extracted interaction force curves, revealed by our measurements, will be analyzed and discussed.

O 43.7 Wed 12:00 MA 043

Structure of V₂O₃ films on Au(111) — ●ERIC MEYER, JAN SEIFERT, and HELMUT WINTER — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin

In recent studies Window et al. [1] have reported on the surface termination of thin V₂O₃ films grown on Au(111). Measurements reveal a reconstructed trilayer with O₃-termination in accord with DFT-calculations. This is in conflict with a complete monolayer of vanadyl

species found by other groups [2].

In this work we present studies on the V_2O_3 surface via scattering of fast atoms under grazing angles of incidence. The measurements are compared with trajectory computer simulations in which electron emission is incorporated for both structural models.

We find clear evidence for the reconstructed trilayer structure. Excellent agreement between experiment and simulation is found so that we can confirm a O_3 termination with slightly modified positions of topmost O atoms compared to [1].

[1] Window et al., Phys. Rev. Lett. 107, 016105 (2011)

[2] Dupuis et al., Surf. Sci. 539, 99 (2003)

O 43.8 Wed 12:15 MA 043

Exploring highly correlated materials via electron pair emission — •LUCIE BEHNKE, FRANK O. SCHUMANN, CHANG-HUI LI, and JÜRGEN KIRSCHNER — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

Metal oxides like NiO are usually termed "highly correlated", because the material properties are decisively determined by the electron-electron interaction. This makes them interesting candidates for electron pair spectroscopy which is particularly sensitive to the electron correlation. We have prepared ultrathin NiO/Ag(100) films and studied the electron pair emission upon electron impact. Compared to metallic Ni we observe an increase of the coincidence intensity by a factor 8-10 for NiO. Thickness dependent measurements prove that this enhancement is an intrinsic effect rather than due to an increased mean free path for NiO. The Neel temperature T_N of NiO films is thickness dependent which allows to tune T_N . We performed temperature dependent measurements for various thicknesses and observed no temperature variation of the coincidence intensity. This proves that the electron pair emission probes the local correlation rather than long-range order. We discuss the prospect of a quantitative characterization of the electron correlation via pair emission spectroscopy.

O 43.9 Wed 12:30 MA 043

Atomistic modeling of electromechanical coupling at metal surfaces — •ANJA MICHL^{1,2}, JÖRG WEISSMÜLLER^{2,3}, and STEFAN MÜLLER¹ — ¹Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany — ²Institute of Materials Mechanics, Helmholtz Zentrum Geesthacht, Geesthacht, Germany — ³Institute of Materials Physics, Hamburg University of Technology, Hamburg,

Germany

Designing functional materials with well-defined catalytic properties requires understanding of the relation between surface structure and reactivity. Electrochemical experiments on pseudomorphic Pd monolayers have revealed the importance of strain for the catalytic activity of metal surfaces. Although the strain response of the electrode potential $\delta E/\delta e$ has been measured for several materials, fundamental understanding of the underlying microscopic processes is far from complete. The variation of the potential of zero charge of an electrode surface in electrolyte is closely linked to the variation of the work function W in vacuum. In order to get further insight, we focus on simple s-p-bonded metals as they connect most readily to theory. We present density functional theory calculations of W for aluminum surfaces for varying tangential strain e which allow the determination of $\delta W/\delta e$ from first-principles. Interestingly, the response parameter is found to be positive in contrast to the negative values reported for e.g. Au experimentally and theoretically. We decompose the work function into a volume and a surface contribution and discuss the response of these contributions in the framework of the Jellium model.

O 43.10 Wed 12:45 MA 043

Dichroism in double photoemission from a Cu surface — ZHENG WEI¹, •FRANK O. SCHUMANN¹, GIANLUCA DIFILIPPO², GIOVANNI STEFANI², and JÜRGEN KIRSCHNER¹ — ¹Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany — ²Dipartimento di Fisica, Università Roma Tre, Rome, Italy

We performed a double photoemission (DPE) experiment with circular polarized light on a Cu(001) surface. The photon energy was chosen to be 125 eV leading to comparable kinetic energies of the 3p photo electron and related Auger electron. We find that the coincidence spectra display circular dichroism while the singles spectra are helicity independent. Usually the emergence of an Auger electron is explained via a two-step process in which the relaxation leading to the Auger emission is preceded by the emission of a photoelectron. This is at odds with a continuous energy sharing [1] and the observation of dichroism in the coincidence spectra only. Our observation can only be explained within a single-step process.

[1] G. van Riessen, Z. Wei, R. S. Dhaka, C. Winkler, F. O. Schumann and J. Kirschner, J. Phys.:Condens. Matter **22**, 092201 (2010).