O 36: Surfaces and Films: Forces, Structure and Manipulation

Time: Tuesday 14:15–16:45 Location: MA 041

O 36.1 Tue 14:15 MA 041

Low-Temperature STM Study of the $(\sqrt{3} \times \sqrt{3})30°$ Reconstructed Ni_2P (0001) Surface - Atomic Resolution and Geometric Model — •Georg Hermann Simon[1], Thomas König[1], Markus Heyde[1], Hans-Joachim Freund[1], Kumiko Kinoshita[2], Yuta Nakagawa[2], Shushi Suzuki[2], and Kiyotaka Asakura[2] — [1]Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, D-14195 Berlin, Germany — [2]Catalysis Research Center, Hokkaido University, Sapporo 001-0021, Japan

New catalysts have to be found to follow the demanding legislation around the world for the reduction of sulfur contents in transportation fuels. A promising candidate is Ni_2P [1], which is fairly new to surface science. Despite several wet-chemical studies, simulation, spectroscopic and the first room-temperature STM characterization [2] there are many open questions to this material. In surface studies (0001) oriented single crystals have been analyzed so far. In our ultrahigh vacuum low-temperature STM study we worked on a deeper understanding of the surface termination, its preparation and mircostructure. We present atomically resolved images of a previously unreported $(\sqrt{3} \times \sqrt{3})30°$ reconstruction of the (0001) surface. We put forward considerations for a geometrical model that is being developed in our cooperation based on the Ni_3P_1 termination of Ni_2P (0001).

[1] X. Wang, P. Clark, S.T. Oyama, J. Catal. 208 (2002) 321.
[2] M.G. Moula, S. Suzuki, W.-J. Chun, S. Otani, S.T. Oyama, K. Asakura, Surf. Interface Anal. 38 (2006) 1611.

O 36.2 Tue 14:30 MA 041

Force measurement with a scanning tunneling microscope — •Kai-Felix Braun[1,2] and Saw-Wai Hla[2] — [1]Physikalisch Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig — [2]Clippinger Laboratories, Ohio University, Athens, Ohio 45701, USA

We present a method to measure the interaction force between single atoms with a scanning tunneling microscope [1]. During experiments for atomic manipulation with a scanning tunneling microscope the tip height curve is recorded. It is shown here that the amplitude of the manipulation curve is a measure for the interaction force between the microscopes tip and a single atom adsorbed on a surface. A simple formula is derived and tested. Extensions of this scheme to different surfaces shall be discussed.

[1] K.-F. Braun and S.W. Hla, Physical Review B 75 (2007), 033406

O 36.3 Tue 14:45 MA 041

The Force to Move an Atom — •Markus Ternes[1], Christopher P. Lutz[1], Cyrus F. Hirjibehedin[1], Franz J. Giessibl[2], and Andreas J. Heinrich[1] — [1]IBM Research Division, Almaden Research Center, San Jose, USA — [2]Institute of Experimental and Applied Physics, University of Regensburg, Regensburg, Germany

Atomic manipulation of single atoms and molecules by scanning probe microscopy enables the assembly of structures at the single-atom scale – the ultimate lower size limit. However, it has been difficult to answer the simple question: How much force does it take to manipulate atoms and molecules on surfaces? To address this question, we used a combined atomic force and scanning tunneling microscope to simultaneously measure the force and the current between an adsorbate and a tip during atomic manipulation.

We found that the force it takes to move an atom depends crucially on the binding between adsorbate and surface. Our results indicate that for moving metal atoms on metal surfaces, the lateral force component plays the dominant role. In contrast, we found that the forces to manipulate molecular adsorbates, such as carbon monoxide (CO), were markedly different.

Measuring the forces during manipulation yielded the full potential energy landscape of the tip-sample interaction. Surprisingly, the potential energy barriers are comparable to diffusion barriers, which are obtained in the absence of a probe tip.

O 36.4 Tue 15:00 MA 041

Lateral Resolution in Piezoresponse Force Microscopy — Tobias Jungk, Akos Hoffmann, and •Elisabeth Soergel — Institute of Physics, University of Bonn, Wegelerstrasse 8, 53115 Bonn, Germany

Among the methods for visualization of ferroelectric domains piezoresponse force microscopy (PFM) has become a very common technique mainly due to its high lateral resolution without any need for specific sample preparation. Although domain structures are easily imaged with this method, the lateral resolution and thus the observed domain wall width is still under discussion. The reported values for the width of 180° domain walls scatter noticeably. These inconsistencies can be explained by the PFM background inherent to the experimental setup that can broaden the observed domain wall widths. In this contribution, we present a quantitative study of the resolution in PFM depending on the tip radius, the type of sample and the thickness of the sample. For bulk single crystals the measured linear dependency of the width of the domain wall on the tip radius using PFM is validated by a simple theoretical model. Independent on the crystal type (BaTiO3, KNbO3, KTP, LiNbO3, LiTaO3, PGO and SBN) the same lateral resolution was measured. Using a Ti-Pt-coated tip with a nominal radius of 15 nm the so far highest lateral resolution in bulk ferroelectric crystals of only 17 nm was obtained.

O 36.5 Tue 15:15 MA 041

Morphology and electronic structure of epitaxially grown $CuInS_2$ films — •Carsten Lehmann[1], Volker Eyert[2], and Christian Pettenkofer[1] — [1]Hahn-Meitner-Institut, SE6, Berlin, Germany — [2]Universität Augsburg, Inst. f. Physik, Augsburg, Germany

The ternary compound semiconductor $CuInS_2$ with a direct band gap of 1.53 finds application as absorber material in modern thin film solar cells. For a better understanding of the parameters determining the properties of a junction detailed information on the electronic structure is necessary. We report on ARUPS measurements on thin epitaxial $CuInS_2$ films prepared on sulfur passivated GaAs(100) and GaAs(111)B. Samples were prepared in a combined UHV GSMBE deposition and analysis system with an organic sulfur precursor. The bandstructure mapping was performed at the beamline TGM7 at BESSY II. The experimentally obtained electronic structure for $CuInS_2$(001) shows good agreement with augmented spherical wave (ASW) calculations based on density functional theory (DFT) and the local density approximation (LDA). For $CuInS_2$(112) films deposited on GaAs(111)B substrates we observe a LEED pattern with a sixfold symmetry which is not in accordance with a simple chalcopyrite (112) structure. We will discuss the observed structure within a domain model of the surface and its implications on our obtained spectra.

O 36.6 Tue 15:30 MA 041

3D force field measurements using non-contact atomic force microscopy on KBr: Theory and Experiment — •Kai Ruschmeier[1,2], Regina Hoffmann[3], and André Schirmeisen[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Wilhelm-Klemm Str. 10, 48149 Münster — [2]CeNTech, Center for Nanotechnology, Heisenbergstr. 11, 48149 Münster — [3]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe

Atomic force microscopy is capable of characterizing surfaces with atomic resolution. Here, we use an ultrahigh vacuum atomic force microscope in non-contact mode to measure the three-dimensional force field [1,2] of a KBr(001) surface at room temperature. On a predefined grid we measure the force distance curves over a wide range of tip-sample distances, from attractive to repulsive forces. Atomic resolution surface scans before and after the 3D force curve measurements showing single atomic defects assured an unmodified atomically sharp tip. The subtraction of long-range van-der-Waals and electrostatic forces allows us to extract the short-range chemical forces. The results show good agreement with site-specific atomistic simulations of short-range tip-sample forces for a K^+-terminated tip [3] and thus allow us to identify the tip apex atom polarity as well as the lattice sites in our AFM images. Furthermore we calculate the lateral tip sample force from the potential energy landscape and compare these results with theoretical predictions.

[1] H. Hölscher et al., APL 81, 4428 (2002) [2] A. Schirmeisen et al., PRL 97, 136101 (2006) [3] R. Hoffmann et al., PRL 92, 146103 (2004)

O 36.7 Tue 15:45 MA 041

Single crystal microcalorimetry: Measuring molecule-surface interactions — •Jan-Henrik Fischer[1], Jason Farmer[2], Jens

Hartmann[1], Swetlana Schauermann[1] und Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Department of Chemistry, University of Washington, Seattle

Determination of the strength of adsorbate-surface interaction is an important fundamental issue in surface science and an essential prerequisite for understanding real catalytic processes. The strength of adsorbate-surface bonding and of lateral adsorbate-adsorbate interactions can be addressed by measurement of heats of adsorption as a function of surface structure, coverage and presence of other co-adsorbates.

Traditional experimental techniques for probing the energetics of adsorption, such as e.g. thermal desorption spectroscopy, provide reliable results only for reversible adsorption systems and cannot be correctly applied for processes including dissociation, clustering, diffusion into the bulk or reaction with other coadsorbates. These restrictions can be overcome by using a direct calorimetric measurement of adsorption energies on surfaces. For this purpose we set up a new microcalorimetry experiment at Fritz-Haber-Institut, which is based on a method previously developed by King and Campbell [1]. The method relies on the measurement of a temperature change upon adsorption of gaseous molecules on ultrathin ($1-10\,\mu$m) single crystals, which is realized by application of a pyroelectric detector and an independent laser-based energy calibration.

[1] Campbell et al., Rev. Sci. Instr. **75**, 11 (2004)

O 36.8 Tue 16:00 MA 041

Investigating surface dynamics with inelastic X-ray scattering — •Bridget Murphy[1], Martin Müller[1], Jochim Stettner[1], Herwig Requardt[2], Jorge Serrano[2], Michael Krisch[2], and Werner Press[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]ESRF, BP 220, F-38043 Grenoble Cedex 9, France

Inelastic x-ray scattering in grazing incidence conditions provides a new tool to selectively study either surface or bulk lattice dynamics in a single experiment. It is possible to study acoustic and optical surface phonon modes currently with a 3meV resolution over a wide range of momentum space and make a direct comparison between surface and bulk dispersion. In particular $2H-NbSe_2$ and $2H-TaSe_2$will be discussed. For these materials a Kohn anomaly has been previously reported. Our data demonstrate that the softening of the Kohn anomaly at the $2H-NbSe_2$ surface is significantly greater that that reported for the bulk [1]. This is an indication of a relaxation in the top most layers of the crystal. Temperature dependent studies will be presented.

[1] B. M. Murphy, H. Requardt, J. Stettner, J. Serrano, M. Krisch, M. Müller, W. Press, Phys. Rev. Lett. 95, 256104 (2005)

O 36.9 Tue 16:15 MA 041

Variations of the electrochemical potential at monoatomic steps resolved by scanning tunneling potentiometry — •Mark Kaspers[1], Alexander Bernhart[1], Bastian Weyers[1], Evgeny Zubkov[1], Rolf Möller[1], Christian Bobisch[2], Jan Homoth[3], Martin Wenderoth[3], Thomas Druga[3], Lars Winking[3], and Rainer-G. Ulbrich[3] — [1]University of Duisburg-Essen, Department of Physics, Duisburg, Germany — [2]University of California, Irvine, USA — [3]Georg-August-University, Physical Institute, Göttingen, Germany

On macroscopic scale the energy dissipation of electrons scattering at phonons, atomic steps, grain boundaries etc. contribute to the total resistivity. To gain access to these effects on the nanoscale scanning tunneling potentiometry was performed on a Si(111)-($\sqrt{3}\times\sqrt{3}$)-Ag surface superstructure. The experimental data show how the variations of the electrochemical potential are correlated to the topography. E.g. the potential drops at step edges on a lengthscale of about 1.2nm.

Our setup consists of an optimized Omicron Nanoprobe equipped with three independent STM-units. Two STM-tips were used to apply a constant lateral current through the Ag adlayer. The third tip maps the topography as well as the local potential simultaneously.

Our experiment gives access to the spatial variations of the potential inside the structure itself right across the obstacles. This provides a new insight in the elementary processes of the electric resistance observed in macroscopic experiments.

O 36.10 Tue 16:30 MA 041

Photoemission experiments using soft x-ray standing waves — •Sven Döring[1,2], Daniel Weier[1,2], Ulf Berges[1,2], Charles S. Fadley[3,4,5], and Carsten Westphal[1,2] — [1]DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, 44221 Dortmund, Germany — [2]Experimentelle Physik 1, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — [3]Materials and Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — [4]University of California, Davis, CA 95616, USA — [5]Forschungszentrum Jülich, IFF-9, 52425 Jülich, Germany

A high depth resolution can be obtained by creating a soft x-ray standing wave field on the sample surface and performing photoemission experiments in this field. A high reflectivity is necessary for a sufficient standing wave modulation. Multilayer samples are used which provide a strong first order Bragg reflection. The standing wave field can be moved through the sample surface by a sample rotation around the Bragg angle. The shape and modulation of these rocking curves contain information about the sample. First measurements on various samples were performed at the TU Dortmund's synchrotron light source DELTA and at higher energies at BESSY II in Berlin. Results from different samples will be presented in the talk: rocking curves from bare multilayers will be shown as well as a first test measurement of a thin layer of MgO on a wedge of Fe on top of a multilayer. The data show depth profiles obtained of the internal interface. Different chemical states of the same element can be identified by their chemical shift in the XPS spectrum and allocated to certain layers.