O 60: Poster Session III (Methods: Atomic and electronic structure; Methods: electronic structure theory; Methods: Molecular simulations and statistical mechanics; Methods: Sanning probe techniques; Methods: other (experimental); Methods: other (theory))

Time: Wednesday 17:45–20:30 Location: Poster B2

O 60.1 Wed 17:45 Poster B2

Two-Photon Photoelectron Spectroscopy using a Display Analyzer — •Daniel Niesner, Tobias Bierlein, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Two-Photon Photoelectron Spectroscopy is a pump and probe technique which allows observation of excited electronic states in solids. After excitation by a first laser pulse a second one removes electrons into vacuum where they are detected by an analyzer. In the display analyzer the sample is placed in one of the focal points of an ellipsoidal mirror which serves as a low pass filter. Subsequently the photoelectrons pass through a retarding high pass filter and are detected by microchannel plates. While most common analyzers are able to detect only electrons emitted in one angular direction, in this setup the two-dimensional angular distribution of electrons emitted into a cone of 90° is measured. We present data from image-potential states on the (001) surfaces of copper and iridium. An energy resolution of 90 meV and an angular resolution of 5° is found.

O 60.2 Wed 17:45 Poster B2

Tight-Binding Parameterizations Derived from Density-Functional Calculations — •Alexander Urban[1], Konstantin Weber[1], Martin Reese[2,3], Matous Mrovec[2,3], Christian Elsässer[2], and Bernd Meyer[1] — [1]Interdisziplinäres Zentrum für Molekulare Materialien ICMM, Universität Erlangen-Nürnberg — [2]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg — [3]Institut für Zuverlässigkeit von Bauteilen und Systemen IZBS, Universität Karlsruhe

With the semiempirical Tight-Binding (TB) method it is possible to compute the electronic structure and total energy of systems with thousands of atoms. We present a straightforward method for the systematic derivation of TB parameters from first-principles DFT calculations of arbitrary model systems. Our method is conceptionally different from previous approaches [1] as it is based on a projection [2] of the fully converged wavefunction from a mixed-basis DFT computation onto an optimized minimal basis of atomic orbitals. The Slater-Koster tables are then calculated within that minimal basis using the fully converged DFT Hamiltonian. The electronic structures, total energies and forces resulting from derived TB models are compared to the DFT reference for different benchmark simulations.

[1] D. Porezag et al. *Phys. Rev. B* 51 (1995) 12947
[2] D. Sanchez-Portal et al. *Sol. State Comm.* 95 (1995) 685

O 60.3 Wed 17:45 Poster B2

Optical properties of LiF, NaF and KF based on self-interaction corrected pseudopotentials — •Christoph Sommer, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster, D-48149 Münster, Germany

Many-body perturbation theory yields optical properties of semiconductors and insulators in good agreement with experiment. In this approach, the Bethe-Salpeter equation is solved for an effective two-particle problem. Very good one-particle excitation energies – as given, e. g., by the GW approximation – are a necessary prerequisite for obtaining reliable results. The GWA is very demanding, however. In turn, self-interaction corrected (SIC) pseudopotential calculations can also provide very accurate electronic energies for ionic wide-band-gap materials. At the same time, they are only about as costly as regular DFT-LDA calculations.

We investigate the applicability of SIC energies and wavefunctions in the Bethe-Salpeter equation using the alkali metal fluorides LiF, NaF and KF as examples. This is done on the basis of SIC pseudopotentials [1] that have been shown to yield bandstructures in good agreement with experiment. We arrive at optical spectra that are in accord with the results available in the literature for these systems.

[1] B. Baumeier, P. Krüger, J. Pollmann, and G. Vajenine, Phys. B **78**, 12511 (2008)

O 60.4 Wed 17:45 Poster B2

Excess electron at the ice surface: an approach via mixed quantum/molecular mechanics simulations — •Volker Mosert and Michel Bockstedte — Theor. Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

Electron solvation shows a rich varity of phenomena, like surface vs. interior bound states in water clusters. *Ab initio* theory greatly helped to understand these phenomena. However, regarding ice-surfaces, it is desirable to go beyond present *ab initio* models of I_h (0001) and to address, for first insight, the complex morphology of ice films as well as the solvation on the long time scale with a less costly approach.[1] Such an alternative is the mixed QM/MM approach.[2] It treats the water-water interaction via classical potentials and the electron-water interaction via a pseudopotential quantum-mechanically. Although its relevance has been demonstrated for water clusters,[2] applications to the electron solvation at the ice surface are scarce [3] and address the temperature regime where pre-melting occurs. For an evaluation of the method, we address the traping of excess electrons at the I_h surface. For prototypical surface defects, the formation energy as well as the electron binding energy are evaluated using different models of the water-interaction. In comparision to recent DFT-calculations, we obtain a good description with TIP4P potentials.

[1] M. Mehlhorn and K. Morgenstern, Phys. Rev.Lett. **99**, 246101 (2007); Bovensiepen *et al* J. Chem. Phys. C **113**, 979 (2009).
[2] L. Turi, W.-S. Sheu, and P. J. Rossky, Science **309**, 914.
[3] A. Madarász *et al*, J. Chem. Phys. **126**, 234707 (2007).

O 60.5 Wed 17:45 Poster B2

Analysis of Neural Network Potential-Energy Surfaces for Atomistic Simulations — •Tobias Morawietz, Nongnuch Artrith, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

In recent years, artificial Neural Networks (NN) have become a promising new method to represent accurate potential energy surfaces (PES) for molecular and condensed systems. NN potentials are constructed using a set of reference points obtained in electronic structure calculations, which are then interpolated to a continuous PES by the very flexible functional form of the NNs. The NN potentials can then be evaluated several orders of magnitude faster than the underlying electronic structure data. Therefore NN potentials are ideal tools to perform long molecular dynamics simulations of large systems. However, because of the a priori non-physical functional form, NN potentials have to be constructed with care. Using various molecules, clusters and solids we analyze how the physical functional form is approximated by NNs and discuss the scope and limitations of the method.

O 60.6 Wed 17:45 Poster B2

Atomic-resolution AFM imaging of single molecules — •Fabian Mohn, Leo Gross, Nikolaj Moll, Peter Liljeroth, and Gerhard Meyer — IBM Research - Zurich, 8803 Rüschlikon, Switzerland

We have recently developed a technique, which enables imaging of individual admolecules with atomic resolution using noncontact atomic force microscopy [L. Gross et al., *Science* **325**, 1110 (2009)]. The key to achieving intramolecular contrast is a controlled functionalization of the microscope's tip apex. We compare the imaging capabilities of different tip terminations and present measurements of the distance-dependence of the imaging contrast. These investigations – along with first-principle density functional theory calculations – indicate, that AFM operation in the regime of maximal attractive forces is crucial for achieving atomic contrast on molecules. Such close-distance operation is facilitated by using oscillation amplitudes in the sub-angstrom range.

O 60.7 Wed 17:45 Poster B2

Atomic charge state determination by AFM — •Leo Gross[1], Fabian Mohn[1], Peter Liljeroth[1], Jascha Repp[2], Franz J. Giessibl[2], and Gerhard Meyer[1] — [1]IBM Research - Zurich, 8803 Rüschlikon, Switzerland — [2]Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

We investigated the charge state switching of individual gold and silver

adatoms on ultrathin NaCl films on Cu(111) using a qPlus tuning fork atomic force microscope (AFM) operated at 5 Kelvin with oscillation amplitudes in the sub-Ångstrom regime. Charging of a gold adatom by one electron charge increased the force on the AFM tip by a few piconewtons. Employing Kelvin probe force microscopy (KPFM) we also measured the local contact potential difference (LCPD) as a function of the tip height above differently charged adatoms. We observed that the LCPD is shifted depending on the sign of the charge and allows the discrimination of positively charged, neutral, and negatively charged atoms. [L. Gross, et al., Science 324, 1428 (2009)]

O 60.8 Wed 17:45 Poster B2

Magnetokraftmikroskopie in starken externen Magnetfeldern — •Lars Ungewitter, Ivo Knittel und Uwe Hartmann — Fachbereich Experimentalphysik, Campus C6.3, 66123 Saarbrücken

In einen Kryostaten mit Raumtemperaturbohrung und supraleitender Magnetfeldspule wird ein modifiziertes kommerzielles Raumtemperatur-Rasterkraftmikroskop eingeführt und als Magnetokraftmikroskop (MFM) bei Feldern bis 1.5 Tesla betrieben. Die Vorteile in der Handhabung sind im Vergleich zum Betrieb eines MFM im variable temperature insert (VTI) ein leichter Zugang zu Probe und Spitze, größere Scanbereiche, und die Abbildung auch ungünstiger Topografien. MFM-Studien über vollständige Hysteresekurven von epitaktischen Magnetitfilmen, SmCo-Filmen und patterned media - Speichermedien werden vorgestellt und diskutiert.

O 60.9 Wed 17:45 Poster B2

The open source scanning probe control software package Gxsm — Percy Zahl[1], •Thorsten Wagner[2], Rolf Möller[3], and Andreas Klust[4] — [1]Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, USA — [2]Institute of Experimental Physics, Johannes Kepler University Linz, Austria — [3]Department of Physics, University Duisburg-Essen, Germany — [4]Lewven, Belgium

Gxsm is a full featured and modern scanning probe microscopy (SPM) software. It can be used for powerful multidimensional image/data processing, analysis and visualization. Connected to an instrument, it is operating many different flavors of SPM, e.g. scanning tunneling microscopy (STM) and atomic force microscopy (AFM) or, in general, two-dimensional multi channel data acquisition systems. The Gxsm core can handle different data types, e.g. integer and floating point numbers. An easily extendable plug-in architecture provides many image analysis and manipulation functions. A digital signal processor (DSP) subsystem runs the feedback loop, generates the scan signals and acquires the data. The programmable Gxsm vector probe engine can perform any thinkable spectroscopy and manipulation task, such as scanning tunneling spectroscopy (STS) and tip formation. Due to the support for a new DSP hardware (SoftdB SR-MK2&A810) new developments like multi channel feedback mixing and adaptive infinite response for the tunneling current had been implemented. The Gxsm software is released under the GNU general public license (GPL) and can be obtained free of charge via internet from http://gxsm.sf.net.

O 60.10 Wed 17:45 Poster B2

Forces in Molecular Electronics — •Mathias Neu, Andreas Pöllmann, and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

In recent years low-temperature scanning tunneling microscopy (STM) and spectroscopy have been very successfully used to study electron transport through individual molecules. However, STM investigations are limited to conducting substrates and the experimental data is determined by both the geometry and the electronic structure of the sample in a complex and often ambiguous manner. To overcome these two limitations we plan to experimentally implement force detection as an additional measure in molecular electronics. To this end a combined STM and scanning force microscope is being build up. The force detection scheme is based on using tuning forks as force sensors [1]. Unlike in the case of cantilever-based AFM, in this setup the scanning tip is not an integral part of the force sensor and can be a metal tip as is usually used in STM, thus making it an ideal force-detection technique to be combined with STM. On our poster we present our progress on the experimental setup.

[1] Giessibl, Appl. Phys. Lett. 73, 3956 (1998)

O 60.11 Wed 17:45 Poster B2

Atomic Force Microscopy meets Field Ion Microscopy — •Jens Falter[1], Daniel-Alexander Braun[1], Udo D. Schwarz[3], Hendrik Hölscher[2], André Schirmeisen[1], and Harald Fuchs[1] — [1]Physikalisches Institut, University of Münster and CeNTech, Center for Nanotechnology, Münster, Germany — [2]IMT, Forschungszentrum Karlsruhe, Germany — [3]Department of Mechanical Engineering, Yale University, New Haven, USA

In atomic force microscopy (AFM), the contrast stems from the interaction between the probing tip and the sample. Although the AFM is even able to measure interaction forces with the force spectroscopy method, the underlying contrast mechanism is still not completely understood. In some extend this is due to the unknown tip shape in an AFM, which is able to resolve atomic resolution of sample surfaces - but not of the tip apex. The Field Ion Microscope (FIM) is a technique which resolves the apex of metal tips with atomic precision. The images of the tip gained with this method allow an atom by atom reconstruction of the foremost atom layers of the tip. We present our home-build system which combines these two microscope techniques: an AFM-head which has been proven to operate at low temperatures in ultra high vacuum [1] and a FIM, which can image the apex of the tungsten tip. The force sensor is based on a tuning fork in the q-plus concept [2] with an electrochemical etched tungsten tip at the end of the free prong. This setup enables us to perform force spectroscopy experiments with well characterized tips from the FIM images. [1] B.Albers et. al., Rev. Sci Instrum. 79 033704 (2008) [2] F.J.Giessibl, APL. 76 1470 (2000)

O 60.12 Wed 17:45 Poster B2

Quantitative Kelvin probe force microscopy imaging on locally doped Si — •Christine Baumgart[1], Anne-Dorothea Müller[2], Falk Müller[2], Manfred Helm[1], and Heidemarie Schmidt[1] — [1]Forschungszentrum Dresden-Rossendorf, Institut für Ionenstrahlphysik und Materialforschung, P.O. Box 510119, 01314 Dresden — [2]Anfatec Instruments AG, Melanchthonstr. 28, 08606 Oelsnitz

Failure analysis and optimization of nanoelectronic devices require knowledge of their electrical properties. Kelvin probe force microscopy (KPFM) is a standard technique for the investigation of the surface potential. Since KPFM was developed in 1991 the measured KPFM signal was attributed to the contact potential difference (CPD) between conductive probe and sample. We show that the CPD is not suitable to describe the measured Kelvin bias in semiconductors quantitatively and introduce a unique KPFM model [1] which successfully correlates the measured Kelvin bias with the difference between Fermi energy and respective band edge. Quantitative dopant profiling is demonstrated on cross-sectionally prepared Si epilayer structures and on a Si dynamic random access memory cell.

[1] C. Baumgart, M. Helm, H. Schmidt, Phys. Rev. B 80 (2009) 085305.

O 60.13 Wed 17:45 Poster B2

Growth of Co-Salen on NiO(001): An atomic force microscopy study in ultrahigh vacuum — •Johannes Hattendorff, Alexander Schwarz, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany

Co-Salen is a paramagnetic metal-organic Schiff-base-complex with a central cobalt atom that carries spin. In previous studies the adsorption and growth of Co-Salen was investigated with atomic force microscopy (AFM) on bulk NaCl(001) [1]. The latter investigation revealed that at room temperature the physisorbed molecules are very mobile on NaCl(001) and exhibit a three-dimensional Vollmer-Weber type of growth. Step decoration and two different well ordered crystalline morphologies with bulk-like structures could be identified.

Here we deposit Co-Salen on NiO(001) which is an insulator like NaCl but with a smaller band gap (3.8 eV instead of 9 eV). First results obtained with AFM for sub-monolayer coverage show a step-flow growth and the formation of islands on terraces. At higher coverage the growth appears to be layer-wise. These observations indicate that the molecule-surface interaction on the transition-metal oxide NiO is very different compared to the alkali-halide NaCl. Note that although both surfaces are ionic with rock salt structure bonds in NiO exhibit a significant covalent character and the lattice constant is much smaller (417 pm instead of 564 pm). Both properties might alter the adsorption geometry and interaction strength drastically.

[1] S. Fremy et al., Nanotechnology 20, 405608 (2009).

O 60.14 Wed 17:45 Poster B2

Observation of Spin Excitation by Inelastic Tunneling Spectroscopy of Fe atoms on a Semiconductor Surface

— •Alexander A. Khajetoorians, Bruno Chilian, Sergei Schuwalow, Frank Lechermann, Jens Wiebe, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Hamburg, Germany

We present a combined experimental and theoretical study of single Fe atoms on a III-V (110) semiconductor surface. Using tunneling spectroscopy at very low temperature (300mK), we observe a zero-field gap in the differential conductivity measured on the Fe atom which can be attributed to magnetic anisotropy. The total spin of the Fe atom as well as its anisotropy is also calculated by first principles calculations within density functional theory and related to the experimental data utilizing a simple quantum magnetic Hamiltonian. In the context of this model, we discuss the predicted magnetic field dependent magnetization and relate it to experimental data in high magnetic fields (12T).

O 60.15 Wed 17:45 Poster B2

Study on automated atom manipulation — •Boris Wolter[1], André Kubetzka[1], Roland Wiesendanger[1], Bernd Schütz[2], and Jianwei Zhang[2] — [1]Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg — [2]Technical Aspects of Multimodal Systems (TAMS), Universität Hamburg, Vogt-Kölln-Str. 30, 22527 Hamburg

Recent years have shown an increasing number of investigations concerning automation of atom manipulation via STM [1, 2]. In our study, we employed a Monte-Carlo simulation to model the interactions between tip, sample and adsorbates [3]. Based on this simulation, we explored the prospects of automated lateral manipulation of single atoms. Required techniques like adsorbate detection, learning of manipulation parameters, path planning with uncertainty [4] and manipulation tracing were developed and tested within the simulated STM environment.

In more recent work, we focus on a local scan method for exact positioning of the tip above specified adsorbates [1]. The primary goals of this method are to prevent time consuming scans of large areas, to counter drift in long-term experiments and to increase experimental accuracy. Once finished, it will be combined with automation techniques for tunneling spectroscopy and atom manipulation.

[1] H. Chen *et al.*, Proc. of ICRA, 169-174 (2005)
[2] T. Knepper *et al.*, Proc. of ROBIO, 95 (2005)
[3] A. Kühnle *et al.*, Surf. Sci. 449, 15 (2001)
[4] J.P. Gonzalez *et al.*, Proc. of IROS, 2435-2442 (2005)

O 60.16 Wed 17:45 Poster B2

Mechanical Behaviour of Graphenes on a Solid Surface — •Stefan Eilers and Jürgen P. Rabe — Department of Physics, Humboldt-Universität zu Berlin, Germany

Graphene is a promising candidate for future generation electronic devices. Structuring and, more general, manipulation of graphenes are needed for the development of possible applications. Scanning force microscope (SFM) techniques are promising for the investigation of single or multilayer graphenes, because of their thinness, flexibility and flatness. Here we demonstrate the manipulation of graphene on a SiO2 surface. Contrary to the cutting of single polymers with an SFM tip, which always results in only one cut, cutting graphenes results in two cuts. Therefore nanogaps and nanoribbons can be readily produced. This effect is attributed to the one- and two-dimensionality of polymers and graphene, respectively. Simple explanations are provided to understand the behaviour. It is demonstrated inhowfar basic models for describing bending and breaking of macroscopic objects are applicable also for these nanoscopic systems.

O 60.17 Wed 17:45 Poster B2

A Dynamic Force and Scanning Tunneling Microscopy Study of Line Defects and Step Edges in the Alumina Film on NiAl(110) — •Lars Heinke, Leonid Lichtenstein, Georg Hermann Simon, Thomas König, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14196 Berlin, Germany

The aluminum oxide thin film on NiAl(110) is an often used model system in catalysis. Line defects in the film like step edges and antiphase domain boundaries are prominent structure elements and they are referred to as active sites [1]. In this study, frequency modulation dynamic force microscopy (FM-DFM) and scanning tunneling microscopy (STM) are applied to determine the atomic structure of the thin film and its line defects in ultra high vacuum at 5 K [2]. By means of bias spectroscopy and contact potential measurement different density of electronic states as well as the electrostatic potential were determined. We would like to link the electronic structure of the line defects to catalytic processes.

[1] S. Schauermann et al., Chem. Phys. Lett. 381 (2003) 298-305
[2] G. H. Simon et al., New J. Phys. 11 (2009), 093009

O 60.18 Wed 17:45 Poster B2

SPM tip cleaning by electron-bombardment for investigation of samples prepared by applying nanospherelithography (NSL) — •David Hellmann, Uli F. Wischnath, and Achim Kittel — EHF, Fak. V, Physik, Carl von Ossietzky Universität Oldenburg

The heat transfer between a sample and a probe can be measured using a Near-field Scanning Thermal Microscope (NSThM) [1,2]. The NSThM combines a STM tip with a thermocouple sensor. Thus data concerning the heat transfer a few nm above the scanned surface can be collected by measuring the thermovoltage. Cleanliness of the tip and the sample is an issue of great importance as the NSThM seems to be more sensitive to adsorbates than traditional STM techniques. By applying nanospherelithography (NSL), structured surfaces have been prepared and subsequently scanned using a NSThM tip. Residues of unknown origin seem to persist on either the tip or the sample though intensive cleaning procedures have been applied to the latter. X-Ray-Photoelectron-Spectroscopy (XPS) conducted on the sample did not reveal the presence of residues. Therefore electron-bombardment has been applied to the tip, as this has been reported in [3] to be an established method to heat a tip to several hundred degrees Celsius. As the tip used here gives a thermovoltage when its temperature is changed, it should be possible to measure the heating effect of the bombardment directly. Interestingly, no clear evidence could be gathered that the tip can be heated up significantly. Literature: [1] A. Kittel et al., PRL 95, 224301 (2005) [2] U. Wischnath, RSI 79, 073708 2008 [3] S. Ernst et al., Science and Technology of Advanced Materials 8 (2007)

O 60.19 Wed 17:45 Poster B2

Investigating structured surfaces with a near-field scanning thermal microscope using a new scanning method — •Lars Hoelzel, Uli F. Wischnath, and Achim Kittel — University of Oldenburg - Energy an Semiconductor Research Laboratory - C. v. Ossietzkystr. - D 26111

The near-field scanning thermal microscope (NSThM) [1] is able to measure the thermal flux between a modified tip of a STM and a heated or cooled sample surface under ultra-high vacuum conditions. Hence, the main contribution is mediated by evanescent electro-magnetic fields. Up to now the heat flux was investigated in constant current mode of the STM on which the NSThM is based [2]. While the tunnelling current decays on a short length scale the heat flux decays on a roughly ten times larger length scale. The new scan mode employs a control loop which keeps the heat current constant. Therefore, it is possible to investigate the influence of the surface morphology on the heat flux at larger distances. The results gained by the constant thermovoltage mode suggest that the evanescent field reaches farther out in trenches compared to a convexly curved surface or even a flat surface.

[1] Uli F. Wischnath et al., Rev. Sci. Instrum. 79, 073708 (2008)
[2] Achim Kittel et al., Appl. Phys. Lett. 93, 193109 (2008)

O 60.20 Wed 17:45 Poster B2

Appearence of Adsorbates in Near-field Scanning Thermal Microscopy — •Ludwig Worbes, Uli F. Wischnath, and Achim Kittel — Universität Oldenburg - EHF - EPKOS

The Near-field Scanning Thermal Microscope (NSThM) is an STM using a probe featuring a miniaturized thermocouple temperature sensor. Therefore it is possible to measure the heat flux between the probe and a heated or cooled sample, in this case Au(111), at distances of a few nanometres [1,2]. By operating in UHV the heat transfer should be restricted to radiation dominated by evanescent electromagnetic fields at this distances.

In reality heat transport measurements turn out to be highly sensitive to adsorbates on the surfaces. Electrically nonconducting adsorbates possibly form a bridge between sample and probe, resulting in phononic heat transfer, without any influence to the electric conductivity of the tunnel gap. Indications can be seen in heat flux versus distance measurements. These measurements are performed with different distance sweep procedures and velocities to survey occurrence and dynamic behaviour of adsorbate bridges.

Even NSThM measurements performed on in situ cleaned samples

display this indications, even though STM images show a clean reconstructed surface. Apparent-barrier-height measurements by STM and XPS measurements display inconsistent results.

[1] Uli F. Wischnath et al., Rev. Sci. Instrum. 79, 073708 (2008)
[2] Achim Kittel et al., Appl. Phys. Lett. 93, 193109 (2008)

O 60.21 Wed 17:45 Poster B2

Infrared near-field nanospectroscopy of SiO2 structures embedded at Si[100] surfaces — Marc Tobias Wenzel[1], •Hans-Georg von Ribbeck[1], Anja Krysztofinski[1], Phillip Olk[1], Andreas Hille[1], Oliver Mieth[1], Peter Milde[1], Lukas M. Eng[1], Rainer Jacob[2], and Manfred Helm[2] — [1]Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Straße 1, 01069 Dresden — [2]Institut für Ionenstrahlphysik und Materialforschung, Forschungszentrum Dresden-Rossendorf, 01214 Dresden

Scattering scanning near-field optical microscopy (s-SNOM, or s-NSOM) allows for optical inspection of nanostructures and materials with a resolution far better than the diffraction-limited resolution of far-field microscopy methods. This is of particular interest in case of mid-infrared investigations. The combination of such an s-SNOM with the wavelength-tunable free-electron laser (FEL) located at the Forschungszentrum Dresden-Rossendorf provides a versatile tool for the nondestructive sample investigation in the IR fingerprint region at nanoscopic resolution.

Here, we present the IR-s-SNOM nanospectroscopy investigations of 400-nm-deep SiO_2 trenches, embedded in intrinsic silicon [100]. Measurements were performed in the wavelength range from 9 to 11 μm (1100 $cm^{-1}$to 910 cm^{-1}). We experimentally demonstrate the expected contrast reversal of the near-field amplitude signals of Si and SiO_2. This contrast reversal is due to the material-specific near-field enhancement at the reststrahlen band of SiO_2. We also present comparative measurements using a CO_2 laser at 10.6 μm (943 cm^{-1}).

O 60.22 Wed 17:45 Poster B2

Development of a modular multiple temperature UHV Scanning Tunneling Microscope — •Carsten Tröppner, Lutz Hammer, and Menko Alexander Schneider — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

We present our newly constructed low temperature scanning tunneling microscope (STM) designed for high resolution scanning tunneling spectroscopy (STS) measurements under ultra high vacuum (UHV) conditions. A standard non-UHV helium bath magnet cryostat is used for cooling the STM down to 4.2K and below (Eigler-Design). With the aim to carry out STM measurements at room temperature as well as low temperature we implemented the STM as a mobile unit, which can be transferred within the UHV chamber between regions of different temperature. The mobility of the STM furthermore provides an easy sample transfer and the possibility to transfer it out of the UHV chamber through a load-lock system. Hence the full instrument or the tip only can be exchanged.

O 60.23 Wed 17:45 Poster B2

Electronic characterisation of thin metallic films using Kelvin Probe Force Microscopy and 4-Point-Probe — •Oliver Ochedowski, Benedict Kleine Bussmann, Florian Meinerzhagen, and Marika Schleberger — Universität Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg

We are investigating the electronic structure of thin metallic films, especially graphene on insulating substrates like siliconoxide. To achieve this, we are combining atomic force microscopy with Kelvin probe technology under UHV conditions and ex situ to map the surface contact potential of these films. This method, first utilized by M. Nonnenbacher, uses the measured force between between the tip and the sample as the control variable [1]: An ac voltage U_{mod} between the tip and sample is modulated on a dc part U_{Bias} until the frequency shift due to electrostatic forces is minimized. As a result the difference in contact potentials can be mapped. We also measure the electrical surface resistance directly by using a four-point-probe mounted on a small micromanipulator. We present first test measurements under ambient conditions.

[1]M.Nonnenmacher, M.P. O Boyle, and H.K.Wickramasinghe Appl. Phys.Lett. 58 (25),2921-2923 (1991)

O 60.24 Wed 17:45 Poster B2

Electronic characterisation of thin metallic films using Kelvin Probe Force Microscopy and 4-Point-Probe — •Oliver Ochedowski, Benedict Kleine Bussmann, Florian Meinerzhagen, and Marika Schleberger — Universität Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg

We are investigating the electronic structure of thin metallic films, especially graphene on insulating substrates like siliconoxide. To achieve this, we are combining atomic force microscopy with Kelvin probe technology under UHV conditions and ex situ to map the surface contact potential of these films. This method, first utilized by M. Nonnenbacher, uses the measured force between between the tip and the sample as the control variable [1]: An ac voltage U_{mod} between the tip and sample is modulated on a dc part U_{Bias} until the frequency shift due to electrostatic forces is minimized. As a result the difference in contact potentials can be mapped. We also measure the electrical surface resistance directly by using a four-point-probe mounted on a small micromanipulator. We present first test measurements under ambient conditions.

[1]M.Nonnenmacher, M.P. O Boyle, and H.K.Wickramasinghe Appl. Phys.Lett. 58 (25),2921-2923 (1991)

O 60.25 Wed 17:45 Poster B2

Near-field infrared microscopy with a broadband light source — •Stefanie Bensmann[1], Christoph Janzen[1], Reinhard Noll[1], Jón Mattis Hoffmann[2], and Thomas Taubner[1,2] — [1]Fraunhofer-Institut für Lasertechnik (ILT), Aachen — [2]I. Physikalisches Institut IA, RWTH Aachen

Scattering-type near-field infrared microscopy offers a wavelength-independent spatial resolution of approximately 30 nm together with chemical sensitivity [1]. Spectra are usually recorded by consecutive measurements that are performed at different wavelengths, which is time-consuming. Additionally, the limited spectral range covered by conventional MIR laser sources does not cover samples like e.g. certain semiconductors (GaAs), polar crystals and different polymers.

Broadband IR light sources allow circumventing these problems by recording a full spectrum with a single measurement in an extended frequency range [2, 3]. However, a laser power of only a few μW restricts measurements to samples with a strong resonance like SiC. We present work on combining a broadband IR laser (power of several mW at $5 - 12$ μm) that is currently developed at the ILT with the NeaSNOM (near-field optical microscope from Neaspec, www2.neaspec.com). This new system will extend the spectral range covered and allow to examine samples with weaker resonances.

[1] F. Keilmann, R. Hillenbrand, in: Nano-optics and Near-field Optical Microscopy, p. 235; X. Zhang, K. Wang (eds), Artech House 2009.
[2] M. Brehm et al., Optics Express 15, p. 11222, 2006.
[3] S. Amarie et al., Optics Express 17, p. 21794, 2009.

O 60.26 Wed 17:45 Poster B2

STM and STS studies of ferroelectric domain structures on $BaTiO_3$(001) and $BaTiO_3$(111) single crystals — •Maik Christl, Christian Hagendorf und Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Germany

A new method of characterizing ferroelectric domain structures on nanometer scale by using a STM is presented. We demonstrate a domain contrast of various domain arrangements based on dI/dV maps. On $BaTiO_3$(001) we can differentiate between ferroelectric c^+, c^-, and a domains based on STM and STS. Additionally domain boundaries between 90° in-plane polarized domains become visible in STS maps. During heating $BaTiO_3$(111) above the Curie temperature, a modified domain pattern is found. The ferroelectric domain structure can be modified locally by tunneling at higher bias voltages. This STM-induced domain nanostructuring will be discussed in comparison to recent AFM studies [1].

[1] A. Gruverman et al., *Scanning Force Microscopy Studies of Domain Structure in $BaTiO_3$ Single Crystals*, Jpn. J. Appl. Phys. Vol. 36 (1997) pp.2207-2211

O 60.27 Wed 17:45 Poster B2

Chirped Pulse Two Photon Photoemission technique to study adsorbate dynamics — •Marianne Bader, Indranil Sarkar, Felix Steeb, Andreas Ruffing, and Martin Aeschlimann — Department of Physics, University of Kaiserslautern, 67663 Kaiserslautern, Germany

Time resolved Two Photon Photoemission (TR 2PPE) is a well-known method in surface physics to study adsorbate dynamics. However, it's

temporal resolution is limited by the Heisenberg uncertainty principle. Here we propose a novel method to observe dynamics of adsorbate states using Chirped Pulse Two Photon Photoemission (CP 2PPE). This method utilizes a suitable modified spectral phase of the exciting femtosecond laser pulse, modulated by a Fork prism pair [1]. We apply this technique in the case of Cs/Cu(111), where we observe significant energy shifts of the excited adsorbate state (Cs*) as well as a peak broadening. The obeserved asymmetry in peak position is suggestive of possible adsorbate motion [2]. We further propose to apply the method of CP 2PPE to systems with shorter time constants where time resolved methods are restricted.

[1] R. L. Fork et al, Opt. Lett. 9 (1984) 150
[2] F. Steeb, PhD Thesis, TU Kaiserslautern, 2008

O 60.28 Wed 17:45 Poster B2

Analysis of XPD-patterns by means of Genetic Algorithms — •Tobias Lühr[1], Daniel Weier[1,2], Frank Schönbohm[1,2], and Carsten Westphal[1,2] — [1]Fakultät Physik - TU Dortmund, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — [2]DELTA - TU Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

Angle-scanned X-Ray Photoelectron Diffraction (XPD) is a powerful technique for the investigation of crystalline interfaces and surfaces. This technique provides the atomic structure of the investigated sample as well as the chemical state of the atoms. In order to determine the accurate structure from the recorded data it is necessary to simulate the XPD-pattern. A genetic algorithm was developed that generates and optimizes different surface structure models. Each structure is defined by a basic model structure and a transformation that depends on a reasonable size of variable parameters (genes). After generating a set of modified structures by variation of the genes the algorithm calculates the multiple scattering pattern for each structure and evaluates the pattern with an R-factor. If no R-factor has reached a specified value, the algorithm creates a new generation of parameter sets by a combination or mutation of the genes of the last generation. In this procedure the genes with a low R-factor are preferred to be chosen. With algorithm we present here it was possible to determine several atomic surface structures like Cyclopentene/Si(100), Pyridine/Si(100), and $ZrSi_2$/Si(100).

O 60.29 Wed 17:45 Poster B2

Analysis of optical systems, caustic formation and contrast depth in mirror electron microscopy — •Sergej Nepijko and Gerd Schönhense — Institute of Physics, University of Mainz, 55099 Mainz, Germany

The conditions of realization of positive and negative contrasts in electron mirror microscope are shown. The contrast depth is analyzed as well, that is the sensitivity of electron mirror microscope to disorders of homogeneity on the object (local magnetic and electric fields, surface relief). Because of these, electron trajectories are distorted and electrons acquire additional velocity components in radial and azimuthal directions. This leads to the shift of the observed point on the screen and, as a consequence, to an image contrast. Since the electron energy, when reflected, is close to zero, electrons are influenced by heterogeneities for a long time. It causes high sensitivity to heterogeneities, up to the crossing of electron trajectories (caustics are generated). The conditions of caustic generation due to local electric or magnetic fields are analyzed: (i) the larger the distance r from the centre of the image, the easier the caustic is generated, (ii) after generation, the caustic expands with growth of distance r from the centre of the image, (iii) the value of azimuthal linear shift $S = \gamma r$ (γ - azimuthal angular shift) reverses sign when passing through the centre ($r = 0$). A dark wedge will be the continuation of the bright wedge opposite the centre. The caustic disappears in the centre of the screen. The contrast increases with growth of r. This differs from the contrast due to electric fields, which does not depend on r.

O 60.30 Wed 17:45 Poster B2

Comparative EELS on carbon-based materials — •Thomas Haensel, Stefan Krischok, Juergen A. Schaefer, and Syed Imad-Uddin Ahmed — Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany

Carbon-based materials are of great interest, due to the many possible applications in various fields. For example regenerative wood-based biopolymers made of cellulose, lignin and additives are expected to be low-cost ground materials for the use in various typical polymer applications such as fuel cells. Additionally, hard synthetic materials like diamond-like (DLC) and nanocrystalline diamond (NCD) films are relevant as transparent protective coatings, use in bio-sensor systems and electron emitters. In contrast to DLC films, graphite (HOPG) is very soft and has a high electric conductivity. In this contribution various carbon-based materials were analyzed with electron energy loss spectroscopy (EELS), which is a surface sensitive technique and provides information about plasmons in the surface and mean surface region. Additionally, these materials were characterized with XPS to extract further information about the chemical composition and functional groups at the surface. The so called π-plasmon as well as other energy losses will be discussed and a comparative survey of EELS of surfaces with different surface preparations will be presented.

O 60.31 Wed 17:45 Poster B2

The High Resolution Diffraction Beamline P08 at PETRA III - First Experiments — •Carsten Deiter, Florian Bertram, Kathrin Pflaum, and Oliver H. Seeck — Hasylab am DESY, Notkestr. 85, 22607 Hamburg, Germany

Since fall 2009 the new synchrotron radiation source PETRA III is operational. At the High Resolution Diffraction Beamline P08 the equipment and the beam parameters are highly suited for surface and interface studies. Different sample cells with heating and cooling capability and the possibility of vacuum (HV and UHV) and gas atmosphere up to 1bar are available. These cells can be installed in the six circle diffractometer (Kohzu) for extreme angular resolution and will be supported by an UHV infrastructure close by in the near future. First user experiments have been performed and the results from first in-house experiments will be presented which show the benefits of the PETRA III beam parameters.

O 60.32 Wed 17:45 Poster B2

Molecular trapping and scattering at ionic liquid surfaces — •Andre Dorsch, Matthias Schöppke, and Reinhard Denecke — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstr. 2, 04103 Leipzig, Germany

Gas uptake in ionic liquids is an important process for the technological use of such substances [1,2]. Using a supersonic molecular beam setup and a moveable quadrupole mass spectrometer, the interaction of CO_2 and N_2 with surfaces of imidazolium-based ionic liquids have been studied. Employing angle-resolved measurements, trapping and inelastic scattering events can be determined. Parameters like the kinetic energy of the impinging molecules, which influence the behaviour, are systematically varied. From the results residence times of gases in ionic liquids are derived.

[1] J. F. Brennecke, E. J. Maginn, Purification of Gas with Liquid Ionic Compounds. US Patent 6,579,343 (2003).
[2] A. Yokozeki, M. B. Shiflett, Appl. Energy 84, 351 (2007).

O 60.33 Wed 17:45 Poster B2

Diffusion of Xe on Multilayer Xe — •Anuschka Schmitt, Matthias Buschmann, Thomas M. Ernst, and Heinz J. Jänsch — Philipps-Universität Marburg

Diffusion of Xe on Xe-multilayers or inside the multilayers is largely unexplored. This mainly reflects a lack of methods. We employ NMR of ^{129}Xe to investigate surface phenomena. The sensitivity is greatly enhanced by the use of laser-polarized ^{129}Xe.

Here we explore different NMR-techniques to study diffusion: surface layer to second layer exchange could be monitored through the strong chemical shift difference ($\Delta\sigma \approx 100$ ppm) of the two; disorder in the solid is spectrally seen by broad lines due to chemical shift fluctuations, so that annealing is detected by line narrowing; direct diffusional motion is measured in pulsed magnetic field gradients.

UHV-compatible gradient coil design was tested and a proof of principle demonstrated by sodium diffusion in a NaCl aqueous solution.

O 60.34 Wed 17:45 Poster B2

Contrast formation in the SEM at lowest landing energy of the electrons — •Philipp Tonndorf, Steffen Schulze, and Michael Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

The primary electrons initially have normal energies of several keV and are slowed down until just before the sample to a few 100 eV by an electric opposing field. This ensures that the chromatic error in the electron optics remains low.

Electron with reduced energy can't penetrate so far into the sample.

So they have a smaller interaction volume, which promises to improve the resolution. For example, you can see the walls of the studied carbon nanotubes, which you can't recognize with higher electron energies.

There is also a change in the secondary electron yield and the backscatter coefficient, which causes other contrasts. For gold on carbon the contrasts reversed under 500eV landing energy.

Even charges of the sample can be reduced. You could represent structures from Al on Si3N4 with opposing field better than without opposing field.

This technique is very surface sensitive and can detect details, which are hidden at higher energies and you can investigate samples that would be destroyed by higher landing energies. Poorly or non-conductive samples can be scanned without the need to evaporate a conductive layer.

O 60.35 Wed 17:45 Poster B2

Real-time simulation of Si(001) 2PPE spectra — •Henning Husser and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, 24098 Kiel, Germany

The photo-current induced by a fs laser-pulse is simulated by real-time *ab initio* TDDFT molecular dynamics. The electronic structure of the Si(001) surface is described within density-functional theory using a slab geometry. To account for the finite escape depth of the photo-electrons emitted from a solid surface like Si(001), an optical potential acting on the conduction states only is included in the integration of the time dependent Kohn-Sham equations. The calculation is carried through at frozen-in effective potential. We note, however, that the time-dependent Kohn-Sham equations could be integrated self-consistently in the case of atoms and small clusters, if no optical potential is included. The photo-emission spectrum is derived from the Fourier transform of the single-particle wave-functions. Normal emission 2PPE spectra from Si(001) for s and p-polarized light are presented. We analyze the photon energy and polarization dependence of the theoretical spectra and we compare to experimental 2PPE spectra by Kentsch *et al.*[1].

[1] C. Kentsch, M. Kutschera, M. Weinelt, T. Fauster, M. Rohlfing, Phys. Rev. B **65**, 035323 (2001).