

O 29 Poster session II (Nanostructures, Magnetism, Particles and clusters, Scanning probe techniques, Time-resolved spectroscopy, Structure and dynamics, Semiconductor surfaces and interfaces, Oxides and insulators, Solid-liquid interfaces)

Time: Wednesday 14:30–17:30

Room: P2

O 29.1 Wed 14:30 P2

Non-paraxial Talbot effect at arrays of microspheres and microstructures — ●MANUEL GONÇALVES, ANDRÉ SIEGEL, ALEXANDER GIGLER, and OTHMAR MARTI — Department of Exp. Physics, University of Ulm, D-89069 Ulm, Germany

The Talbot effect, known in optics since the middle of the 19th century was observed in atom optics in 1995. Since then, an increasing attention has been drawn to this effect in both classical and atom optics. One of the reasons for that is the connection between the Talbot effect and the optical coherence. However, most of the theoretical analysis has been based on the paraxial approximation of optical rays. In some cases this approach is inadequate.

We have measured the Talbot effect for two-dimensional arrays of microspheres, on flat surfaces, and for microstructured surfaces using colloidal crystals as templates. These structures can focus strongly plane waves generating very sharp light sources. We show that if the size of light sources is of the order of the wavelength, or even smaller, the conventional paraxial approach to calculate the Talbot length z_T fails.

We have developed a theoretical model based on the scalar diffraction theory to calculate the field in the Fresnel region, without using the paraxial approximation. The results obtained are in good agreement with the experimental measurements. By contrary, the simulations based on the Fresnel diffraction were not observed experimentally.

O 29.2 Wed 14:30 P2

Ultraflat Ternary Nanopatterns Fabricated via Colloidal Lithography — ●MICHAEL HIMMELHAUS, OLIVER WORSFOLD, CONOR WHITEHOUSE, and JONATHAN WRIGHT — Bionanotechnology Research Project, R&D Division, Fujirebio, Inc., 51 Komiya-cho, Hachioji-shi, Tokyo 192-0031, Japan

Colloidal lithography on mica has been combined with subsequent thermal evaporation, sputtering, and template-stripping processes to produce ultraflat ternary nanopatterns of large lateral extension. As confirmed by atomic/friction force microscopy (AFM/FFM) the patterns provide a new type of model surface particularly useful for applications that demand proper distinction between surface chemistry and topography. By right choice of materials for fabrication of the inorganic pattern, the resulting features can be selectively functionalized with self-assembled monolayers, thereby altering surface properties of the addressed regions only. We found that the size of the circular patches, which can be fabricated by our method, is reduced to 60% of the nominal diameter of the colloidal particles used to produce the colloidal mask. Accordingly, the minimum size of circular features that can be fabricated by colloidal lithography is significantly reduced.

O 29.3 Wed 14:30 P2

Electronic properties of the Si(557)-Au surface investigated by STM and STS — ●M. SAUTER¹, R. HOFFMANN¹, C. SÜRGER¹, and H. v. LÖHNEYSSEN^{1,2} — ¹Physikalisches Institut und DFG Center for Functionale Nanostructures (CFN), Universität Karlsruhe, D-76128 Karlsruhe — ²Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe

The Si(557)-Au surface is investigated by scanning tunneling microscopy (STM) and spectroscopy (STS) at different temperatures. Previous photoemission data were interpreted in terms of a one-dimensional metallic band at room temperature [1]. However, at $T = 260$ K the photoemission intensity near the Fermi energy vanishes. This has been attributed either to a Peierls transition [1] or to a shift of the Fermi energy [2]. At room temperature our STM images confirm the chainlike structure due to adatoms adjacent to a diffuse row attributed to the step edge. At $T = 77$ K images of unoccupied electronic states show a splitting of the step-edge structure but no doubling of periodicity in contradiction with the interpretation of a Peierls transition. In addition, we present high-resolution images that reveal a substructure at the location of the Au-Si bonds. Current-distance measurements have been performed in order to investigate the k -dependence of the tunneling spectra.

[1] J. R. Ahn *et al.*, Phys. Rev. Lett. **91**, 196403 (2003).

[2] D. Sánchez-Portal *et al.*, Phys. Rev. Lett. **93**, 146803 (2004).

O 29.4 Wed 14:30 P2

Preparation und characterization of molecular Ag nano contacts via electromigration — ●JEDRZEJ SCHMEIDEL, GERNOT GARDINOWSKI, CHRISTOPH TEGENKAMP, and HERBERT PFNÜR — Institut für Festkörperphysik, Universität Hannover, Abteilung Oberflächen, Appelstrasse 2, 30167 Hannover, Germany

In order to obtain electrical characteristics from molecules and nanostructures, atomically well-defined and stable contacts are of high importance, which can be manufactured reproducibly, e.g. under UHV conditions to minimize further contamination.

We create nanogaps using an electromigration technique. For heat dissipation different geometries have been fabricated by using e-beam lithography on mono(PMMA)- and bi-layer(PMMA/LOR3B) photo-resist systems. The latter is used to create nano-bridges due to underetching. In a following step Ag is evaporated on H-terminated Si(100) or Si(111) surfaces at different angles, thus forming flat Ag films in between thicker Ag contacts, which are around 50nm high and laterally separated by 200nm. The evaporation is done at 80K, i.e. continuous Ag films are obtained already for 10ML in the central part. The widths of the initial structure is around 30nm. The chemistry and the structure on the mesoscopic scale is controlled by AES, SEM and AFM. In a final step, after bonding the structures, computer-controlled electromigration is performed using a high precision current source. For excluding thermal mobility and reducing the breakdown speed, the sample has been cooled down to LN₂ temperature. As revealed from I-V characteristics, gaps of around 1nm are formed.

O 29.5 Wed 14:30 P2

Preparation of metal nanodroplets and solidification under zero-g conditions — ●ANJA HABENICHT, PAUL LEIDERER, and JOHANNES BONEBERG — Universität Konstanz, Fachbereich Physik, LS Leiderer, 78457 Konstanz

Flat metal nanostructures on inert substrates (e.g. glass) are illuminated by single intensive laser pulses with fluences above the melting threshold. The liquid structures produced in this way are far from their equilibrium shape and a dewetting process sets in. On a timescale of a few nanoseconds the liquid contracts toward a sphere. During this contraction the center of mass moves upward, which can lead to detachment of droplets from the surface due to inertia. The velocity of the detaching nanodroplets is measured with a light barrier technique and compared with the velocity deduced from simple estimations for the dewetting process [1].

Further we show impact experiments where the droplets are landed on another substrate. The particles cool down during the flight due to thermal radiation. They solidify either during flight or when impacting on the substrate. By catching at different distances, the landing temperature and thus, if still liquid, the time on the substrate while liquid can be varied. Snapshots of different stages of droplet impact are shown.

[1] A. Habenicht, M. Olapinski, F. Burmeister, P. Leiderer, J. Boneberg. Science 309 (2005) 2043

O 29.6 Wed 14:30 P2

Double layers from polycyclic aromatic hydrocarbons as studied by STM and STS — ●MIN AI¹, FRANK JÄCKEL¹, JI SHAN WU², KLAUS MÜLLEN², and JÜRGEN P. RABE¹ — ¹Humboldt University Berlin, Department of Physics, Newtonstr. 15, 12489 Berlin — ²Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz

We present the investigation of functionalized hexa-perihexabenzocoronenes (HBC) by scanning tunneling microscopy (STM) and spectroscopy (STS) at the liquid-solid interface. For star-shaped HBC derivatives different mono- and double layer structures were observed depending on the solvent that can be incorporated [1]. For composites of electron rich HBC derivatives (donors) with electron acceptors different architectures were observed, some of which can be solved with atomic precision using as additional information the spectroscopic data obtained from STS [2]. The potential for prototypical single-molecule electronic devices is discussed.

[1] Jäckel, F.; Ai, M.; Wu, J.; Müllen, K.; Rabe, J.P. *J. Am. Chem. Soc.* 2005, 127, 14580. [2] Jäckel, F.; Watson, M.D.; Müllen, K.; Rabe, J.P. submitted.

O 29.7 Wed 14:30 P2

Lithographic Fabrication of Clean Nanostructures by Means of Electron-Beam Induced Deposition (EBID) — ●M. SCHIRMER, T. LUKASCZYK, H. MARBACH, and H.-P. STEINRÜCK — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstraße 3, D-91058 Erlangen, Germany

EBID is the electron induced decomposition of chemical compounds and the resulting deposition of the non-volatile fragments. By utilizing a sharp spot of electrons well defined deposit structures in the nanometer range can be achieved in a controlled manner. A common difficulty is the contamination of the deposits due to e.g. residual gases. To avoid this problem an ultra high vacuum chamber is utilized. The integrated UHV electron column creates an electron-beam approximately 2 nm in diameter. This instrument in combination with a lithographic package enables the controlled fabrication of clean nanostructures via EBID. For the characterization of the obtained structures the following probe techniques are housed in the same UHV chamber: scanning tunnelling microscopy, scanning Auger electron microscopy and scanning electron microscopy. To generate pure carbon structures the hydrocarbon ethylene (C_2H_4) is tested. Other promising candidates for EBID are chemical compounds like silane (SiH_4), metal hydrides or organometallic compounds. The concept of the project and first results will be discussed.

O 29.8 Wed 14:30 P2

Influence of pulsed laser light on gold triangles: Experiment vs. theory — ●JULIANE KÖNIG-BIRK¹, KEVIN SHUFORD², GEORGE SCHATZ², JOHANNES BONEBERG¹, and PAUL LEIDERER¹ — ¹Fachbereich Physik, LS Prof. Dr. Leiderer, Universität Konstanz, 78457 Konstanz — ²Chemistry Department, Northwestern University

The optical properties of nanostructures are a topic of current investigations. In analogy to the near-fields around a Hertz dipole we expect near-fields in the surrounding of all nanostructures. To visualize these near-fields we use a method called "optical near-field photography". In our experiments we use e.g. silicon as substrate. The nanostructures, in this case gold triangles, on the substrate are illuminated with femtosecond laserpulses. The intensity is adjusted such that no influence of the illumination is detectable on the bare substrate. When illuminating ARRAYS of nanostructures we observe ablation of the substrate below the gold triangles due to the local intensity enhancement in the optical near-field. Depending on the polarization of the laser light, two or one corner of the triangle show ablation holes. In contrast to simulations on single triangles these effects are rotated at 90°. When illuminating SINGLE nanostructures we observe good agreement with the simulation.

O 29.9 Wed 14:30 P2

Fabrication of Gold Nanoparticles using Nanosphere Lithography in Combination with Laser Tailoring — ●RODICA MORARESCU, FRANK HUBENTHAL, and FRANK TRÄGER — Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology- CINSaT, Universität Kassel, Heinrich-Plett Strasse 40

In order to overcome the classical limits of silicon technology the use of molecular circuits is a challenging new possibility. The idea behind this is to use molecular wires as active elements, thus reducing circuit dimensions to the molecular scale. As a possible approach to realize such structures, we describe exploratory experiments for the preparation of regular arrays of metal nanoparticles by nanosphere lithography (NSL) and their exploitation as anchor points for the formation of uni- and bi-directional molecular nanowires with a high degree of lateral orientation. Depending on the molecular species and length of the nanowires to be oriented on a substrate surface, the distance between the metal nanoparticles as well as their size and shape have to be chosen independently. For these purpose we apply nanosphere lithography in combination with laser based tailoring of the dimensions of the nanoparticles. In the past we have already achieved laser manipulation of the size and shape of gold and silver nanoparticles. Here we have further produced hexagonally close packed monolayers of latex spheres by the tilt coating method, gold atoms being deposited using electron beam evaporation under ultra high vacuum conditions. An array of triangularly shaped gold nanoparticles remains on the substrate, after the mask is removed. Subsequently, the interparticle spacing and particle shape are varied by laser tailoring.

O 29.10 Wed 14:30 P2

IR-spectroscopy of Pb films and nanowires — ●F. KOST¹, T. KOLB¹, R. LOVRINCIC¹, F. NEUBRECH¹, A. PUCCI¹, M. JALOCHOWSKI², and G. FAHSOLD¹ — ¹Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität, 69120 Heidelberg, Germany — ²Institute of Physics, Maria Curie-Skłodowska University, 20031 Lublin, Poland

The conductivity of metal films and nanowires can be specified via IR spectroscopic measurements which allow analysing these structures in a non-contact mode. The experimental setup enables in-situ investigation in an UHV chamber and therefore, the growth during lead evaporation to a silicon substrate can be investigated. Since the mean free path of electrons at Fermi energy and at room temperature for lead is roughly ten nanometers, classical size effects occur as the film thickness is of this order of magnitude. Quantum size effects are expected as well since the diameter of the nanostructure reaches the range of several ten times the Fermi wavelength [1]. Using a model for charge transport, we describe the measured spectra and explore the development of relaxation rate and plasma frequency and hence get information about scattering effects, band structure and film morphology [2]. In order to obtain nanowires for IR spectroscopic studies, lead is evaporated onto a single-domain stepped silicon substrate. Thereby, solid like nanowires of Pb align parallel to the step edges of the silicon due to self-organization processes [3].

[1] Trivedi, N. and Ashcroft, N.W., *Phys. Rev. B* 38 (1988), 12298 [2] G. Fahsold and A. Pucci, *Adv. in Solid State Physics*, Vol. 43, ed. by B. Kramer (Springer, 2003) 833. [3] M. Jalochowski, M. Strozak, R. Zdyb, *Appl. Surf. Sci.* 211 (2003) 209-215.

O 29.11 Wed 14:30 P2

Angle-resolved photoelectron spectroscopy on self-assembled dysprosium-silicide nanowires on vicinal Si(001) — ●SYLVIA HAGEDORN¹, MARTINA WANKE¹, GERD PRUSKIL¹, MARIO DÄHNE¹, DENIS VYALIKH², FRIEDRICH SCHILLER², SERGEIJ MOLODTSOV², and CLEMENS LAUBSCHAT² — ¹Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin — ²Institut für Festkörperphysik, Technische Universität Dresden, D-01219 Dresden

Rare-earth silicide nanowires attract considerable interest due to their simple preparation and their anisotropic electronic properties. We report on angle-resolved photoelectron spectroscopy investigations of the electronic structure of dysprosium-silicide nanowires on vicinal Si(001) surfaces at BESSY II. Two types of nanowires are found depending on the specific preparation conditions. Different electronic properties of these nanowires depending on the wiretype will be presented. In nanowire direction strongly dispersing bands are found crossing the Fermi energy, while also a slight dispersion in perpendicular direction will be discussed in detail. Hence dysprosium-silicide nanowires could be interesting for contacting devices in future nanocircuit technologies.

This project was supported by DFG, project number DA 408/11.

O 29.12 Wed 14:30 P2

Electrochemically Fabricated Nanoscale Copper Wires: Investigation of Wire Morphology and Composition — ●THOMAS KOCH^{1,2}, SHENG ZHONG^{1,2}, EBERHARD NOLD³, TORSTEN SCHERER², HARALD ROESNER², HORST HAHN², STEFAN WALHEIM², MU WANG⁴, and THOMAS SCHIMMEL^{1,2} — ¹Institute of Applied Physics, University of Karlsruhe, D-76128 Karlsruhe, Germany — ²Institute of Nanotechnology (INT), Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany — ³Institute for Materials Research I (IMF I), Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany — ⁴National Laboratory of Solid-State Microstructures, Nanjing University, Nanjing 21009, China

Metallic nanostructures, especially made from copper, have attracted considerable attention in recent years due to their potential use both as interconnects and as components for future generations of electronics. Here we report on the investigation of electrochemically self-assembled copper wires by SEM, TEM and SAMS. The wires were found to be straight, regular, without branches and more than 100 micrometer long. These wires align spontaneously to form ordered arrays, covering the insulated substrate in large numbers. The thickness of the wires can be controlled by the experimental parameters down to 120 nm. The SAMS results show that the investigated stable structures consist of pure copper. The TEM results point out that the wires consist of stacked single crystalline copper lamellae, which have a thickness of down to a few monolayers. The SAMS depth profiles show that the wires are surrounded by an oxide layer with a thickness of less than 15 nm.

O 29.13 Wed 14:30 P2

Crescent-shaped noble-metal structures: preparation, optical properties and applications — ●NOELIA BOCCHIO, HEIKO ROCHHOLZ, JENIFFER SHUMAKER-PARRY, NATALIE HORN, and MAXIMILIAN KREITER — Max Planck Institut für Polymerforschung, Ackermannweg 10, D-55128, Mainz, Germany

Crescent-shaped metallic nanoparticles in the 60 nm - 400 nm size range were developed applying a combination of nanosphere lithography, metal deposition and ion-milling techniques. They were characterized by scanning electron microscopy and UV-Vis/NIR extinction spectroscopy (1). As expected from the symmetry of the system, the structure exhibits different responses to illumination polarised along the two symmetry axes. For both cases, distinct resonances are observed. A systematic study of the impact of variations of the most relevant geometrical parameters on the optical response is presented.

In the search for an explanation of these experiments and a full understanding of the optical response of the system, a first approach to the resonant responses through a simplified multipole model is presented and discussed.

Finally, single entity scattering and fluorescence measurements on the particles are introduced, laying the basis for applications in near-field enhanced spectroscopy.

(1) Adv. Mater. , 2005, 17, 2131 - 2134

O 29.14 Wed 14:30 P2

Surface Plasmon Polariton excitation on gratings with tunable grating constant — ●MICHAEL BERNDT^{1,2}, STEPHANIE REHWALD^{1,2}, FRANK KATZENBERG³, KLAUS SCHIERBAUM², and DOMINIC ZERULLA¹ — ¹UCD Dublin, School of Physics, Dublin 4, Ireland — ²Heinrich-Heine-Universität Düsseldorf, Materialwissenschaft, 40225 Düsseldorf, Germany — ³Universität Dortmund, Werkstoffe und Korrosion, 44227 Dortmund, Germany

For the excitation of Surface Plasmon Polaritons (SPP) grating couplers with tunable periodicity have been developed. Since the excitation of SPPs for a given grating period is restricted to a single, fixed wavelength at a certain angle of incidence, the possibility of adjusting the grating period provides much more flexibility to match resonance conditions, e. g. with respect to changes in the excitation wavelength.

Therefore the polymer based gratings present a well adapted substrate for extremely surface sensitive spectroscopic methods like Surface Plasmon Resonance (SPR) or Surface Enhanced Raman Scattering (SERS). The grating coupler consists of a polymer base upon which a sinusoidal structure is generated. Subsequently, the system is coated with a suitable metal (e.g. silver, gold, or aluminium).

Even though the metal stripes are separated by a nonconducting polymer, a strong surface plasmon resonance is observed. The experimentally obtained SPP dispersion relation is in good agreement with theoretical predictions with respect to an effective dielectrical constant for the metal-polymer surface.

O 29.15 Wed 14:30 P2

Optical Effects of Surface Plasmons Confinement in Planar Nanoparticles — ●MANUEL GONÇALVES, ANDRÉ SIEGEL, and OTHMAR MARTI — Department of Exp. Physics, University of Ulm, D-89069 Ulm, Germany

The scattering of light by metallic nanoparticles and nanostructures is intimately related with the surface plasmon-polaritons (SPP). Material, shape and size of the particles influence the confinement of the SPPs and their resonances. When the k-vector of the SPPs and the k-vector of light match a radiative process occurs. Small particles of the size of the wavelength, with sharp corners and edges, generate scattered waves with large k-vector and, therefore, are appropriate to study the scattering of light by SPPs.

We have investigated arrays of planar metallic particles of triangular shape, with different thicknesses and of different materials. The optical far-field characterization was done using a Total-Internal-Reflection illumination setup and a confocal microscope. The near-field was investigated using a SNOM microscope in illumination mode. It was observed that the scattering of laser light is strongly dependent on the material of the particle, on its orientation and on the polarization of light. We present an overview of the optical effects observed.

O 29.16 Wed 14:30 P2

Observation of Ferromagnetic Coupling in Eu/Gd(0001) by Spin-Resolved Photoelectron Spectroscopy — ●YURY DEDKOV¹, ELENA VOLOSHINA², THOMAS KLEISSNER¹, STEFFEN DANZENBAEHER¹, SERGUEI MOLODTSOV¹, and CLEMENS LAUBSCHAT¹ — ¹Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany — ²Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany

We report on a magnetic analysis by means of spin-resolved photoelectron spectroscopy of an atomically flat heteromagnetic rare-earth interface of 1 ML Eu/Gd(0001). The measurements reveal a high net Eu magnetization at low temperatures reflected by a spin polarization of about +15% of the Eu 4f state. This magnetic Eu configuration is due to a strong ferromagnetic interlayer exchange coupling across the Eu/Gd interface which overcomes a weak negative intralayer coupling between Eu spins in the hexagonal two-dimensional lattice.

O 29.17 Wed 14:30 P2

Optical properties of ultrathin magnetic layers on Cu(110) — ●RICHARD DENK, ROBERT MITTERMAIR, MICHAEL HOHAGE, LIDONG SUN, and PETER ZEPPENFELD — Institut für Experimentalphysik, Johannes Kepler Universität Linz, A-4040 Linz, Austria

Magnetic thin films of Ni and Co on Cu(110)(2x1)O have been studied by means of Reflectance Difference Spectroscopy (RDS). The regular optical anisotropy signal has been used to monitor the morphology of the Co and Ni films during growth. In addition the magnetization of these films has been addressed by the RD-spectrometer via Magneto-Optical Kerr Effect (MOKE) measurements [1]. To perform the magnetic measurements the UHV chamber is equipped with an in-situ electromagnet. The present RD-MOKE setup allows conducting spectroscopic measurements of the magnetization of the films at photon energies between 1.5 eV and 5.5 eV. By applying the RD-technique at opposite magnetization (M^+ , M^-) of the film, the optical anisotropy signal $(\Delta r/r(M^+) + \Delta r/r(M^-))/2$ can be separated from the MOKE signal $(\Delta r/r(M^+) - \Delta r/r(M^-))/2$. Hysteresis curves at any desired photon energy between 1.5 eV and 5.5 eV can be recorded online. For characterization of the film morphology, the chamber is equipped with a STM and a LEED/AES system. A major focus of the study has been the temperature dependence of the magnetization of Ni on the oxygen precovered Cu(110) surface, as well as the way how the remanent polar magnetization develops within the ultrathin Ni films. References [1] M. Wahl, Th. Herrmann, N. Esser, and W. Richter, phys. stat. sol. 0, 3002 (2003)

O 29.18 Wed 14:30 P2

Monte Carlo simulations of small transition metal oxide clusters: a comparison of numerical efficiency — ●RALF GEHRKE and KARSTEN REUTER — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany

Structural information is a key prerequisite to understand the peculiar chemical, optical, magnetic and materials properties of small transition metal oxide clusters. This concerns not only the ground state structure, but also all lowest-energy isomers within a thermally accessible energy range. Identification of these states requires proper sampling of the vast configurational space, suitably carried out by Monte Carlo (MC) based schemes. In order to make such simulations quantitative, they have to be based on reliable first-principles energetics, e.g. from density-functional theory. Due to the high computational cost of the latter techniques, utmost efficiency of the MC algorithms in terms of energy and force calls is mandatory.

As a prelude to targeted first-principles MC simulations, we therefore assess and optimize the efficiency of different MC schemes like basin hopping [1] or Wang-Landau sampling [2]. As representative test systems we use M_3O , M_5O_3 and M_7O_7 ($M = Ru, Pd$) oxide clusters described by a model Lennard-Jones potential. Since the evaluation of forces in first-principles methods is computationally more expensive than the calculation of energies, special emphasis is put on minimizing the number of required structural relaxations in the MC algorithms.

[1] D. Wales *et al.*, Science **285**, 1368 (1999).

[2] M. Scott Shell *et al.*, Phys. Rev. E **66**, 056703 (2002).

O 29.19 Wed 14:30 P2

DFT-Investigations of Coalescence Behaviour of small magic Si Clusters on Surfaces — ●WOLFRAM QUESTER and PETER NIELABA — Fachbereich Physik, Universität Konstanz, 78457 Konstanz

Experimental results indicate that small magic Si clusters do not form islands of bulk Si on weakly interacting surfaces (HOPG). For Si₄ this was confirmed in earlier calculations [1].

These investigations were extended to Si₇. Potential energy curves of two approaching Si₇ clusters were calculated for different reaction channels using Density Functional Theory implemented in the CPMD code available at [2]. It could be shown that there are fusion barriers higher than room temperature. This can be understood looking at the distribution of the electron density in the clusters.

The next step will be to model the graphite surface and investigate their influence on the cluster energetics.

[1] M. Grass, D. Fischer, M. Mathes, G. Ganteför and P. Nielaba, *Appl. Phys. Lett.*, **81**, 3810 (2002)
[2] www.cpmd.org

O 29.20 Wed 14:30 P2

Investigation of the morphology and electronic properties of small gold clusters and the impact of different organic ligands — ●MATHIS GRUBER^{1,2}, GEORG HEIMEL², LORENZ ROMANER^{1,2}, JEAN-LUC BRÉDAS², and EGBERT ZOJER^{1,2} — ¹Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria — ²School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400

The synthesis and characterization of small metal clusters, both neutral and charged, have been the focus of vast experimental and theoretical efforts. Recently, small noble-metal clusters coated with a shell of organic ligands have received a lot of attention in the context of nanotechnology and molecular electronics. The motivation for the present theoretical study is to gain a basic understanding of the electronic structure of gold nanoclusters, its dependence on the geometric shape of the clusters, and the modification induced by organic ligands covalently bound to the particles. To that end, we performed density functional theory calculations on small gold clusters. We employed quantum-mechanical molecular dynamics simulations in order to find favored (low-energy) geometric structures with and without symmetry constraints. For all conformations, we performed a detailed analysis of the electronic properties focusing on the relation between morphology and total electronic spin. When studying clusters bearing conjugated organic ligands, we paid particular attention to the alignment of their molecular levels relative to the quasimetallic states of the gold nanoparticles.

O 29.21 Wed 14:30 P2

Calculation of radiation damping of plasmons in prolate gold nanoparticles — ●CHRISTIAN DAHMEN, STEFAN BECKER, and GERO VON PLESSEN — Nanostructure Optics Group, I. Physikalisches Institut (IA), RWTH Aachen, 52056 Aachen

Plasmon resonances of non-spherical noble-metal nanoparticles are of interest for possible applications in plasmon-enhanced spectroscopy, such as surface-enhanced Raman scattering. Theoretical work has mainly focussed on calculating the spectral position of the plasmon resonance and the optical field enhancement for irregularly shaped particles. In this work, we discuss how the radiation damping rate of prolate spheroidal gold nanoparticles depends on volume and shape of the particles. The separation of variables method [1] is employed to calculate their scattering cross sections. The contribution of the radiative plasmon decay to the total linewidth of the plasmon resonance is determined. We find that the radiative decay rate depends sensitively on both the particle volume and the aspect ratio.

[1] S. Asano and G. Yamamoto, *Appl. Opt.* **14**, 29-49 (1975)

O 29.22 Wed 14:30 P2

Fabrication and characterization of gold nanocrystals for use as probes in the diffracted x-ray tracking technique — ●ARMIN BRECHLING, JAWAD SLIEH, WIEBKE HACHMANN, ULF KLEINEBERG, and ULRICH HEINZMANN — University of Bielefeld, Molecular and Surface Science, D-33615 Bielefeld

Diffracted x-ray tracking (DXT), a new single molecule experiment, uses x-rays to monitor the rotating motions of a labeled nanocrystal. This technique has the potential to resolve intramolecular conformation changes in the scale of few picometers with a time resolution in the ms interval [1].

For this technique it is essential to prepare stable, highly ordered nanocrystals. Further it is advantageous to use a biocompatible material. Gold is a suitable material in biophysical studies because it can

be directly linked to the thiol groups of cystein in protein molecules [2].

We report the fabrication of dispersive gold nanocrystals using a vacuum evaporation technique. Gold has been evaporated under ultra high vacuum conditions on a freshly cleaved NaCl (100) surface at a substrate temperature of approximately 350°C. The substrate with the gold layer, grown in an island-type structure, was subsequently dissolved in an aqueous CHAPS-solution in order to get dispersed gold crystals.

The gold nanocrystals have been characterized by means of different techniques such as Atomic Force Microscopy (AFM), Transmission Electron Microscopy (TEM) and X-Ray Diffraction (XRD).

[1] Y. C. Sasaki et al. *Phys. Rev. Lett.* **87** (2001) 248102-1

[2] Y. C. Sasaki et al. *Biophys. J.* **72** (1997) 1842

O 29.23 Wed 14:30 P2

Scanning Tunnelling Microscopy and Photoemission of Clusters at Surfaces — ●MARKUS BIELETZKI¹, THOMAS IRAWAN¹, STEFANIE KRAUSE¹, HEINZ HÖVEL¹, CHUNRONG YIN², and BERND VON ISSENDORFF² — ¹Universität Dortmund, Experimentelle Physik I, 44221 Dortmund, Germany — ²Universität Freiburg, Fakultät für Physik, 79104 Freiburg, Germany

We study the electronic structure of cluster/surface systems and the nature of charge transfer processes between the cluster and the surface. STM/STS and UPS on size selected large clusters in contact with a surface will be combined with photoelectron spectroscopy on the same clusters in the gas phase. The direct comparison of the three different techniques is expected to improve the understanding of the cluster-surface interaction. For metal islands (gold and lead) on different surfaces (HOPG, Au(111) and Pb(111)) the electronic coupling to the surface and charging effects in the photoemission process were studied with UPS. We observed significant energetic shifts if the islands were decoupled from the surface by a thick rare gas layer and different materials for the substrate and the islands were used [1]. C₆₀ is a promising model system for STS on clusters at surfaces.

[1] T. Irawan, D. Boecker, F. Ghaleh, C. Yin, B. v. Issendorff and H. Hövel, "Metal Clusters on Rare Gas Layers - Growth and Spectroscopy", *Appl. Phys. A* (published online Sept. 2005)

O 29.24 Wed 14:30 P2

Oxidation of Au/Ag-nanoparticles and clusters on HOPG/SiO₂ surfaces — ●RAINER DIETSCHKE, DONG CHAN LIM, MORITZ BUBEK, IGNACIO LOPEZ-SALIDO, YOUNG DOK KIM, and GERD GANTEFÖR — Fachbereich Physik, Universität Konstanz, 78464 Konstanz

Au nanostructures were prepared on HOPG and SiO₂ surfaces. Size distribution was studied using STM. Oxidation and reduction of the particles was performed with atomic oxygen and carbonmonoxide under UHV conditions. XPS spectra of the Au 4f level show different behaviour depending on particle size.

On HOPG Au nanoparticles smaller than ~10 nm two different oxygen species were detected, suggested to be Au-oxide and subsurface oxygen. Both species show different reactivity towards CO.

On silica layers the oxidation/reduction behaviour of Au nanoparticles show a strong size dependency. Larger particles exhibit additional features of the Au 4f level. Whereas particles smaller than ~7 nm in height show a much less reactive type of Au-O bond.

Au and Ag clusters were deposited and studied with the same method. Small Au clusters on SiO₂ show a significant even-odd size dependency in CO oxidation.

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[3] Lopez-Salido, Lim and Kim, *Surface Science*, **588** (1-3) 6-18, 2005

O 29.25 Wed 14:30 P2

Mo_nS_m- and W_nS_m-clusters: Nano-platelets and nano-wires — ●WILKO WESTHÄUSER, TIM FISCHER, NILS BERTRAM, JÖRN CORDES, RAINER DIETSCHKE, MORITZ BUBEK, and GERD GANTEFÖR — University of Konstanz, Department of Physics, D-78457 Konstanz

Clusters of the layered semiconductor materials MoS₂ and WS₂ may form fullerenes similar to carbon. Therefore, we used gas phase mass and photoelectron spectroscopy in combination with Density Functional Theory calculations in order to investigate small Mo_nS_m- and W_nS_m-clusters. E. g. the Mo₄S₆-clusters revealed a large HOMO-LUMO gap

(about 2eV) indicating to be a so-called “magic cluster” with a high stability and chemical inertness [1,2].

In mass spectra of Mo_nS_{m-} and W_nS_{m-} clusters with $n>5$ atoms the theoretically predicted stable 2-d triangular platelet structures were detected and 1-d chain-like clusters of the stoichiometry $Mo_{3n}S_{3n+2}$ were identified and characterised with PES. In addition, selected clusters were deposited in soft-landing mode on HOPG-, Au- and Ag- substrates in order to study the interaction of the clusters with the metal surfaces via XPS, AES and HREELS.

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O 29.26 Wed 14:30 P2

Preparation of bimetallic AuAg/TiO₂ model catalysts — ●C. WEILACH, S. KIELBASSA, J. BANSMANN, and R.J. BEHM — Dept. of Surface Chemistry and Catalysis, University of Ulm

Studies on powder catalysts revealed, that using AuAg bimetallic particles instead of monometallic particles on metal oxides may enhance the performance and the stability of the catalytic system. Exploiting model catalysts with nm-sized bimetallic particles on flat TiO₂(110) single crystal surfaces will give new insights on the significance of particle composition and size with respect to catalyst activity and stability. Therefore, we examined the growth of AuAg nanoparticles by subsequent evaporation and the influence of substrate temperature and evaporation order on this process. Furthermore we developed a new preparation method resulting in samples with metal particles of different composition. This creates the opportunity to investigate the morphology with AFM and the catalytic activity with a newly designed scanning-mass spectrometer setup at chemically different regions on one substrate.

O 29.27 Wed 14:30 P2

Particle removal by laser-induced acoustic waves — ●TOBIAS GELDHÄUSER, FLORIAN ZIESE, JOHANNES BONEBERG, and PAUL LEIDERER — University of Konstanz, Fach M676, Universitaetsstrasse 10, 78457 Konstanz

Different approaches can be used for particle removal from surfaces like ultra-/megasonics or Dry / Steam Laser Cleaning. Here we analyze an alternative approach where a laser pulse hits the back of a wafer and thereby initiates a bulk acoustic wave which travels towards the wafer surface, leading to surface displacements and particle removal. We relate the cleaning efficiency for colloidal contaminants of different diameters (measured by light scattering) to the surface expansion, and hence the acceleration, which is measured with a ns-time-resolved Michelson Interferometer. Furthermore the backside configuration is modified by sacrificial layers in order to enhance the intensity of the acoustic wave.

O 29.28 Wed 14:30 P2

Studying the dewetting behaviour of Ni-films on oxidized Si(001) by GISAXS — ●F. GARONE¹, ANDREA TOMA¹, FRANCESCO BUATIER¹, CORRADO BORAGNO¹, UGO VALBUSA¹, IAN K. ROBINSON², WEI ZHANG², NICOLE M. JEUTTER³, and ROBERTO FELICI³ — ¹Dipartimento di Fisica, Università di Genova, via Dodecaneso 33, 16146 Genova, Italy — ²Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, IL 61801-3080, USA — ³ESRF, 6 Rue Jules Horowitz, 38000 Grenoble France

The development of materials with new electronic and/or chemical properties is pushing the research through the study of nano-objects. For obtaining surfaces with morphology features on the nano-meters scale, we can take advantage of self-aggregation phenomena, which is generally easier to integrate in industrial processes. However the size uniformity and control, they offer, are more complex. A method for obtaining metal nano-objects at the surface of oxides is based on dewetting phenomena. In this case a thin metal film grown on an inert substrate is heated up at high temperatures, until the surface tension of the metal becomes higher than the adhesive force of the film onto the substrate. At this point the metal forms small droplets. In this study we present real-time in-situ studies of the nucleation and formation of Ni metal clusters starting from an uniform metal film deposited on an oxidized Si(001) substrate. Films of different thicknesses have been annealed at different temperatures in the range 400-800 K. By following in time the evolution of the grazing incidence small angle scattering pattern we gained unique information on the dynamics at the base of the nano-particles formation.

O 29.29 Wed 14:30 P2

Femtosecond Pump-Probe Measurements of Silver Nano-Clusters on Quartz (0001) — ●ALEXANDER GRUJIC, KONRAD VON VOLKMAN, and MARTIN WOLF — Fachbereich Physik der Freien Universität Berlin, Arnimallee 14, 14195 Berlin

We have measured the energy relaxation of supported silver nano-clusters by time resolved transient absorption spectroscopy. The clusters are prepared in UHV via VOLMER-WEBER growth by evaporation of silver on a single crystal quartz (0001) sample at room temperature, resulting in a mean cluster size of ≈ 12 nm. The sample was excited by 400-nm pump pulses with 40-fs duration, and the transmission was probed with a beam of the same wavelength. In-situ temperature, size and fluence dependent transmission measurements have been performed and a fast ($\approx 2 \dots 3$ ps) and a slow (≈ 150 ps) decay channel have been identified. They are attributed to the electron-phonon relaxation within the silver cluster and the much slower heat transfer of the cluster lattice to the quartz substrate.

O 29.30 Wed 14:30 P2

Oxidation of electrochemically deposited nanocrystalline aluminium — ●FABIAN BEBENSEE^{1,2}, WOLFGANG MAUS-FRIEDRICHS¹, and FRANK ENDRES² — ¹Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, D-38678 Clausthal-Zellerfeld — ²Institut für Metallurgie, TU Clausthal, Robert-Koch-Str. 42, D-38678 Clausthal-Zellerfeld

The applicability of nanocrystalline aluminium in semiconductor devices and corrosion protection is crucially dependent on the oxidation behaviour and interaction of nanocrystalline aluminium with molecules from the ambient atmosphere. Nanocrystalline aluminium with grain sizes around 20 nm was deposited onto Si(100) substrates via electrodeposition in the ionic liquid 1-butyl-1-methylpyrrolidinium-bis(trifluoromethylsulfonyl)imide, saturated with anhydrous AlCl₃. The interaction of nanocrystalline aluminium with oxygen was studied with Metastable Impact Electron Spectroscopy (MIES), Ultraviolet Photoelectron Spectroscopy (UPS) and X-Ray Photoelectron Spectroscopy (XPS). The oxidation behaviour of nanocrystalline aluminium is compared to the oxidation behaviour of aluminium films prepared by physical vapour deposition (PVD). The topography of the films being strongly dependent on the deposition parameters was investigated with microscopic techniques.

O 29.31 Wed 14:30 P2

Non-Destructive Trace Element Analysis of Presolar Stardust via XANES-PEEM — ●THOMAS BERG¹, PASQUAL BERNHARD¹, JOCHEN MAUL¹, NICOLE ERDMANN², CHRISTA SUDEK³, ULRICH OTT³, and GERD SCHÖNHENSE¹ — ¹Universität Mainz, Institut für Physik, D-55099 Mainz — ²Universität Mainz, Institut für Kernchemie, D-55099 Mainz — ³Max-Planck-Institut für Chemie, D-55128 Mainz

Meteorites contain small amounts of presolar dust that survived the formation of the solar system without being affected by the isotope homogenisation. Therefore the isotopic composition not only of bulk elements, but also of trace elements(1) is anomalous. Isotopic analysis via SIMS(2) / RIMS(3) often reveals the fingerprint of the nucleosynthetic s-process that occurred in the grain's origin star. The disadvantage of SIMS/RIMS, however, is that only a small number of isotopes can be investigated, because the sample grain is being destroyed. We present non-destructive synchrotron based XANES measurements using PEEM. Prior to isotopic analysis this technique is suitable for identification of interesting trace elements present in single stardust grains. In addition, XANES-PEEM provides information on the chemical environment in which the different elements occur within the particles. Supplementing TOF-SIMS measurements(4) confirming the XANES-PEEM results are also presented.

- (1) E.Zinner, Annu.Rev.Earth Planet.Sci.26(1998)147
- (2) K.K.Marhas, P.Hoppe, U.Ott, Meteorit.Planet.Sci.38(2003)A58
- (3) M.R.Savina et al., Geochim.Cosmichim.Acta67(2003)3201
- (4) T.Stephan, Planetary Space Sci.49(2001)859

O 29.32 Wed 14:30 P2

A Scanning Probe Microscope (SPM) with quasi in-situ Sample Treatment Capabilities — ●MARKUS HUND¹ and HANS HEROLD² — ¹Physikalische Chemie II, Universität Bayreuth, D-95440 Bayreuth — ²Elektronikwerkstatt der Universität Bayreuth, D-95440 Bayreuth

State-of-the-art SPMs have limited *in-situ* sample treatment capabilities. Aggressive treatments like plasma etching or etching in aggressive

liquids typically require to remove the sample from the microscope. In consequence, time consuming procedures are required if the same spot of the sample is to be imaged after successive processing steps. We have developed a first prototype of an SPM with quasi *in-situ* sample treatment capabilities based on a commercial atomic force microscope (AFM; Model Dimension 3100, Veeco Instruments Inc.). A sample holder is positioned in a special reactor chamber. The tip can be retracted by several millimeters such that the chamber can be closed for sample treatment. Most importantly, after the treatment the tip is moved back to sample with a lateral drift per process step in the 20 nanometer regime. We discuss recent experiments involving consecutive plasma etching of nanostructured polymer films.

O 29.33 Wed 14:30 P2

Two dimensional dopant profiling of semiconductor microdevices with high spatial resolution using High Speed Scanning Capacitance Spectroscopy — •MARTIN VON SPREKELSEN and ROLAND WIESENDANGER — University of Hamburg, Institute of Applied Physics and Microstructure Research Center, Jungiusstrasse 11, D-20355 Hamburg, Germany

For the analysis of semiconductor devices tools with high spatial resolution down to the nanometer scale become increasingly important. Scanning capacitance microscopy (SCM) is an established method to obtain 2D-dopant profiles of charge carrier concentrations. These profiles are usually taken at a constant bias voltage (V_{bias}).

However unavoidable side effects such as mobile surface charges or the strong influence of V_{bias} on the SCM profiles are limiting factors for the spatial resolution of SCM. To overcome these restrictions we modulate the V_{bias} voltage at a frequency in the kHz-range. The modulated electric field virtually traps mobile surface charges. We use High Speed Scanning Capacitance Spectroscopy (HSSCS) to obtain capacitance spectra for V_{bias} , by which we can analytically get rid of the influence of V_{bias} .

The method can be used on Si- and III-V-semiconductors. On ultrashallow junctions on Si-semiconductor samples a high spatial resolution down to 10 nm can be achieved. Examples of practical applications of HSSCS will be shown.

O 29.34 Wed 14:30 P2

Manipulation of nanometer-scale metallic islands in ultrahigh vacuum by dynamic force microscopy techniques — •DIRK DIETZEL¹, ANDRE SCHIRMEISEN¹, HARALD FUCHS¹, and UDO SCHWARZ² — ¹Institute of Physics, University of Münster, Münster, Germany — ²Department of Mechanical Engineering, Yale University, New Haven CT, USA

The fundamentals of friction are still insufficiently understood on the nanometer-scale. Recently, a new technique for systematic island manipulation using dynamic force microscopy (DFM) in air has been introduced by Ritter et al. [1], which allows the correlation between contact area, energy dissipation during motion, and crystalline structure. However, under ambient conditions, oxidation and contamination might influence the frictional properties of the interface. To avoid this, experiments have been performed entirely under UHV conditions. Metallic islands with diameters between 10-50 nm have been grown by thermal evaporation of aluminum on highly oriented pyrolytic graphite (HOPG). The experimental protocol by Ritter et al. was adapted to UHV conditions and frequency modulation detection by gradually reducing the frequency shift setpoint. This allows determining the threshold value for energy dissipation necessary to initiate manipulation. In addition, information about the dissipated energy can be obtained even during the lateral movement. First results show that the manipulation of the islands strongly depends on their size and on the strength of the interaction between the oscillating cantilever tip and the islands.

[1] Ritter et al., Phys. Rev. B 71, 085405 (2005)

O 29.35 Wed 14:30 P2

Design of a low temperature Tuning Fork Atomic Force Microscope combined with a Field Ion Microscope — •THOMAS KÖNIG¹, DANIEL BRAUN¹, JENS FALTER², ANDRÉ SCHIRMEISEN^{1,3}, HENDRIK HÖLSCHER³, MARCUS LIEBMANN⁴, UDO D. SCHWARZ², and HARALD FUCHS^{1,3} — ¹Institute of Physics, University of Münster, Münster, Germany — ²Department of Mechanical Engineering, Yale University, New Haven, CT, USA — ³Center of Nanotechnology (CeN-Tech), University of Münster, Münster, Germany — ⁴Institute of Physics, RWTH-Aachen, Aachen, Germany

The atomic force microscope (AFM) has been established as a tool for the imaging of surfaces with atomic resolution. However, an inter-

pretation of the forces which act between tip and surface atoms is only possible if the exact configuration of the tip apex atoms is known. The last atom layers of the tip can be analyzed by field ion microscopy (FIM). We have built a non-contact mode AFM by implementing a tuning fork as force sensor [1] in a low temperature, ultra high vacuum (UHV) design [2]. This setup allows us to choose an appropriate FIM material, such as tungsten for the tip, while maintaining atomic-scale resolution capabilities. The high stability of the setup has been proven by scanning tunneling microscopy investigations. Furthermore, we present a special home-built transfer design for the tuning fork exchange between the FIM and AFM chambers in the UHV system and first atomic resolution images of tungsten tips with the FIM are shown.

[1] F. J. Giessibl, Appl. Phys. Lett. 76 1470 (2000)

[2] W. Allers et al., Rev. Sci. Instrum. 69, 221 (1998)

O 29.36 Wed 14:30 P2

Towards Automatisation of Nanotomography Imaging — •CHRISTIAN DIETZ, NICOLAUS REHSE, MECHTHILD DÖRING, SABINE SCHERDEL, and ROBERT MAGERLE — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

Nanotomography is a layer-by-layer imaging technique based on scanning probe microscopy. We present our approach to automate the process for successive etching and imaging. Thermal drift and non-linearities of the piezo scanners make it difficult to image exactly the same spot of the specimen. We correct this problem by applying an appropriate offset to the piezo scanners which is calculated from the offset between two successive images using the cross correlation coefficient. As an example, we image a thin film of polypropylene with tapping mode scanning force microscopy (SFM) and etch it successively with potassium permanganate. The etching and imaging is done *in-situ* in a liquid cell of a MultiMode SFM connected to reservoirs of etchants and water for flushing after each etching step. The flow of the different liquids is controlled with solenoid valves which allow for an automated measuring protocol. We will present first results and discuss our concepts for adjusting the imaging parameters to maintain a good imaging quality.

O 29.37 Wed 14:30 P2

Frequency Modulated Atomic Force Microscopy: Atomic Resolution and Force Spectroscopy — •GEORG SIMON, MARKUS HEYDE, HANS-PETER RUST, and HANS-JOACHIM FREUND — Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, D-14195 Berlin, Germany

Images with atomic resolution by frequency modulated atomic force microscopy (FM-AFM) on different materials have been presented. However, proper descriptions of the tip-sample interaction and contrast mechanisms are still under discussion. The understanding of these issues leads toward new insights of specific surface properties and to an extension of FM-AFM beyond topography measurements. In contrast to the simple relation connecting the static deflection of a cantilever to the interaction force, the corresponding relation for FM-AFM is significantly more complex and depends on both the spring constant and amplitude of oscillation. Here we present an experimental method for quantitative determination of the spring constant and the amplitude oscillation for a double tuning fork sensor operated at low temperature in ultra-high vacuum [1]. The quantitatively characterized measurements will be shown in combination with atomically resolved images.

[1] M. Heyde, M. Kulawik, H.-P. Rust, H.-J. Freund, Rev. Sci. Instrum. 75, 2446 (2004).

O 29.38 Wed 14:30 P2

Optimization of the preparation process for tips used in Scanning Tunneling Spectroscopy (STS) — •STEFAN ERNST¹, STEFFEN WIRTH¹, MICHAL RAMS^{1,2}, and FRANK STEGLICH¹ — ¹Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — ²Institute of Physics, Jagiellonian University, 30-059 Kraków, Poland

Scanning Tunneling Spectroscopy (STS) is a powerful method to investigate the electronic structure of material surfaces. By means of STS, it is possible to probe the local density of states of a sample with sub-nanometre spatial resolution.

One prerequisite for high resolution and stability is a good tunneling tip. In our UHV STM systems, we plan on working predominantly with tips made of tungsten. A well-established way of producing tungsten tips is electrochemical etching. However, such tips are covered with a disturbing oxide layer and are usually not sufficiently sharp. Thus, facilities for further *in-situ* tip conditioning had to be added to our UHV-STM sys-

tems. The techniques for tip conditioning which have been investigated include direct annealing, electron beam heating and self-sputtering with light ions such as neon. Differently treated tips have been characterized by means of electron microscopy, field emission and STM experiments.

O 29.39 Wed 14:30 P2

Design of an UHV-STM with a Split Coil Magnet for Low Temperature Applications — •MIKE GYAMFI, OSWALD PIETZSCH, JULIAN C. CHEN, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg

To study the spin dependent local electronic structure of single magnetic nanowires and nanoislands a new STM will be installed in a three chamber ultra high vacuum system. The STM will be operated in a liquid helium bath cryostat (expected base temperature 6 K) with a split-coil-magnet which assures good access for sample and tip exchange. A magnetic field of 5 T in z-direction will be available. A new feature of the system is a mechanism which will enable the controlled rotation of the magnetic tunnelling tip. It will provide the unique opportunity to tune the azimuth angle of an in-plane magnetised tip to a collinear configuration with the sample magnetisation in order to maximise the magnetic contrast. A further feature is the possibility to rotate the sample about the x-axis. This will allow evaporation onto the cold substrate and immediate STM measurements without loss of the microscopic position on the sample. We will discuss the design concept of the system.

O 29.40 Wed 14:30 P2

Digital Pulsed Force Mode in Ambient and Liquid Environment - Indentation of Soft Condensed Matter — •ALEXANDER GIGLER, CLAUDIA GNAHM, MICHAEL HOLZWARH, KATRIN HÜBNER, and OTHMAR MARTI — Department of Experimental Physics, Ulm University, D-89069 Ulm, Germany

AFM measurements can be conducted in every kind of environment, which makes it very suitable for material science investigations. The Digital Pulsed Force Mode (DPFM) allows the detailed investigation of the elastic and viscoelastic material parameters of samples. Thus, it is also a possible candidate for the determination of the mechanical properties of more difficult and complex structures such as biopolymers or even living cells. In this contribution the capability of the DPFM to investigate very delicate samples is demonstrated.

Due to the high volume of information acquired during the experiments, automated evaluation has been developed recently to allow a thorough physical testing of the sample materials. The possibilities of data evaluation of the force traces collected during these measurements will also be shown.

O 29.41 Wed 14:30 P2

Work function differences of C_{60} on oriented metal surfaces — •ULRICH ZERWECK, CHRISTIAN LOPPACHER, and LUKAS M. ENG — Institute of Applied Photophysics, University of Technology Dresden, 01062 Dresden

Organic semiconductors have gained increased interest with respect to their use in organic light emitting diodes. For the efficient injection of charge carriers from the metal electrodes into the organic semiconductor, a low dipole barrier height is required. Similar to most organic molecules, C_{60} also shows a linear dependence between the workfunction of the metal substrate and the dipole barrier formed between molecule and substrate. Such evidence stems from macroscopically measurements using UPS [1]. In this work, we compare these findings to microscopic inspections of local barrier heights investigating individual C_{60} molecules by the use of Kelvin probe force microscopy.

In a previous publication [2] we showed the agreement between dipole barrier heights acquired with macroscopic UPS on one hand and, on the other hand, quantitative Kelvin probe force microscopy on the nanometer scale. Recently, we were able to push the lateral resolution forward down to ≈ 10 nm, still being quantitative.

[1] I. G. Hill et al., *Appl. Phys. Lett.* **73**, 662(1998)

[2] U. Zerweck et al., *Phys. Rev. B* **71**, 125424 (2005)

O 29.42 Wed 14:30 P2

Near-field-optical investigation of surface plasmons in metal-insulator-semiconductor tunnel junctions — •TINO GÖHLER¹, JAN SEIDEL¹, STEFAN GRAFSTRÖM¹, LUKAS ENG¹, BORIS CHICHKOV², and ALAIN DEREUX³ — ¹Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Str. 1, 01069 Dresden, Germany — ²Laser Zentrum Hannover e.V., Hollerithallee 8, 30419 Hannover, Germany — ³Laboratoire de Physique de l'Université de Bourgogne, UMR CNRS 5027, 9 avenue Alain Savary, Boîte Postale 47870, F-21078 Dijon, France

In layered metal-insulator-semiconductor (MIS) structures electrons can excite surface plasmon (SP) oscillations in the metal layer via inelastic tunnelling [1]. In our experiments these structures consist of a silicon substrate covered by a thin oxide layer onto which a top metal electrode is deposited. This type of structure supports different SP modes for which the electromagnetic field is concentrated to different interfaces, namely the top metal-air interface and the bottom metal-oxide interface. SP excitation in the gap is supposed to be quite efficient with the inelastic tunnelling rate reaching $\sim 10\%$ of the elastic rate. Therefore, such MIS structures appear highly attractive as electrically pumped plasmon sources for integrated optoelectronic devices. We report here on SP emission directly investigated by scanning near-field optical microscopy (SNOM). Emphasis is placed on spectral characteristics of SPs in defined structures and at metal electrode edges.

[1] McCarthy, S. L., Lambe, J., *Appl. Phys. Lett.* **33**, 858 (1978)

O 29.43 Wed 14:30 P2

Dynamic Force Microscopy - Manifestations of Rare Atomic Jumps: Experiment and Simulation — •B. ITTERMANN¹, R. HOFFMANN¹, A. BARATOFF², L. KANTOROVICH³, T. TREVETHAN³, and H. v. LÖHNEISEN^{1,4} — ¹Physikalisches Institut und DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe, D-76128 Karlsruhe — ²NCCR on Nanoscale Science, Institute of Physics, University of Basel — ³Department of Physics, Kings College London — ⁴Institut für Festkörperphysik, Forschungszentrum Karlsruhe, D-76021 Karlsruhe

In recent non-contact scanning force microscopy experiments, jumps of the resonance frequency shift were observed below a critical tip-sample distance above specific atomic sites on a KBr (001) surface [1]. At the same distance additional energy dissipation related to the jumps sets in. The two branches of the frequency vs. distance curves between which the jumps occur are interpreted as the interaction of the surface with the tip being in two different configurational states. We proposed a model of the tip where an atom can hop from position A to position B in a double well potential. This proposal is checked with atomistic simulations for a small KBr cluster representing the tip and a KBr slab with a planar surface as sample [2]. The force as a function of distance obtained from the simulations is compatible with a double minimum potential for the different states A and B of the tip. Molecular dynamics simulations are planned in order to study the process at finite temperatures. [1] R. Hoffmann et al., to be published [2] R. Hoffmann et al., *Phys. Rev. Lett.* **92**, 146103 (2004)

O 29.44 Wed 14:30 P2

Imaging local potentials and thermovoltages with the STM — •J. HOMOTH, M. WENDEROTH, L. WINKING, T. DRUGA, and R. G. ULBRICH — IV. Physikalisches Institut der Universität Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

If tip and sample of an STM are at different temperatures, a thermovoltage arises which is correlated with the derivative of the sample's and tip's density of electronic states at the fermi level.

If the temperature difference between tip and sample is caused by a current parallel to the sample surface an additional potential component can be measured. The resulting tip-sample voltage is the sum of the local potential and the local thermovoltage.

This voltage is measured by a second interlaced feedback loop, which brings the average current from tip to sample to zero, while the tip height is kept constant. We show results for three different sample systems (semiconducting, semi-metallic and metallic) and distinguish between potential components caused by thermovoltage and the local potential.

In the case of a Si(111) surface the local thermovoltage represents the atomic corrugation in the Si(111)-7x7 reconstruction. Local potentials connected to the macroscopic field applied to the sample were measured in the case of thin metallic films. Potential components caused by ther-

movoltages were separated and potential gradients across grain boundaries and percolation structures are presented.

The work was financially supported by the SFB 602 TP A7.

O 29.45 Wed 14:30 P2

Improved design for a variable temperature scanning tunneling microscope — ●JAN WIENHAUSEN, GERMAR HOFFMANN, and ROLAND WIESENDANGER — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, 20355 Hamburg, Germany

Variable temperature scanning tunneling microscopy (VT-STM) is a versatile tool to study locally the growth of molecular systems on a carrier substrate. A recently installed VT-STM operated in ultra-high vacuum demonstrated high vertical and lateral stability down to 30 K sufficient for single molecule spectroscopy. To increase the available temperature range further we studied numerically the heat flow in the STM design. Whereas the rigid STM design itself is kept unmodified the design is optimized in terms of the heat balance. Heat transfer from a liquid helium flow cryostat is increased and heat losses to the environment are reduced. Here we will discuss the numerical results along with the detailed instrumental realization in comparison with its precursor. First applications to insitu prepared molecular films will be presented.

O 29.46 Wed 14:30 P2

The thermal resistance of a thermocouple tip in a scanning thermal microscope — ●ANDREAS KNÜBEL, ULRICH FLEISCHMANN-WISCHNATH, and ACHIM KITTEL — University of Oldenburg, D-26111 Oldenburg

The fabrication of a novel thermocouple sensor as a thermal profiler has enabled us to set up a very sensible scanning thermal microscope (SThM) based on a scanning tunnelling microscope (STM) under ultra-high vacuum conditions with high spatial resolution. This provides the possibility to an improved analysis of the frequently discussed near-field heat transfer on a nanometer scale. Because theory already provides a statement for the distance dependence of the heat transfer this quantity has to be determined experimentally for comparison. Therefore, it is essential to characterize the thermal resistance. By means of the thermal resistivity of the microscope tip its possible to quantify the heat transfer through the vacuum gap between the thermocouple tip and a cooled planar material surface from the measured temperatures. With a specially designed set-up we were able to evaluate the thermal resistance of the thermocouple.

O 29.47 Wed 14:30 P2

Video-rate Scanning Probe Microscopes: problems and solutions — ●M.J. ROST^{1,2}, G.J.C. VAN BAARLE^{1,2}, W.A. VAN LOO¹, L. CRAMA¹, P. SCHAKEL¹, E. VAN TOL¹, T.H. OOSTERKAMP¹, and J.W.M. FRENKEN¹ — ¹Kamerlingh Onnes Laboratory, Leiden University, P.O.Box 9504, 2300 RA Leiden, The Netherlands — ²Leiden Probe Microscopy, KOL, Leiden University, Niels Bohrweg 2, 2333 CA Leiden, The Netherlands

For a wide variety of surface and interface phenomena, in both fundamental and applied contexts, it is becoming increasingly important to visualize them with atomic or molecular resolution combined with high imaging speeds. We have recently developed a video-rate control system for scanning probe microscopes, including high-bandwidth amplifiers and fast data handling. From different tests, where we connected the new control electronics with several home-built and commercial instruments, we conclude that the current bottle neck in high-speed imaging is solely formed by the mechanical behaviour of the microscopes. We present new concepts and first, promising tests for high-frequency scanners, involving compact designs, new piezo geometries, and local damping solutions.

O 29.48 Wed 14:30 P2

A Besocke-type double-probe STM — ●PHILIPP JASCHINSKY, FRANZ-PETER COENEN, HELMUT STOLLWERK, GERHARD PIRUG, and BERT VOIGTLÄNDER — Institut für Schichten und Grenzflächen (ISG 3), Forschungszentrum Jülich, 52425 Jülich, Germany

A combination of a double-probe scanning tunnelling microscope (STM) with a scanning electron microscope (SEM) in ultrahigh vacuum (UHV) environment is presented. Due to a compact Besocke beetle-type design with two stages it was possible to integrate two independently driven STMs on small space. The positioning of the two tips can be controlled from macroscopic range down to 50 nm by an add-on electron column. This apparatus is a promising tool for manipulation and charac-

terizations of nanostructures on surfaces. The operation and performance of the instrument will be illustrated by several examples.

O 29.49 Wed 14:30 P2

Contact potential reading with a high-resolution tuning-fork AFM using a cantilever tip — ●SEBASTIAN TEICH, STEFAN GRAFSTRÖM, CHRISTIAN LOPPACHER, ULRICH ZERWECK, and LUKAS M. ENG — Institute of Applied Photophysics, University of Technology Dresden, 01062 Dresden

We report on a home-built tuning-fork non-contact atomic force microscope (AFM) operated with phase-sensitive electronics in the FM demodulation mode. One prong of the tuning fork is glued to a support mounted on the scanner piezo [1]. An ac voltage applied to the tuning fork electrodes induces a vibration of the free prong with an amplitude of 1-5 nm normal to the sample surface. We measure the oscillation amplitude by detecting the induced current using a lock-in amplifier. An electronic circuit compensates for the background signal originating from direct capacitive pick-up of the drive voltage. The probe-sample distance is controlled by a feedback loop such that the resonance frequency coincides with the given driving frequency. A second feedback keeps the mechanical oscillation amplitude constant, thereby providing information on the dissipation caused by the tip-sample interaction. As a probe, a commercial cantilever tip is glued to the tuning fork [2]. Various topographic structures with characteristic length scales down to 10 nm could be resolved. Furthermore, aiming for Kelvin probe force microscopy, we made the tip conductive and contacted it to one of the electrodes of the tuning fork by evaporating a metal layer onto the tip.

[1] F.J. Giessibl et al., *Nanotechnology* 15 (2004) S79

[2] S. Rozhok and V. Chandrasekhar, *Sol. Stat. Comm.* 121 (2002) 683

O 29.50 Wed 14:30 P2

Fluctuations and jump dynamics in atomic friction experiments — ●SABINE MAIER^{1,2}, YI SANG¹, TOBIN FILLETTER¹, MARTIN GRANT¹, ROLAND BENNEWITZ¹, ENRICO GNECCO², and ERNST MEYER² — ¹Department of Physics, McGill University, Montreal, Quebec, Canada — ²Department of Physics and Astronomy, University of Basel, Switzerland

We studied atomic stick-slip processes by means of friction force microscopy with high spatial and temporal resolution on KBr(100) in ultra-high vacuum. These processes are caused by the jump of the tip from one atomic position to the next. The occurrence of such stick-slip behavior is one-to-one related to energy loss in the sliding process. Thermal fluctuations in the combined system of tip, surface, and force sensor play a crucial role in the dynamics of the stick-slip behavior.

We characterized the influence of the tip-sample contact on the thermal fluctuations of the force sensor and on the dynamics of the stick-slip process. Results are compared with simulations based on an extended Tomlinson model including thermal fluctuations. A correlation between the duration of the atomic slip event and the atomic structure of the contact is established.

O 29.51 Wed 14:30 P2

Lateral and electrical forces during the manipulation of organic molecules — ●LARS ZIMMERLI, OLIVER PFEIFFER, THILO GLATZEL, SABINE MAIER, ENRICO GNECCO, ALEXIS BARATOFF, and ERNST MEYER — Institute of Physics, Klingelbergstr 82, 4056 Basel, Switzerland

The measurement of lateral forces between the tip of a force microscope and atomic scale features on a surface is an important issue in manipulation experiments. Feedback-controlled excitation of the torsional eigenmode of a rectangular cantilever beam forces the tip to oscillate parallel to the surface. We already reported the general capability to measure lateral forces using this technique [1, 2] at a step edge and we now observe these forces during the manipulation of organic molecules.

We have studied the lateral forces while manipulating single Cu-TBPP molecules on Cu[100]. Conservative and dissipative lateral interactions will be discussed while the tip is close or even directly above one porphyrine molecule. These results will be compared with those measured over a step edge or an impurity on the surface. We also studied Kelvin probe force microscopy which yields detailed information of topography and local work function on the nanometer scale. We identified distinct differences in energetics between the Cu-TBPP molecules and the substrate surface.

[1] O. Pfeiffer et al., *Phys. Rev. B* 65, 161403 (2002) [2] Ch. Loppacher et al., *Phys. Rev.* 90, 066107 (2003)

O 29.52 Wed 14:30 P2

Chirped-Pulse Two Photon Photoemission spectroscopy from surfaces — ●FELIX STEEB, STEFAN MATHIAS, MICHAEL BAUER, and MARTIN AESCHLIMANN — FB Physik, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern

Two-Photon Photoemission (2PPE) with ultrashort laser pulses is a well-established technique which has been successfully applied to the investigation of the structure and dynamics of electron excitations at surfaces. In this paper, we show that the spectral chirp of the exciting laser pulse is an additional experimental parameter which can be utilised to gather further information on the electron states involved in the 2PPE process.

A well-defined amount of spectral chirp is applied to the ultrashort laser pulse. For a series of differently chirped pulses, the appropriate 2PPE spectra were recorded. In the case of a clean and a cesium covered Cu(111) surface, we observe significant energy shifts as large as 40 meV from the occupied shockley surface state and from the unoccupied cesium resonance respectively.

Model calculations within the framework of the Liouville-von-Neumann equations reproduce the experimental results for the photoexcited adsorbate and enable us to relate this shift to the finite lifetime of the adsorbate resonance. On the other hand, a lack of any energy shift of the shockley surface state in the simulations point to a need for further development of the theoretical model. The results and future prospects, e.g. the interaction of spectral chirp and adsorbate motion are discussed.

O 29.53 Wed 14:30 P2

Theoretical Study of the Electron Dynamics at the Silicon (100) 2x1-Surface — ●NORBERT BÜCKING^{1,2}, MARTIN SLOWIK¹, PETER KRATZER², MATTHIAS SCHEFFLER², and ANDREAS KNORR¹ — ¹Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — ²Fritz-Haber-Institut der Max-Planck-Gesellschaft, Abt. Theorie, Faradayweg 4-6, 14195 Berlin, Germany

Recent photoemission experiments call for a detailed study of the temporal surface dynamics on silicon surfaces. We use a model for the phonon based short-time dynamics where the electron-phonon interaction of both bulk and surface states is described by Density-Functional-Theory (DFT). The surface band structure of Si(100), including the surface states D^{up} and D^{down} , is calculated using a slab geometry in local density approximation (LDA). For the bands contributing to the surface dynamics, the corresponding Kohn-Sham wave functions are used to compute electron phonon coupling matrix elements. Density matrix formalism is used to evaluate the population dynamics of excited conduction band states. Different theoretical approaches, such as Markovian and time-convolutionless (TCL) methods are compared.

O 29.54 Wed 14:30 P2

Quasiparticle lifetimes of rare-earth elements, transition metals and noble metals — ●ALEXANDER MÖNNICH, JÖRG LANGE, MICHAEL BAUER, and MARTIN AESCHLIMANN — FB Physik, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern

The dynamics of excited (hot) electrons play an important role in surface physics and chemistry. It is therefore important to address the question of how the bulk electronic structure influence the mean free path and the excited electron lifetimes. For excitation energies > 10 eV the so called universal curve allows a rather good estimate of these quantities. However, at low excitation energies ($E - E_F < 10$ eV) there can be significant deviations from this approximation.

With the time resolved two-photon photoelectron spectroscopy (TR-2PPE) method we investigated the electron dynamics in various noble, transition and rare earth metals up to excitation energies $E - E_F = 3$ eV. The characteristics of the electronic structure of the respective metal classes responsible for energy dissipation processes of hot electrons will be analyzed by comparing our experimental data in to different theoretical results.

O 29.55 Wed 14:30 P2

ARUPS with higher harmonics using a 2D hemispherical energy analyser — ●STEFAN MATHIAS¹, RALF FRESE², MARTIN WIESENMAYER¹, SVEN PASSLACK¹, DOROTHEA HOFFMANN¹, MARTIN AESCHLIMANN¹, and MICHAEL BAUER¹ — ¹Department of Physics, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — ²Physics Department, University of Southern Denmark, Campusvej 55, 5230 Odense M, Denmark

Time-resolved UPS is an attractive experimental tool to study the ultra-fast dynamics of processes at surfaces [1]. Next to the photoelectron energy distribution also the time and angular dependence of the photoemission spectrum can contain important information, for instance the dynamics related to the coupling between molecules adsorbed on a surface. Short pulse EUV-light sources, such as higher harmonic generation (HHG), are typically driven at rather low repetition rates. Therefore, highly efficient parallel detection schemes are necessary to achieve time and angle resolved photoemission data (TR-ARUPS). Here we present first ARUPS experiments performed with a 1 kHz HHG light source using a hemispherical energy analyser, equipped with a 2D-detector for parallel energy and momentum detection. The HHG light source provides photon energies up to 45 eV and the photoelectrons are collected between $+/- 7^\circ$ ($k_{||} = +/- 0,42 1/\text{Å}$ at 45 eV) with an angle resolution of better than $0,2^\circ$. We discuss limitations, advantages and disadvantages of this detection scheme in comparison to a time of flight electron analyser, typically used for this kind of experiments. [1] M. Bauer, J. Phys. D: Appl. Phys. 38 (2005) R1-R15

O 29.56 Wed 14:30 P2

TDDFT simulation of Si(001) dimer excitation by intense fs laser-pulses — ●ECKHARD PEHLKE and JAN VAN HEYS — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität Kiel, 24098 Kiel

The surface band-structure of the Si(001) surface is characterized by either fully occupied or fully unoccupied dangling-bond orbitals located at the Si-dimer atoms. The population dynamics of the initially unoccupied states after laser excitation and the surface response has been studied by Weinelt *et al.* [1]. Here we present simulations of the dynamics of the Si(001) surface atoms, in particular the dimer-buckling angle, after very strong electron-hole pair excitation in the surface states by an intense fs laser-pulse. The dynamics of the electrons is described within time-dependent density functional theory while the nuclei follow classical Ehrenfest dynamics. The electric field representing the laser excitation is restricted to the direction perpendicular to the surface. Different laser-pulse shapes and intensities have been studied. The buckling angle decreases on a timescale of about 150 fs. A coupling between the dimer buckling angle and the total number of excited electrons is observed. Initial state contributions to the time-dependent surface core-level shifts have been calculated (screening effects, however, are still lacking). Additionally, the lifetime of the induced surface-atom vibrations has been investigated by molecular dynamics simulations on the Born-Oppenheimer surface.

[1] M. Weinelt *et al.*, Phys. Rev. Lett. **92**, 126801 (2004) and Appl. Phys. A **80**, 995 (2005).

O 29.57 Wed 14:30 P2

Description of femtosecond laser induced diffusion within the electronic friction model — ●J. GÜDDE¹, K. STEPAN¹, A.C. LUNTZ², and U. HÖFER¹ — ¹Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg — ²Physics Department, Odense University, 5230 Odense M, Denmark

It has been recently shown that diffusion of atomic oxygen on a Pt(111) surface can be induced by femtosecond laser excitation [1]. The energy flow from the optical excitation to the adsorbate has been modeled in the same way as the well-studied process of desorption induced by femtosecond laser excitation is frequently described. Three coupled temperatures for electrons, substrate ions and the adsorbate are introduced and the electronic coupling between adsorbate and metal surface is represented by an electronic friction coefficient η_e . In this way a fast energy transfer to the adsorbate and a nonlinear dependence of the corresponding rate on laser fluence can be reproduced. We have made different approaches for η_e : Ab initio calculations give the correct order of magnitude for the response time, but cannot reproduce the extremely strong nonlinear fluence dependence of the hopping-rate, which has been observed in the experiment [1]. Satisfactory agreement with the experimental data can be achieved only if a strong dependence of η_e on electron temper-

ature is assumed, which is not supported by the ab initio calculations. We will discuss alternative excitation pathways including an anharmonic coupling between different vibrational modes, which may be responsible for an effective temperature dependence of the electronic friction.

[1] K. Stepan *et al.* Phys. Rev. Lett. **94**, 236103 (2005).

O 29.58 Wed 14:30 P2

Positron induced Auger electron spectroscopy — ●STEFAN LEGL and CHRISTOPH HUGENSCHMIDT — Technische Universität München, Lichtenbergstraße 1, 85747 München

Positron annihilation induced Auger electron spectroscopy (PAES) uses the annihilation of a positron with an electron of the inner shell of atoms whereas X-rays or high energy electrons are used in conventional AES for ionisation. Advantages of PAES are the higher surface sensitivity and the better signal to noise ratio. In order to benefit from PAES one has to use a low-energy positron beam of high intensity, which is available at NEPOMUC at FRM-II. However, the positron intensity amounts to a few picoampere whereas up to 1mA electron current is used in AES. To overcome this lack of intensity a novel time-of-flight spectrometer (TOF-PAES) was developed, which efficiently collects the emitted Auger electrons. In the TOF-PAES the energy of the Auger electrons is determined by the measurement of the electron flight time with an accuracy of 1eV. The detection of one annihilation quantum (511keV) delivers the start signal for the timing. After a flight of about 1.1m the Auger electron hits a micro channel plate detector which creates a stop signal. The features of this new spectrometer as well as first results will be presented.

O 29.59 Wed 14:30 P2

Electron Transfer Dynamics from Perylene to ZnO Semiconductor: A comparative study between TiO₂ and ZnO — ●CHARAF CHERKOUK, JODI SZARKO, LARS GUNDLACH, LIANA SOCACIU-SIEBERT, ANTJE NEUBAUER, and FRANK WILLIG — Hahn-Meitner-Institute, Department: Dynamics of Interfacial Reactions SE4, Glienickestrasse 100, 14109 Berlin

Heterogeneous electron transfer (ET) between different molecules adsorbed on semiconductor surfaces has been investigated mainly with TiO₂ as the substrate [1,2]. The (10-10) surface of ZnO was used here as a substrate in order to investigate the influence of the nature of the semiconductor on the injection and relaxation dynamics. For both substrates electron transfer and relaxation dynamics were measured using time resolved two-photon photoelectron spectroscopy (TR-2PPE). Angular dependent 2PPE intensity was measured in order to extract information on the orientation of the molecules on the surface of the semiconductor. Others techniques such as XPS, UPS, and LEED were used in addition to characterize the surface of the clean and the dye-covered ZnO (10-10) single crystal surface, respectively. These results are compared with measurements on identical systems using TiO₂ as a substrate.

[1] L. Gundlach, S. Felber, W. Störck, E. Galoppini, Q. Wei, and F. Willig, Res. Chem. Intermed. **31**, 39, 2005.

[2] R. Huber, J.-E. Moser, M. Grätzel, and J. Wachtveitl, J. Phys. Chem. B **106**, 6494, 2002.

O 29.60 Wed 14:30 P2

Design and Setup of a Butterfly X-Ray Reflectometer for the Investigation of Liquid Surfaces and Interfaces — ●VOLKER SCHÖN and PATRICK HUBER — Technische Physik, Universität des Saarlandes, 66123 Saarbrücken, Germany

We present the design and setup of a tabletop x-ray reflectometer suitable for the investigation of the microscopic structure of liquid surfaces and interfaces. First measurements from the bare surface of water and liquid hydrocarbons as well as polymer/lipid/vapor interfaces demonstrate its functionality.

O 29.61 Wed 14:30 P2

Experimental and theoretical studies of the structure and dynamics of the CaF₂(111) surface — ●A. GOTTE¹, M. BAUDIN¹, K. HERMANSSON¹, A. CABELLO², J. VOGT², and H. WEISS² — ¹Department of Materials Chemistry, The Ångström Laboratory, Box 538, 752 21 Uppsala, Sweden — ²Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

The structure and dynamics of the CaF₂(111) surface was investigated by means of low-energy electron diffraction (LEED) and molecular dynamics (MD) simulations at 300 K. LEED beam intensities were recorded as a function of electron energy and were analyzed with the tensor LEED

approach. Positions as well as mean square amplitudes (MSA) of the ions in the first layers were fitted to the experimental I(E) curves. The MD simulations were performed using a 2-dimensional slab representation of the surface. Short-range interactions were described by a Buckingham potential and long-range interactions were calculated using a 2-D Ewald summation technique. Ionic polarizations were included by the shell-model. All parameters of the force field were fitted to the experimental bulk structure and elastic and dielectric data. According to experiment and theory the structure of the CaF₂(111) surface is close to the bulk-terminated geometry with only small vertical displacements of the top-most ions. Moreover it is found that the MSAs of the anions are larger than those of the cations. Enhanced vibrational amplitudes of the ions in the surface layers are supported by both studies, although with different values of the respective MSAs.

O 29.62 Wed 14:30 P2

Jumping atom rows on Au(110) observed with video-rate STM — ●RICHARD VAN RIJN, JOOST W.M. FRENKEN, and MARCEL J. ROST — Kamerlingh Onnes Laboratory, Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands

When depositing gold on a Au(110) surface, we find the formation of atom rows with a width of only one atom and surprisingly large lengths up to hundreds of atoms. This length scale is roughly a factor ten larger than we expect on the basis of two-dimensional equilibrium shape theory (Wulff construction). In addition we observe a large spread in row lengths. Next to the unusual island form, we also find that these atom rows are mobile at room temperature. Using standard STM imaging speeds, we observe atom rows with lots of kinks. But at video rate it seems, as if the whole atom row jumps back and forth in the [001] direction via a collective movement of all (hundreds of) atoms. As this collective movement is highly unlikely, we suggest that the basic mechanism for the jumps is given by the creation and the diffusion of an individual kink within the row, but on a very fast time scale. This system is a perfect model for one-dimensional diffusion related to the 'classical ruin problem'. We analyze the row diffusion via the frequency and temporal correlations of kink passages, as a function of position along the row, row length and temperature.

O 29.63 Wed 14:30 P2

Surface conductivity induced by fullerenes on diamond — ●PAUL STROBEL, JÜRGEN RISTEIN, and LOTHAR LEY — Institut für Technische Physik, Universität Erlangen-Nürnberg, Germany

The surface conductivity of hydrogen terminated diamond under atmospheric conditions is a well known phenomenon. The atmospheric adsorbents induce a near-surface hole gas resulting in a surface conductivity of diamond. In the present work we investigated C60 and fluorinated derivatives C60F18, C60F36, and C60F48 as alternative electron acceptors on the diamond surface. The electron affinity of the fluorinated fullerenes increases with the number of F-atoms from 2.7eV for C60 up to 4.1eV for C60F48. As a consequence, the doping efficiency increases in the same order and reaches unity for C60F48, i.e. each adsorbed C60F48 accepts one electron from the diamond. With device applications in mind, we further investigated the thermal stability of fullerene induced surface conductivity on diamond. Due to the increasing vapour pressure of the fullerenes with increasing fluorination the desorption temperature in high vacuum decreases from 200°C for C60 to RT for C60F48. A notable improvement of thermal stability was achieved by passivation of fluorinated fullerenes by different dielectric layers (SiO, CaF₂). In the case of C60 we observed an auto stabilisation up to 350°C in high vacuum after light, air, and temperature promoted polymerisation.

O 29.64 Wed 14:30 P2

STM-investigations of metal films near the percolation threshold on GaAs(110) — ●J. HOMOTH, M. WENDEROTH, T. DRUGA, L. WINKING, and R. G. ULBRICH — IV. Physikalisches Institut der Universität Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

The resistance of thin Ag and Cu films on insulating GaAs(110) was measured in-situ during UHV deposition at different sample temperatures (80K - 300K). The onset of conductance is seen in the thickness range of d=2 monatomic layers (ML). At thicknesses of more than 2ML an increase of conductance as a function of d with a power law behaviour of an exponent grater 1 is found.

We present scanning tunnelling topographies of films near the percolation thickness. The overall film morphology resembles a 3D cluster growth. Spatially resolved scanning tunnelling spectroscopy reveals addi-

tional states in the band gap region of the clean GaAs(110) surface. The additional states are localised around the metal clusters with a lateral decay length of less than 5 Angstroms.

The work was financially supported by the SFB 602 TP A7.

O 29.65 Wed 14:30 P2

Structural and electronic analysis of Hf on Si(111) surface studied by angle-scanned photoelectron diffraction — ●M. F. CARAZZOLLE^{1,2}, M. SCHÜRMAN^{1,3}, U. BERGES³, C. FLÜCHTER^{1,3}, D. WEIER^{1,3}, A. DE SIERVO⁴, R. LANDERS^{2,4}, G. G. KLEIMAN², and C. WESTPHAL^{1,3} — ¹Experimentelle Physik 1 - Universität Dortmund, Otto-Hahn-Str. 4, D44221-Dortmund, Germany — ²Instituto de Fisica - Universidade Estadual de Campinas, C.P.6165, 1083-970-Campinas, SP, Brazil — ³DELTA-Dortmunder Elektronenspeicherring Test Anlage, Maria-Goeppert-Mayer-Str. 2, D44227-Dortmund, Germany — ⁴Laboratorio Nacional de Luz Sincrotron, C.P. 6192, 13084-971-Campinas, SP, Brazil

The development of alternative high-k gate dielectrics for future complementary metal-oxide-semiconductor (CMOS) devices is indispensable in achieving both low leakage current and small equivalent oxide thickness. HfO₂ is one possible candidate because of its high dielectric constant and high conduction band offset. On the other hand the formation of metallic Hf-silicide during the annealing process for activation is one of the most serious problems, because the electrical characteristics will be influenced drastically due to the leakage current. In this work we present a systematic electronic and structural study of the Hf-silicide formation upon annealing. We utilized XPS, LEED and angular XPD to study the surface of ultra-thin films of the Hf on Si(111). The work was performed at DELTA (Accelerator Facility at the University Dortmund) using an undulator beam line with a photon energy of 200 eV.

O 29.66 Wed 14:30 P2

A Photoelectron Diffraction Investigation of the SiO₂/4H-SiC(0001) Interface — ●MARK SCHÜRMAN, STEFAN DREINER, ULF BERGES, and CARSTEN WESTPHAL — Universität Dortmund, Experimentelle Physik 1, Otto-Hahn-Straße 4, 44227 Dortmund, Germany

In our study we used photoelectron diffraction to investigate ultrathin SiO₂-films on 4H-SiC(0001). Synchrotron radiation with high flux and sufficient spectral resolution of the U41-PGM beamline at BESSY 2 (Berlin) was used. It was possible to separate individual spectral components in the XPS spectra. These components display different diffraction patterns due to the different local atomic environments of the respective emitters. We present a comparison between experimental data of a thermally oxidized ultrathin oxide layer showing no long-range order and an ordered silicate layer. From the diffraction patterns of the Si⁺ component originating from silicon emitters at the interface it is possible to conclude that the local atomic structure at the interface is very similar for both samples. However, the diffraction of the SiO₂ component is different for both patterns and a comparison with simulations shows, that this difference is a result of the local order within the oxide film. Furtheron, an R-factor analysis of the Si⁺ diffraction reveals details about the local atomic structure of the interface between bulk SiC and non-ordered SiO₂.

O 29.67 Wed 14:30 P2

Initial stages of the graphite/SiC interface formation studied by photoelectron spectroscopy — ●K. EMTSEV¹, TH. SEYLLER¹, L. LEY¹, L. BROEKMAN², J.D. RILEY², and R.G.C. LECKEY² — ¹Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Erwin-Rommel-Str. 1, 91058 Erlangen — ²Department of Physics, La Trobe University, Bundoora, Victoria 3083, Australia

Nowadays graphite layers grown on SiC(0001) surface are widely accepted as an alternative to the samples of natural graphite. Single-crystalline graphite multilayers result from the decomposition of SiC upon annealing at high temperatures. As an initial stage of graphitization a complex $(6\sqrt{3} \times 6\sqrt{3})R30^\circ$ surface reconstruction occurs after annealing of 6H-SiC(0001) at T=1150°C. The nature of this reconstruction is discussed controversially. Fingerprints of graphitization (π^* and σ^* bands) were observed in inverse photoelectron spectroscopy [1], while the energies of C1s surface shifted components differ from that of graphite [2]. The early models suggested a monolayer of graphite on top of either the unreconstructed surface or the $(\sqrt{3} \times \sqrt{3})R30^\circ$ reconstructed surface. The latest model proposes that the surface is covered by the graphene-like islands arranged in a honeycomb structure [3]. In the present work we

analyze in detail the electronic structure of the $6\sqrt{3}$ reconstructed surface of 6H-SiC(0001) by means of angle-resolved photoelectron spectroscopy.

[1] I. Forbeaux et al., Phys. Rev. B, 58 16396 (1998)

[2] L.I. Johansson et al., Phys. Rev. B, 53 13793 (1996)

[3] W.Chen et al., Surf.Sci., in press (2005)

O 29.68 Wed 14:30 P2

Surface characterization of InN grown by PIMBE — ●MARCEL HIMMERLICH^{1,2}, VADIM LEBEDEV², STEFAN KRISCHOK^{1,2}, OLIVER AMBACHER², and JUERGEN A. SCHAEFER^{1,2} — ¹Institut für Physik, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — ²Zentrum für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany

Indium nitride (InN) layers were grown by plasma-induced molecular beam epitaxy using a conventional effusion cell for In and an rf nitrogen plasma source to supply active N radicals. The growth was monitored by a quadrupole mass spectrometer and reflection high energy electron diffraction (RHEED). After removal from the growth chamber, the samples were directly cut and loaded to a second UHV system to reduce the exposure to contaminants from ambient air. The InN layers were investigated using X-ray and ultra-violet photoelectron spectroscopy (XPS, UPS) and atomic force microscopy (AFM). Although the surface is quite rough (rms 4.5nm), surface steps with a height of 6Å can be observed. The amount of carbon and oxygen on the surface is relatively low compared to samples which have been exposed to air for a few days. Heating of the samples to 170°C-230°C resulted in a further reduction of oxygen along with a removal of the oxide related feature in the In3d and In4d core levels. However, this procedure did not succeed in removing any carbon. The binding energy of the InN related peaks are 443.9eV, 396.3eV and 17.4eV for In3d_{5/2}, N1s and In4d_{5/2}, respectively. Additionally, a structure in the valence band emerges at 3.1eV which can be attributed to a nitrogen related contribution.

O 29.69 Wed 14:30 P2

SiC Pore Surfaces: Surface Studies of 4H-SiC(1102) and 4H-SiC(1102) — ●U. STARKE¹, W.Y. LEE¹, M. HETZEL¹, C. VIROJANADARA¹, C. COLETTI², S.E. SADDOW², R.P. DEVATY³, and W.J. CHOYKE³ — ¹Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — ²University of South Florida, Tampa, USA — ³University of Pittsburgh, USA

Porous SiC has shown intriguing perspectives for a variety of possible applications in electronics, sensors, fuel cells and bio-technology. One important pore type found is a triangular shaped channel with surfaces inclined by about 62° with respect to SiC(0001). The respective single crystal surface, 4H-SiC($\bar{1}10\bar{2}$), and its isomorphous opposite, i.e. the 4H-SiC(1102) surface have been studied in this work using AFM, LEED, STM and AES. The mechanically polished samples were etched in hydrogen flux at about 1500°C which eliminates the polishing damage as monitored by AFM. Both surfaces immediately display a sharp LEED pattern of bulk-like periodicity. An apparent thin oxide layer termination is inferred from AES. Further annealing in UHV leads to the removal of oxygen after flashing to about 1200°C. Si deposition and subsequent annealing lead to a well ordered surface with the best LEED pattern obtained after heating to about 1120 and 1000°C, respectively. Also the Si/C composition ratio increases up to this temperature regime until it drops at higher temperatures. A tendency towards a (2×1) reconstruction is observed. The interpretation of LEED spot intensity curves indicates a different structure for the UHV treated surface as compared to the 'as-etched' surface condition.

O 29.70 Wed 14:30 P2

Temperature Induced Phase Transformation on the 4H-SiC(1120) Surface — ●U. STARKE¹, W.Y. LEE¹, and S. SOUBATCH^{1,2} — ¹Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — ²present address: International University Bremen, Germany

The demand for better SiC devices has initiated an increased focus the non-polar 4H-SiC(1120) surface which has a lower defect density than basal-plane surfaces and can serve as alternative growth orientation. In the present work, we have studied this surface after hydrogen etching as well as after Si deposition as a function of temperature using XPS, LEED, AES and AFM. Results show that despite having a smooth, featureless surface (as observed by AFM), the 'just-loaded' hydrogen etched surface exhibits a (1×1) LEED pattern, although weak. Chemically, the surface appears to be C-rich, indicated by XPS and AES spectra with an additional small amount of oxygen present. The oxygen peak vanishes upon

heating to about 1150°C. A well ordered surface can be obtained by Si deposition and subsequent annealing. The LEED pattern remains (1×1). However, the LEED intensities show a sharp change around 1000°C indicating a structural phase transformation. The chemical composition also changes during annealing, however in a more gradual manner. The results will be discussed in detail, focusing on the chemical and structural properties of the two distinct phases observed.

O 29.71 Wed 14:30 P2

Growth and morphology of ZnO on Fe(110) — ●CHRISTIAN TUSCHE, HOLGER L. MEYERHEIM, and JÜRGEN KIRSCHNER — MPI für Mikrostrukturphysik Halle, D-06120 Halle, Germany

The Fe/ZnO/Fe tri-layer system is a potentially promising system for tunneling magneto-resistance (TMR) and future spintronic applications. Since the tunneling properties sensitively depend on the details of the interface[1], the study of the growth, morphology and structure of ZnO on Fe and vice versa is of primary importance.

Ultrathin films of ZnO were deposited on Fe(110) from a ZnO-rod heated by electron bombardment and by pulsed laser deposition using a stoichiometric ZnO target. For the ZnO(0001)/Fe(110) epitaxy the lattice mismatch is 12% for $[11\bar{2}0]_{\text{ZnO}} \parallel [001]_{\text{Fe}}$. ZnO films up to 3 monolayers thickness exhibit a (1x1) pattern in low energy electron diffraction (LEED), although with reduced spot sharpness as compared to the clean Fe(110) surface. Structural order improves upon annealing to 520K, however at higher temperatures, the interface is subject to a reduction-oxidation reaction. Scanning tunneling microscopy on films in the same thickness range reveals a two dimensional growth of the ZnO.

For ZnO-deposition in ambient oxygen atmosphere ($p(\text{O}_2) = 10^{-7} \text{ mbar}$) photo electron spectroscopy indicates an oxidation of the Fe substrate. This goes in parallel with the observation of extra spots in the LEED-pattern, indicative for a relaxed ZnO adlayer (hexagonal a-axis = 3.25 Å).

[1] C. Tusche et al., Phys. Rev. Lett. **95** (2005) 176101

O 29.72 Wed 14:30 P2

Morphology and electronic structure of ultrathin manganese oxide films — ●MATHIAS NAGEL, LEI ZHANG, HEIKO PEISERT, and THOMAS CHASSÉ — Institute of Physical and Theoretical Chemistry, University of Tübingen, Auf der Morgenstelle 8, 72076 Tübingen, Germany.

Binary transition metal monoxides have been of basic scientific interest for many years. Due to their high electronic correlation they reveal interesting properties. Of particular interest besides their electronic properties are magnetic phenomena in layer systems which are already utilised in technical applications. As a consequence of the trend in miniaturising devices questions about the influence of the reduced dimensionality on the properties arise. In layered systems the influence of the morphology and the reactions directly at the specific interface have to be evaluated.

The MnO/Ag(100) is an interesting model system due to the lattice mismatch which is quite high (9 %). By choosing the optimal preparation method either pseudomorphic growth or relaxed growth of MnO on Ag(100) can be obtained. This defined growth method is giving the possibility of studying separately the interface strain and the effect of the reduced dimensionality. Ultrathin, epitaxial layers of MnO were prepared at Ag(100) and characterised in-situ by means of XPS, XPD and LEED. Additionally, in-situ grown samples were investigated with XES and XAS measurements. By combining these techniques a detailed understanding of the morphology and electronic structure of the evolving film can be obtained and is discussed.

O 29.73 Wed 14:30 P2

Growth, atomic structure and vibrational properties of thin MnO films on Pt(111) — ●STEFFEN SACHERT¹, CHRISTIAN HAGEDORF¹, KRASSMIR KOSTOV², and WOLF WIDDRA¹ — ¹Martin-Luther-Universität Halle-Wittenberg, FB Physik, D-06120 Halle (Salle) — ²Institute of General and Inorganic Chemistry, Bulgarian Academy of Science, BG-1113 Sofia

Thin MnO layers (from 0.2 to 4 monolayers) have been grown on Pt(111) by reactive deposition of Mn in an O₂ atmosphere. High-resolution electron energy loss spectroscopy (HREELS), low energy electron diffraction (LEED) and variable-temperature scanning tunneling microscopy (STM) have been used to investigate surface vibrational and structural properties of various thin manganese oxide films.

Submonolayer coverages of MnO grown at 375 K are characterized by strong Fuchs-Kliwer phonons. The corresponding MnO coverages

within the monolayer are estimated by CO adsorption at 85 K and thermal desorption. For the completed MnO monolayer on Pt(111) a well-ordered (19×1) superstructure is observed in LEED and in atomically resolved STM. The related HREEL spectrum shows a narrow Fuchs-Kliwer phonon at 365 cm⁻¹.

Further growth of MnO occurs layer-by-layer as found by STM. The layer-dependent vibrational properties and their changes with annealing to higher temperatures will be discussed: Heating the films to 700 K improves ordering in the 2D film. At 800 K, annealing leads to the well-defined monolayer with few, larger 3D MnO clusters, whereas at about 1100 K alloy formation takes place.

O 29.74 Wed 14:30 P2

Epitaxial Cobalt Oxide Films on Ir(100) — ●CHIARA GIOVANNARDI, LUTZ HAMMER, and KLAUS HEINZ — Lehrstuhl für Festkörperphysik, Universität Erlangen Nürnberg, Staudtstr. 7, D-91058 Erlangen

On various modifications of the Ir(100) surface (1×1, 5×1, 2×1-O) cobalt grows pseudomorphically up to several monolayers. Post-oxidizing a 2ML Co film grown on the 1×1 surface and subsequent annealing at around 500K leads to the formation of flat epitaxial CoO-films with rock-salt structure. In contrast to substrates like Fe(100) and Ag(100) [1,2] these CoO-films cannot grow in (100) orientation on the Ir(100) surface due to the large lattice misfit (2.72 Å vs. 3.04 Å). Instead, the film grows slightly distorted in (111) orientation giving rise to a c(10×2) superstructure. For other thicknesses and surface preparations fully relaxed CoO patches are found as well as patches with Co₂O₃ structure.

[1] S. Valeri et al., Surf. Sci. 423 (1999) 346

[2] Ch. Hagedorf et al., Surf. Sci. 532-535 (2003) 346

O 29.75 Wed 14:30 P2

Surface morphology of epitaxial lattice-matched Ba_{0.7}Sr_{0.3}O on the Si(001) surface — ●DIRK MÜLLER-SAJAK, JAN ZACHARIAE, and HERBERT PFÜR — Institut für Festkörperphysik, Abtl. Oberflächen, Universität Hannover, Appelstr. 2, 30167 Hannover

Recently we have shown that Ba_{0.7}Sr_{0.3}O as a high K gate dielectric offers an adequate band gap, an appropriate band alignment and an atomically sharp interface to the Si(001) substrate [1].

Here we will present a SPA-LEED (Spot Profil Analysis LEED) study of the Ba_{0.7}Sr_{0.3}O surface morphology. The vertical roughness was determined to be ≤ 2ML at up to 15 nm layer thickness. In addition, local variations of the lattice spacing due to fluctuations of the local composition were detected in our G(S) analysis.

Growth of Ba_{0.7}Sr_{0.3}O on vicinal Si(001)-[011]4° leads to stepped oxide surfaces. The spot splitting is 4% of the surface Brillouin zone for the oxide surface in contrast to 10% for vicinal Si(001). This indicates an uncorrelated mixture of terraces separated by triple steps and double steps in molecular units. This is mainly caused by a rearrangement of the vicinal Si(001) surface due to the preadsorbed Sr layers, which is necessary for the crystalline growth of Ba_{0.7}Sr_{0.3}O [1].

Pd chains which nucleate along these steps were investigated by ARUPS and SPA-LEED. The structure of this 1D electronic system will be discussed.

[1] J. Zachariae and H. Pfnür, Phys. Rev. B 72, 075410 (2005)

O 29.76 Wed 14:30 P2

Ultrathin vanadium oxide films on W(110) investigated by LEEM — ●BENJAMIN BORKENHAGEN, GERHARD LILIENKAMP, and WINFRIED DAUM — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, D-38678 Clausthal-Zellerfeld

Vanadium oxide films with thicknesses in the range between submonolayer and several monolayers were epitaxially grown on a W(110) single crystal under UHV conditions. Depending on the growth conditions, LEED investigations revealed various well-ordered superstructures, e. g. with 2x2 symmetry, and a hexagonal film in Kurdjumov-Sachs orientation. Cleanness and composition of the films were checked by Auger spectroscopy. Low energy electron microscopy (LEEM) of the vanadium oxide-covered tungsten surface showed a flat surface with monoatomic steps. Dark field images using one or more diffraction spots revealed the growth process and the distribution of different domains of the vanadium oxide. The sample was also investigated in situ during annealing under oxidizing and reducing conditions, respectively. Structural transitions are correlated with the oxygen content in the film and alloying of vanadium with the tungsten substrate.

O 29.77 Wed 14:30 P2

Thermally and Electron-Induced Processes in Condensed Acetic Acid–Water Films between 80 and 200K studied with MIES, UPS(HeI and II), FTIR and TPD — ●S. BAHR¹, O. HÖFFT¹, A. BORODIN¹, V. KEMPTER¹, F. BORGET², T. CHIAVASSA², and A. ALLOUCHE² — ¹Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, D-38678 Clausthal-Zellerfeld — ²Physique des Interactions Ioniques et Moléculaires, CNRS-UMR6633 Campus Universitaire de Saint Jérôme, Marseille, France

Thermally and electron-induced processes in condensed acetic acid (AA)-water films, deposited on tungsten and gold at 80K and 120K, were studied with Metastable Impact Electron Spectroscopy (MIES), UPS(HeI and II), FTIR-Spectroscopy and TPD in a temperature range between 80K (120K) and 200K. The results are interpreted with the help of cluster DFT calculations. The prepared interfaces, namely AA layers on thin films of solid water and H₂O adlayers on thin AA films, were characterised with the above mentioned techniques at 80K (120K) and additionally with TPD during annealing. By the combination of electron spectroscopy with FTIR and TPD we are able to get informations about inter and intra species binding strengths in addition to structural changes (in the case of AA from cyclic dimers to chain like structures at 150K) and desorption behaviour of both species in the films during annealing. Currently, we study the electron-induced modification of the AA film structure as well as processes initiated by the radiation-induced H₂O fragments (OH, H₃O⁺ etc).

O 29.78 Wed 14:30 P2

Segregation of salt ions at surfaces of polar liquids and the corresponding amorphous solids — ●O. HÖFFT¹, U. KAHNERT¹, V. KEMPTER¹, P. JUNGWIRTH², and L.X. DANG³ — ¹Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4 38678 Clausthal-Zellerfeld — ²Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague — ³EMSL, Pacific Northwest National Lab

Surface segregation of iodide, but not of fluoride, or cesium, is observed by a combination of metastable impact electron spectroscopy (MIES) and ultraviolet photoelectron spectroscopy (UPS(HeI)) of amorphous solid water exposed to CsI and NaI on one side and NaF and CsF vapour on the other side. The same surface ionic behavior is also derived from molecular dynamics (MD) simulations of the analogous aqueous salt solutions. These results give a strong support to the suggested surface propensity of heavier halides (iodide, bromide) in water and confirm the structural similarity between the amorphous solid and the corresponding liquid. In contrast, no appreciable surface segregation of ions is observed in methanol, neither in the experiment nor in the simulation, which points to the remarkable surface properties of water among polar solvents. The propensity of heavier halides for the air/solution interface has important implications for heterogeneous chemical processes, particularly in the atmosphere.

O 29.79 Wed 14:30 P2

The structure of ordered iodine layers on Pt(100) in electrolyte and air — ●BJÖRN BRAUNSCHWEIG and WINFRIED DAUM — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, D-38678 Clausthal-Zellerfeld

Well-defined iodine adlayers, prepared by flame annealing and subsequently quenching in iodine vapor, were studied by scanning tunneling microscopy (STM) in air and a 0.1M HClO₄ electrolyte with atomic-resolution. The I-Pt(100) surface showed atomically flat terraces with monoatomic steps mainly along the [010] direction. At low iodine coverage STM in air reveals domains of clean reconstructed Pt(100)-hex and domains of an ordered ($\sqrt{2} \times 5\sqrt{2}$)R45°-I adlattice on Pt(100)-(1x1). At high coverage iodine forms a complete ($\sqrt{2} \times 5\sqrt{2}$)R45° layer on the Pt(100) surface which consists of a defect-free phase with iodine rows perpendicular to the main direction of the terrace steps, and a defect-rich phase with iodine rows parallel to the steps and with quasi-one-dimensional defects along the [010] direction. The boundary between the two phases is found to be atomically abrupt. Contrary to our STM data in 0.1M HClO₄ which are in agreement with previous work [1], STM imaging in air reveals buckled iodine double-rows. The strength of buckling depends on tunneling resistance and on the orientation of the ($\sqrt{2} \times 5\sqrt{2}$)R45° domains.

[1] R. Vogel and H. Baltruschat; Surf. Sci. Lett. 259,L739-42(1991)

O 29.80 Wed 14:30 P2

Reactivity studies of formic acid oxidation on the bare and the Cu modified Pd(111) surface — ●KLAUS WANDEL, KATRIN BRANDT, and MARCO STEINHAUSEN — Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, D-53115 Bonn, Germany

FTIRS, CV and AES have been used to investigate the reactivity of formic acid oxidation on the bare and the Cu modified Pd(111) surface as a function of potential, electrolyte and surface composition. This reaction has thus been studied in pure formic acid as well as in 10 M and 5 mM aqueous formic acid solution. Carbon dioxide evolution which was characterised by the asymmetric O=C=O stretching vibration at 2345 cm⁻¹ has been employed as "probe" for the surface reactivity.

The spectroscopic characterisation of HCOOH/Pd(111) points to an extraordinary acceleration of CO₂ evolution at the electrode as the potential is increased above 0.45 V. Analysis of IR-measurements at constant potentials lead to the assumption that the electronic state of the solid/liquid interface in the open-circuit HCOOH/Pd(111)-H₂SO₄-system corresponds to that at about 0.4 V vs. RHE. Water as solvent plays an important role in formic acid oxidation as a decrease in formic acid concentration in the electrolyte results in an augmentation of the relative reactivity normalized to the number of formic acid molecules in solution. Depending on the direction of the potential scan the rate of formic acid oxidation is inhibited or accelerated by electrochemically deposited Cu on the Pd(111)-surface.

O 29.81 Wed 14:30 P2

Immobilization of cationic porphyrins (H2TMPyP) on sulfate modified Cu(111): An ECSTM study — ●MINH HAI NGUYEN THI, KLAUS WANDEL, and PETER BROEKMANN — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, D-53115 Bonn, Germany

The immobilization of cationic porphyrins (Meso-Tetra (N-methyl-4-pyridyl) Porphyrine Tetratosylat (H2TMPyP)) on sulfate modified Cu(111) surface has been studied by means of Cyclic Voltammetry (CV) and in-situ Scanning Tunnelling Microscopy (STM). Therefore a Cu(111) electrode surface was exposed to dilute sulfuric acid (5 mM H₂SO₄). Sweeping the electrode potential into the anodic direction starting from the regime of hydrogen evolution initiates the adsorption and subsequent ordering of a hydrophilic sulfate/water coadsorption layer. This adlayer formation follows a nucleation and growth mechanism so that even submonolayer coverages of this sulfate/water can be obtained depending on the applied electrode potential. Adsorption and immobilization of the cationic porphyrins takes place exclusively on the negatively charged sulfate/water coadsorption layer but not on the bare sulfate-free copper surface. This preferential adsorption is explained in terms of enhanced electrostatic interactions between the anion/water layer on the one hand and the cationic porphyrins layer on the other hand.

O 29.82 Wed 14:30 P2

Organized Chirality at the Solid/Liquid Interface: An In-Situ STM Study — ●MINH HAI NGUYEN THI¹, NAKCHEOL JEONG², BARBARA KIRCHNER¹, MAKUS REIHER³, CHRISTOPH A. SCHALLEY⁴, KLAUS WANDEL¹, and PETER BROEKMANN¹ — ¹Institut f. Physikalische und Theoretische Chemie, Universität Bonn — ²Department of Chemistry and Division of Molecular Engineering and Chemistry, Korea University — ³Institut f. Physikalische Chemie, Universität Jena — ⁴Institut f. Chemie und Biochemie, Freie Universität Berlin

The phase behavior of chiral metallo-supramolecular rhomboids of the Fujita type has been studied under electrochemical conditions by means of in-situ STM. A Cu(100) electrode which is pre-covered by a well ordered c(2 x 2) chloride layer served as substrate for the subsequent adsorption of positively charged metal complexes of the Fujita type. Characteristically, these metallo-supramolecular cages exhibit a molecular cavity of about 1.6 nm diameter and can therefore be regarded as potential model systems for the inclusion of small aromatic molecules in terms of supramolecular host/guest chemistry. On the c(2 x 2) chloride lattice these rhomboids adsorb flat lying with their cavity oriented to the solution phase. The racemic mixture of the chiral rhomboids spontaneously separates at the surface into two laterally well ordered mirror domains of enantiomerically pure rhomboids. When only one of both enantiomers is added to the supporting electrolyte we consequently observe only one of both mirror domains leading to a truly chiral electrode surface. Submolecular features of the chiral rhomboids in the STM experiment can be understood with the help of additional DFT calculations.

O 29.83 Wed 14:30 P2

Solid-liquid surfaces under potential control studied by X-ray diffraction — •FRANK UWE RENNER, YVONNE GRÜNDER, and JÖRG ZEGENHAGEN — ESRF, BP220, 38043 Grenoble, France

At modern synchrotron radiation sources (e.g. ESRF in Grenoble) it is possible to study structures of surfaces in contact with liquids or electrolytes by in-situ X-ray diffraction with atomic resolution. On a conducting (metal or semiconductor) surface in contact with electrolyte it is possible to control the chemical potential of surface atoms by adjusting the electrical potential. Thus adsorption and desorption processes as well as structural phase changes of the bare crystal surfaces can be initiated close to or far from the equilibrium depending on the choice of potential. At the X-ray Standing Waves Surface Science Beamline ID32 at the ESRF we are studying these phenomena with newly developed electrochemical cells in-situ with X-ray diffraction and X-ray standing waves. Especially for metal alloy and semiconductor systems that have to be prepared by surface science vacuum methods a new UHV transfer electrochemical cell for in-situ X-ray diffraction has been developed using and controlling a droplet of electrolyte solution on the sample surface. We will present latest results for potential induced corrosion of low-index single crystal surfaces of the metal alloy systems Cu-Au and Cu-Pd, as well as metal deposition on semiconductors.

O 29.84 Wed 14:30 P2

Video STM Observation on A(111) Surface and Cu upd Layer in Aqueous Solution — •KOJI SUTO and OLAF MAGNUSSEN — Institut für Experimentelle und Angewandte Physik, Universität Kiel

Dynamics of atom or ion on the electrified interface has been a hot topic on physics and nanotechnology over decades, but there are only a few reports on electrochemical systems. This time we will present some investigation on Au(111) surface in aqueous solution by Video STM (acquiring up to 30 images/s). First, electrochemically induced lifting of reconstruction was investigated in sulfuric acid. Herringbone structure was observed to disappear line by line, and its decay rate was analysed quantitatively. Next, Cu electrodeposition was investigated. It is well known that, by under potential deposition (upd), submonolayer of Cu is formed on Au(111) reductively at slight positive potential towards bulk deposition. Sulfate ($\sqrt{3} \times \sqrt{3}$) structure, which covered Cu upd layer was seen and the motion of the boundary fluctuating in between two parallel ($\sqrt{3} \times \sqrt{3}$) domains was observed by Video STM. Dynamic state of bulk deposition was also considered.