O 28 Methodisches (Exp. und Theorie)

Zeit: Samstag 15:00–17:00 Raum: TU EB407

O 28.1 Sa 15:00 TU EB407

Coherent x-ray reflectivity using white synchrotron radiation — •Tobias Panzner[1], Ivan Vartanyants[2], Gudrun Gleber[1], and Ullrich Pietsch[1] — [1]Institut für Physik, Universität Potsdam, Am Neuen Palais 10, D-14415 Posdam — [2]HASYLAB at DESY, D- 22603 Hamburg, Germany

In this talk we will present results of x-ray reflectivity measurements with coherent synchrotron radiation. Before application of this method to particular samples one has to analyse precisely the apparatus function of the experimental set-up.

We used a pink beam of 5-20keV and a circular aperture to define the incident wave. Therefore we studied the influence of the diffraction from a circular aperture and the resulting shape of the illumination function approaching the sample. In particular we compare calculated and experimental apparatus function measured at the EDR beamline at BESSY II.

Using this function we show the possibilities and advantages of an energy dispersive set up for static and time resolved coherence experiments and give first results of the investigation of a smooth polymer film covered on silicon.

O 28.2 Sa 15:15 TU EB407

Calculations for a matched photon and photoelectron energy dispersive soft x-ray beamline — •D.R. Batchelor[1], Th. Schmidt[1], R. Follath[2], C. Jung[2], R. Fink[3], and E. Umbach[1] — [1]EP2, Univ. Würzburg — [2]BESSY Gmbh — [3]Phys.Chem. II, Univ. Erlangen

The high brilliance of third generation synchrotron radiation sources and modern developments in monochromator design, combined with 2d-detecting electron energy analysers, allow the simultaneous detection of photoelectron and photon energy: the photon dispersion of the monochromator is imaged onto the specimen, and the 1d-laterally resolving analyser is used to detect this dispersion. Such a combination opens up exploitation of CFS and CIS techniques such as NEXAFS, resonant Auger, and photoelectron spectroscopy. The parallel detection enables the large parameter space to be efficiently sampled such that high energy resolution can be combined with short time scales in the ms range. However, the electron and photon optics of monochromator and electron energy analyser have to be matched and optimised, considering imaging and dispersion characteristics of both. We present calculations for the combination of a collimated, variable cff, PGM monochromator and a Scienta SES 200 analyser with a 2d-detector at the UE52 Undulator at BESSY II, evaluating the limitations and developments necessary to realise the full potential of such an experiment.

Funded by BMBF under contract no. 05KS4WWC/2

O 28.3 Sa 15:30 TU EB407

Resonant inelastic soft x-ray scattering probing semiconductor surface adsorbate dynamics — •Franz Hennies[1], Alexander Föhlisch[1], Annette Pietzsch[1], Mitusuru Nagasono[1], Nadine Wittkowski[2], Stina Matsson[3], Maria-Novella Piancastelli[3], and Wilfried Wurth[1] — [1]Universität Hamburg, Institut für Experimentalphysik, Luruper Chaussee 149, D-22761 Hamburg — [2]Laboratoire d' Optique des Solides, Université Pierre et Marie Curie, Paris, France — [3]Department of Physics, Uppsala University, Sweden

Resonant inelastic x-ray scattering (RIXS) probes the valence electronic structure of a system in an atom specific and symmetry selective manner. Furthermore, the method is sensitive to dynamic properties of the core excited intermediate state. In recent years the method has been utilized to investigate adsorbates on metal surfaces, leading to an improved understanding of the surface chemical bond [1].

We have now investigated adsorbates on a semiconductor surface, i.e. simple hydrocarbons on the Si(001)-(2x1) surface with selectively excited, fully polarization and symmetry resolved RIXS at beamline I511 at MAXLab in Lund, Sweden. The electronic structure information which we obtain supports theoretical adsorption models. In contrast to metals a clear signature of dynamic processes in the core-excited state has been observed. We will present our results and suggest theoretical interpretation schemes. This work is supported by grant Fo343/1-1 of the Deutsche Forschungsgemeinschaft.

[1] A. Nilsson and L.G.M. Pettersson, Surf. Sci. Rep. **55**, 49 (2004)

O 28.4 Sa 15:45 TU EB407

Two-Photon Photoemission Microscopy of Self-organized Ag-Nanostructures on Si(001) — •L. I. Chelaru, O. Heinz, P. Zhou, M. Horn-von Hoegen, D. von der Linde, and and F. Meyer zu Heringdorf — Institut für Laser-und Plasmaphysik, Universität Duisburg-Essen (Campus Essen), 45117 Essen

During epitaxial growth of Silver on Si(001), compact islands and quasi-one-dimensional nanowires are formed. These self-organized nanostructures have been investigated by photoemission electron microscopy (PEEM) where the electrons are generated by femtosecond laser pulses through a two-photon photoemission process (2PPE). Shadow like features are observed around the nanostructures when the Ag islands and wires exceed a certain lateral dimension. The features are different for both directions of the polarization of the incoming light (s- and p-polarization, respectively). In p-polarization the shadows consist of several interference fringes. We interpret the shadows to represent the near field around the islands that is strongly emphasized in photoemission through the nature of the non-linear 2 photon photoemission process. The Ag-nanowire photoemission yield also shows a dependence on the polarization direction of the incoming light with respect to the orientation of the nanowire. Ag-nanowires oriented parallel to the polarization vector of the incoming light are not visible in the microscope images, in contrast to Ag-nanowires that are oriented normal to the vector of polarization. Also, the photoemission yield depends on the size of the islands. We explain these findings with a plasmon state in the silver nanostructures that is the intermediate state for 2 photon photoemission.

O 28.5 Sa 16:00 TU EB407

GW quasiparticle energy calculations for surfaces: the influence of dynamic polarization in a repeated-slab approach — •Philipp Eggert[1], Christoph Freysoldt[1], Patrick Rinke[1], Arno Schindlmayr[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

The combination of density functional theory (DFT) and many-body perturbation theory in the GW approximation has become an important tool for *ab-initio* band structure calculations typically in good agreement with experiment. In order to treat surfaces one often employs a repeated slab geometry for computational convenience. However, electric multipole moments may occur in the slabs which then lead to a slowly decaying electrostatic interaction. If present, static dipoles must be corrected for in DFT [1]. In GW however, dynamic dipoles are always created. We present calculations for the hydrogen-saturated silicon (001) slabs and show that slabs smaller than 10 layers are not converged fully with 10-20 Å vacuum thickness. The effect of the dynamic dipoles is slowly decreasing with slab thickness, in accordance with an extension of a simple electrostatic model, that includes these polarization effects [2]. Therefore it is essential to monitor the convergence carefully and if necessary to extrapolate to infinite separation.

[1] J. Neugebauer, M. Scheffler, Phys. Rev. B **46**, 16067 (1992)
[2] C. Delerue, G. Allan and M. Lannoo, Phys. Rev. Lett. **90**, 076803 (2003)

O 28.6 Sa 16:15 TU EB407

The multipole compensation method for slab geometry — •Ferenc Tasnadi — IFW Dresden, ITF Group Numerical Solid State Physics and Simulation

The multipole compensation method developed by M. Weinert[1] to solve the Poisson equation for 3-dimensional periodic crystalline systems is extended for slabs, layer symmetric[2] structures. Unlike in Ref.[1] the presented method assumes localized (compact support), overlapping original charge distributions as introduced in Ref.[3] and non-local (no compact support) Ewald density distributions. The Poisson equation is solved with periodic boundary conditions in the plane and with finite voltage boundary condition in the perpendicular (z) direction. For the $K_{||} \neq 0$ case a Fourier transformation helps to calculate the solution in a three dimensional periodic sense. While for the $K_{||} = 0$ case, the required charge neutrality is the starting point to find the solution. The $K_{||} = 0$ solution connects the z directional potential step with the surface density of the dipole z component. For both cases suitable representations

of the spherical harmonics are needed to arrive at expressions that are convenient for numerical implementation.

[1]M.Weinert, J. Math. Phys. **22**,11 (1981).
[2]V. Kopsky and D.B. Litvin, eds., *Subperiodic Groups,* vol. E of *International Tables for Crystallography* (Kluwer Academic Publisher, Dordrecht/Boston/London, 2002).
[3]K. Koepernik and H. Eschrig, Phys. Rev. B. **59**, 1743 (1999).

O 28.7 Sa 16:30 TU EB407

Genetic algorithms in surface cluster expansions — •Ole Wieckhorst und Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik, Staudtstr. 7, 91058 Erlangen

The cluster expansion treats the binary alloy problem by mapping DFT-based formation enthalpies of a number of selected input structures onto a finite set of pair and multibody interactions corresponding to characteristic figures like triangulars, tetrahedron, etc. The two critical points of this concept are the selection of an appropriate set of figures and input structures used for the construction, especially when the surface comes into play: The lifting of the symmetry due to the surface causes a lifting of the degeneracy of the figures, thus creating a huge repository of figures and structures to choose from. An effective way of treating such a selection problem are genetic algorithms. It will be demonstrated how the implementation of genetic algorithms in surface cluster expansions allows for a much more efficient and accurate determination of both, energetically relevant figures and input structures compared to conventional fitting procedures. As a first example, we apply this concept to construct a cluster expansion for the (100) surface of the B2-CoAl phase. Here, the segregation profile is controlled by so-called antisite atoms, as we have shown recently [1,2]. (supported by DFG)

[1] V. Blum et al., Phys. Rev. Lett. 89, 266102 (2002)
[2] O. Wieckhorst et al., Phys. Rev. Lett. 92, 195503 (2004)

O 28.8 Sa 16:45 TU EB407

The Nanoworkbench: A Tool to Probe Electronic Properties of Surfaces and Small Structures — •Hubertus Marbach[1,2,3,4], Olivier Guise[1,2,3], Jeremy Levy[2,5], Joachim Ahner[2,6] und John T. Yates, Jr.[1,2,3,5] — [1]Surface Science Center — [2]Center for Oxide Semiconductor Materials for Quantum Computation — [3]Department of Chemistry — [4]Lehrstuhl für Pysikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen — [5]Department of Physics, University of Pittsburgh, Pittsburgh, PA 15260 — [6]Seagate Technology, Pittsburgh, PA 15222

To investigate the properties of surfaces and small particles in the sub-micrometer range we developed a novel experimental setup: the nanoworkbench (NWB). The core of the NWB consists of an array of four manipulators in UHV which can be positioned individually with nanometer precision. Equipped with sharp metal tips we can use the manipulators to contact the sample electrically. Four terminal measurements like van der Pauw or four-point probe measurements can be performed with the setup. Part of the design is an electron focusing column which enables us to image the sample and the four tips in situ by means of scanning electron microscopy. Running the nanomanipulators in scanning tunnelling microscopy mode provides an additional imaging method. The design of the NWB and first measurements will be presented. Work supported by AFOSR and DARPA