

## HIGHLIGHTS IN SYNCHROTRON RADIATION RESEARCH (SYSR)

Das fachverbandübergreifende, interdisziplinäre Symposium wird von den beiden Arbeitskreisen AKF und AMOP gemeinsam veranstaltet. Es wird auf Anregung des Komitees Forschung mit Synchrotronstrahlung durchgeführt und soll die besondere Bedeutung der Synchrotronstrahlung für die Physik und die Nachbarwissenschaften zum Ausdruck bringen, insbesondere im Hinblick auf die Möglichkeiten, die sich in Bezug auf den Ausbau existierender Quellen und das Potential der Freien Elektronen Laser (FEL) in Deutschland ergeben.

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### ÜBERSICHT DER HAUPTVORTRÄGE

(Hörsal TU HE101)

#### Hauptvorträge

SYSR 1.1	Sa	08:30	(TU HE101)	<b>Transient structures in chemical reactions determined by picosecond x-ray diffraction</b> , <u>Michael Wulff</u>
SYSR 2.1	Sa	09:00	(TU HE101)	<b>Biological x-ray microscopy: biochemical mapping of sperm and lensless imaging of yeast</b> , <u>Chris Jacobsen</u>
SYSR 3.1	Sa	09:30	(TU HE101)	<b>In-situ High Pressure XPS of Heterogeneous Catalysts</b> , <u>Robert Schlögl</u> , Axel Knop-Gericke
SYSR 4.1	Sa	10:00	(TU HE101)	<b>Photoelectron spectroscopy of solids with soft and hard x-rays: Towards enhanced bulk sensitivity</b> , <u>Ralph Claessen</u>
SYSR 5.1	Sa	11:00	(TU HE101)	<b>Investigation of buried interfaces and surface structures</b> , <u>Harald Reichert</u>
SYSR 6.1	Sa	11:30	(TU HE101)	<b>Magnetism and Dynamics Probed via Nuclear Excitation: Applications and Perspectives</b> , Ralf Röhlsberger
SYSR 7.1	Sa	12:00	(TU HE101)	<b>X-ray Spectroscopy of Nanoclusters: State of the art and perspectives at the new VUV - Free Electron Laser in Hamburg</b> , <u>Wilfried Wurth</u>
SYSR 8.1	Sa	12:30	(TU HE101)	<b>X-ray Holography, Femtosecond Snapshots and the Potential of the BESSY Free Electron Laser</b> , <u>Stefan Eisebitt</u>

Kaffeepause: 10:30 - 11:00

## Fachsitzungen

– Hauptvorträge –

### SYSR 1 Hauptvortrag

Zeit: Samstag 08:30–09:00

Raum: TU HE101

#### Hauptvortrag

SYSR 1.1 Sa 08:30 TU HE101

**Transient structures in chemical reactions determined by picosecond x-ray diffraction** — ●MICHAEL WULFF — European Synchrotron Radiation Facility, Grenoble Cedex 38043, FRANCE

The excited-state structure of small molecules in solution has been studied by combining ultrafast laser techniques with x-ray diffraction. The experiments are done using the pump and probe method: ultra short laser pulses excite a subset of molecules in the sample and delayed x-ray pulses (100 ps) record the structure at a given delay. The diffraction patterns are recorded on a CCD detector in pairs *with* and *without* excitation. The change in the intensity  $\delta S(q,t)$  is then Fourier transformed to  $\delta S[r,t]$ , the real-space image of the excited system. There are two contributions to  $\delta S[r,t]$ : the *change* in intramolecular structure of the solute in its case

and the *change* in intermolecular structure in the bulk liquid. We have studied these phenomena for some simple photo reactions in liquids: the dissociation and recombination of  $I_2$  [1],  $HgI_2$ ,  $C_2H_4I_2$  and  $Br_2$  in polar and non-polar liquids. The experimental data will be compared to Molecular Dynamics simulations and we will discuss methods to separate the two contributions.

Finally we will discuss our myoglobin project, specifically the migration of CO in native myoglobin and in the mutant L29F. In both cases the difference maps show how CO moves away from the binding site in jumps between cavities in the protein [2].

[1] A. Plech et al., Phys. Rev. Lett. 92 (2004) 125505; S. Rice, Nature 429 (2004) 255.

[2] F. Schotte et al., Science 300 (2003) 1944.

### SYSR 2 Hauptvortrag

Zeit: Samstag 09:00–09:30

Raum: TU HE101

#### Hauptvortrag

SYSR 2.1 Sa 09:00 TU HE101

**Biological x-ray microscopy: biochemical mapping of sperm and lensless imaging of yeast** — ●CHRIS JACOBSEN — Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY, USA

What's inside a cell? Much is known, thanks to light and electron microscopy. However, x rays offer new insights, by imaging whole cells at 20-40 nm resolution using zone plate lenses, and in particular by combining this with spectroscopic sensitivity to organic functional groups. While spectra of single compounds can provide exquisite information on electronic states, a cell is much more complex. Pattern recognition algo-

gorithms provide a way to deal with this complexity and obtain insights into biochemical organization at a fine spatial scale, as illustrated in an ongoing study of the correlation of morphology with biochemical content in sperm. Can one obtain better resolution than present x-ray lens technology allows? The purest form of measurement is to collect x rays scattered by a cell with no optics-imposed losses. By using iterative phasing algorithms, this diffraction data can be phased to deliver a real-space image of a complex cell (at present, 30 nm resolution in studies of freeze-dried yeast) with a possible ultimate extension to atomic resolution imaging of proteins using x-ray free electron lasers.

### SYSR 3 Hauptvortrag

Zeit: Samstag 09:30–10:00

Raum: TU HE101

#### Hauptvortrag

SYSR 3.1 Sa 09:30 TU HE101

**In-situ High Pressure XPS of Heterogeneous Catalysts** — ●ROBERT SCHLÖGL and AXEL KNOP-GERICKE — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin

Heterogeneous catalysts are dynamical systems that can be studied in their correct function only when subjected to appropriate reaction conditions taking into consideration the coupling between the catalyst structure and its reaction environment. Consequently we studied structural and catalytic properties simultaneously by applying in-situ methods and using synchrotron radiation. Facing a deficit in truly surface-sensitive in-situ- techniques in collaboration with the University of Berkeley we de-

veloped a high pressure XPS system allowing photoemission and photoabsorption studies of all kinds of heterogeneous catalysts under flow-through conditions at pressures up to ca. 10 mbar. This and the tunability of SR radiation allowing non-destructive depth profiling provide substantial information about the interaction of catalytic material with its reaction environment. Examples of studies on metals (Cu, Ag, Ru) and oxides (vanadium oxides, molybdates) are used to highlight the type of information that can be gathered. The data clearly show the metastable nature of the systems and their decomposition behaviour upon removal of the reaction conditions. It is shown that a new quality of insights into the function of catalyst is obtained by using SR-based in-situ XPS that is now mature enough for applications to complex practical systems.

### SYSR 4 Hauptvortrag

Zeit: Samstag 10:00–10:30

Raum: TU HE101

#### Hauptvortrag

SYSR 4.1 Sa 10:00 TU HE101

**Photoelectron spectroscopy of solids with soft and hard x-rays: Towards enhanced bulk sensitivity** — ●RALPH CLAESSEN — Experimentalphysik II, Universität Augsburg, D-86135 Augsburg, Germany

Photoelectron spectroscopy (PES) is a powerful tool for electronic structure determination in solids, allowing direct access to densities of states, band structures, and Fermi surfaces. However, a serious drawback of the method is its extreme surface sensitivity of only a few atomic layers, which results from the rather low photoelectron mean free path when using vacuum ultraviolet radiation, as is usually the case. This problem can be overcome by using high-energy x-ray photons at third generation

synchrotron radiation sources, leading to much higher probing depths. I will present examples of soft x-ray PES (SX-PES,  $h\nu \approx 700..1000$  eV) on selected transition metal oxides with large unit cells, where strong surface effects would prevent the use of conventional PES for a reliable determination of their *bulk* electronic structure. It will also be shown that SX-PES spectra still contain substantial k-space information. The bulk sensitivity can be further enhanced by using hard x-rays (HX-PES,  $h\nu \approx 6..10$  keV), where probing depths of more than 100Å can be achieved. This not only helps to overcome the surface barrier, but also opens an opportunity for PES on *buried* interfaces and nanostructures. I will discuss first pilot experiments in this direction and plans for a possible HX-PES beamline at the new x-ray source PETRA-III at Hasylab.

## SYSR 5 Hauptvortrag

Zeit: Samstag 11:00–11:30

Raum: TU HE101

### Hauptvortrag

SYSR 5.1 Sa 11:00 TU HE101

**Investigation of buried interfaces and surface structures** — ●HARALD REICHERT — Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, D-70569 Stuttgart

Surfaces and interfaces are of fundamental interest in condensed matter physics and the availability of highly brilliant synchrotron radiation has boosted our understanding of the structure of surfaces and interfaces in the last decades, especially in the case of liquid materials. Nevertheless, the characterization of the structure of liquid and amorphous interfaces,

which is already elusive in bulk system, still presents a challenge to experimental physics. We have recently developed a new transmission-reflection scheme using high energy microbeams in a high resolution setup which allows us to resolve the structure of deeply buried interfaces in diffraction experiments. In a series of pilot experiments we have investigated a variety of solid-liquid interfaces. A common feature we found in most systems are pronounced density anomalies at the interfaces. Most prominent examples are Schottky contacts and the interface ice-SiO<sub>2</sub> which develops a high density liquid water layer upon approaching the melting temperature of ice.

## SYSR 6 Hauptvortrag

Zeit: Samstag 11:30–12:00

Raum: TU HE101

### Hauptvortrag

SYSR 6.1 Sa 11:30 TU HE101

**Magnetism and Dynamics Probed via Nuclear Excitation: Applications and Perspectives** — ●RALF RÖHLSBERGER — HASY-LAB@DESY, Notkestr. 85, 22607 Hamburg

The outstanding brilliance of 3rd-generation synchrotron radiation sources has rendered several x-ray scattering techniques sensitive to smallest amounts of material. This applies in particular for nuclear resonant x-ray scattering. It is the virtue of this technique to be capable of probing magnetic as well as vibrational properties, basically in the same experimental setup.

Magnetic properties are studied via elastic resonant scattering: Ultra-

thin layers of the resonant isotope are employed to directly probe magnetic spin structures on an atomic scale. This allows one to image the internal magnetic structure of nanoscale systems with very high depth resolution. Recent studies have been applied to exchange-coupled thin films like exchange-spring magnets, exchange-bias systems and coupled metal/oxide heterostructures.

Using inelastic resonant scattering, the vibrational density of states can be determined with energy resolutions in the sub-meV range. In thin films and nanostructured systems, the microscopic origin of excitations that are strongly influenced by the reduced dimensionality can be explored. Finally, the talk illuminates new possibilities at future sources like PETRA III and the XFEL.

## SYSR 7 Hauptvortrag

Zeit: Samstag 12:00–12:30

Raum: TU HE101

### Hauptvortrag

SYSR 7.1 Sa 12:00 TU HE101

**X-ray Spectroscopy of Nanoclusters: State of the art and perspectives at the new VUV - Free Electron Laser in Hamburg** — ●WILFRIED WURTH — Institut für Experimentalphysik, Universität Hamburg

Third generation synchrotron sources provide high brilliance radiation in the soft X-ray regime with variable polarisation. Soft X-ray spectroscopy at these sources is an ideal tool to study the detailed evolution of static physical properties of nanoclusters from the atom to the bulk. Re-

cent examples for the magnetic properties of supported transition metal clusters obtained at BESSY in Berlin will be given. With the free electron laser in the XUV spectral regime at DESY in Hamburg (VUV-FEL) operational from 2005 a new research tool will be available which offers unique opportunities. In the talk I will review some of the prospects of this new source for the investigation of nanoclusters. In particular I will discuss the possibility to obtain detailed electronic structure information as a function of the number of atoms in small free clusters as well as possible approaches to study ultrafast dynamical processes in nanoclusters with the VUV-FEL.

## SYSR 8 Hauptvortrag

Zeit: Samstag 12:30–13:00

Raum: TU HE101

### Hauptvortrag

SYSR 8.1 Sa 12:30 TU HE101

**X-ray Holography, Femtosecond Snapshots and the Potential of the BESSY Free Electron Laser** — ●STEFAN EISEBITT — BESSY m.b.H., Albert-Einstein-Str. 15, 12489 Berlin

While holography has evolved to a powerful technique in the visible spectral range, it is difficult to apply at shorter wavelength as no intrinsically coherent (soft) x-ray laser is yet available as a light source. The progression from visible light towards shorter wavelength is motivated by the increase in spatial resolution that can be achieved. Of equal importance is the possibility to exploit special contrast mechanisms provided by scattering in resonance with transitions between electronic core and valence levels. We demonstrate magnetic imaging by x-ray spectro-holography at 50 nm spatial resolution, imaging magnetic domain patterns forming

in thin film Co-Pt multilayers. Holography at this wavelength was made possible by combining the sample with a nanostructured mask [1]. This approach is particularly valuable for future *single shot* imaging experiments at free electron x-ray lasers. At such sources, the coherent x-ray flux will be sufficient to record a holographic snapshot using a single x-ray pulse with a duration of a few femtoseconds. Snapshots and pump-probe schemes will thus allow the study of dynamic processes on ultrafast time scales. The future prospects of imaging techniques based on coherent scattering will be discussed in the context of the current development of x-ray lasers, such as the BESSY HGHG free electron laser.

[1] S. Eisebitt, J. Lüning, W. F. Schlotter, M. Lörger, O. Hellwig, W. Eberhardt, J. Stöhr, Nature, accepted (2004)