

poly(glycidyl methacrylate). The PSA films were prepared with solution casting on pre-cleaned glass surfaces. From a naive point of view, one would have expected homogenous films which are characterized by the average monomer composition. To investigate the surface structure, we probed the density profile perpendicular to the PSA surface using x-ray reflectivity (XRR). We detected the presence of an enrichment layer of one type of monomer at the surface, followed by an enrichment of the other monomer type underneath. Which type of monomer of the statistical copolymer is enriched at the free surface depends on the choice of the minority component. The lateral structure of the detected enrichment layers is probed with grazing incidence small angle x-ray scattering (GISAXS).

Keywords: surface analysis, X-ray reflectivity, polymer films

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Coordination effects in magnetic nanostructures

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Advanced synchrotron radiation techniques are able to provide high sensitivity to the study of very diluted magnetic systems, unveiling thus novel properties hardly accessible by other experimental techniques. X-ray circular dichroism, in particular, has been successfully used to track the evolution of the magnetic properties in nanostructures constructed at surfaces, from finite-sized particles to isolated adatoms. This presentation will illustrate how x-ray circular magnetic dichroism carried out in high magnetic fields and cryogenic conditions can be employed to simultaneously measure the valence state and magnetic moment of individual atoms and small clusters on surfaces. The results show how Hund's rule magnetic moments of a free atom change upon adsorption on a surface, the appearance of magnetic anisotropy, the dependence of the magnetic and electronic configuration on the substrate interaction and the atomic coordination.

Keywords: nanomagnetism, surfaces, X-ray circular magnetic dichroism

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Structural effects and the spin reorientation in Au/Co/Au films

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Ultrathin Au/Co/Au films are known to exhibit Spin Reorientation Transitions (SRT) from in- to out-of plane as a function of the

Co-film thickness, Au cap-layer thickness and temperature. We performed an in-situ systematic study of the magnetic, electronic and structural properties of Co/Au and Au/Co/Au films grown on W(110), by means of soft x-ray absorption and photoemission experiments with synchrotron radiation. Our recent X-Ray Magnetic Circular Dichroism (XMCD) measurements on this system establish that, contrary to a widely accepted opinion, the perpendicular magnetic anisotropy is not necessarily accompanied by an increase of the orbital moment along the easy magnetic direction [1]. This experimental observation is confirmed by theoretical considerations, showing that the magneto-crystalline anisotropy is system-dependent [1]. Here, we furthermore, study the correlation of structural effects with the magnetic properties in these films. We present Co L-edge Extended X-ray Absorption Fine Structure (EXAFS) results on the local structure for the same in-situ grown films, whose magnetic properties were characterized using XMCD and X-ray resonant reflectivity experiments. We apply the Bayes-Turchin approach developed by Krappe and Rossner [2,3] to analyze EXAFS spectra. From this analysis we obtain quantitative information on the structural strain and disorder of the Co layers, for both the in- and the out-of-plane magnetic phases. We are, for the first time, able to perform a systematic investigation of the interplay between local structural changes and the occurrence of the SRT [1].

[1] C. Andersson et al., *Phys. Rev. Lett.* 99, 177207 (2007)

[2] H. J. Krappe and H. H. Rossner, *Phys. Rev. B* 70, 104102 (2004)

[3] H. H. Rossner et al., *Phys. Rev. B* 74, 134107 (2006)

Keywords: XAFS data analysis, crystal and magnetic structure, magnetic phase transitions

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Quantum phase transitions using non-resonant X-ray magnetic scattering at high pressures

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Over the last decade or two, quantum phase transitions (QPT) and their associated critical behavior have provided an accessible experimental approach and also an expressive language to our understanding of quantum fluctuation and correlation. Correlation between electrons is responsible for kaleidoscopic forms of novel phases in important materials of both technological interest and intellectual challenges, while fluctuation from Heisenberg's uncertainty principle rather than a thermal exploration of states drives phase transitions at absolute zero of temperature. Traditionally, experimental approaches of QPT rely on tuning via magnetic field or alloying. However, hydrostatic pressure serves as a cleaner method than doping because it retains a constant chemical environment and, unlike a magnetic field, does not break any symmetries. Through a combination of cryogenics, diamond anvil cell, and synchrotron x-ray diffraction techniques, we directly measure the spin and charge orders in pure Cr metal as it is driven through the spin-density-wave/paramagnet QPT. We observe that both the spin and charge orders are suppressed exponentially with pressure, well beyond the region where disorder cuts off such a simple evolution. The evolution of the magnetic wavevector reveals a rigid band structure under pressure, and ascribes the destruction of antiferromagnetism to the growth in electron kinetic energy. The observed order parameter behavior follows a weak-coupling BCS theory for the ground state, even though strong correlations were observed in Cr to surprisingly high

temperatures and energies in dynamic fluctuations. This duality points to the fundamental issue of how mean-field behavior can describe so successfully important aspects of highly correlated electron systems.

Keywords: quantum phase transition, magnetic X-ray diffraction, high pressure diamond anvil cells

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High pressure induced charge ordering in lithium vanadate spinel

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The spinel oxide LiV_2O_4 has been attracting considerable interest as the first heavy fermion oxide [1]. Although the low temperature properties of LiV_2O_4 are in striking parallel with those of intermetallic heavy fermions, it is not clear whether their similar properties have similar origins. LiV_2O_4 has a face-centered-cubic (FCC), spinel structure, and the formal oxidation of V ion is 3.5+. Previous studies showed that LiV_2O_4 remains cubic down to low temperature and that no magnetic ordering occurs down to 20 mK, indicating that all V sites are crystallographically equivalent even at low temperatures. We found that this system shows a metal-insulator transition under pressure. The metal-insulator transition can be attributed to charge ordering of V ions, similar to one observed in AlV_2O_4 [2]. EXAFS measurements under high pressure for LiV_2O_4 (vanadium K edge at SLS, up to 22 GPa) indicated that a phase transition occurs probably associated with a charge ordered state[3]. It is probable that the phase transition we observed is of the same type as that of vanadium clusters, an interesting model proposed recently[4]. Experiments performed at the ESRF synchrotron (powder diffraction function of temperature and pressure) showed also a structural transition but at lower temperatures than that inferred from EXAFS measurements, and similar to the work reported earlier by Takeda et al[5].

References

- [1] S. Kondo et al., *Phys. Rev. Lett.* 78, 3723 (1997), C. Urano et al. *Phys. Rev. Lett* 85, 1052 (2000).
 [2] K. Matsumo et al., *J. Phys. Soc. Jap.* 70, 1456 (2001).
 [3] N. Dragoe et al. *High Pressure Research*, 26, 427-431 (2006). L. Pinsard-Gaudart et al. *Phys Rev B* 76, 045119 (2007).
 [4] Y. Horibe et al. *Phys. Rev. Lett.* 96, 086406 (2006).
 [5] K. Takeda et al. *Physica B*359-361, 1312 (2005).

Keywords: high pressure, charge order, spinel

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Pressure-induced hydration and order-disorder transition in a synthetic gismondine zeolite

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Two high pressure phases of a potassium gallosilicate with a gismondine framework (K-GaSi-GIS) were characterized using Rietveld refinements of in-situ high-pressure, high-resolution synchrotron X-ray powder diffraction data. The observed response of the K-GaSi-GIS framework under hydrostatic pressure is a gradual flattening of the so-called 'double crankshaft' structural chain units. At pressures below 1.0(1) GPa, additional water molecules from the hydrostatic pressure-transmitting medium are inserted into the potassium-water guest network ('pressure-induced hydration') resulting in a 'super-hydrated' high pressure phase I. As the flattening of the 'double crankshaft' structural units in the GIS-framework continues above 1.6 GPa, the ellipticity of the cross-linking 8-ring windows is reduced below a certain threshold and a disordering of the potassium-water guest structure along the 8-ring channel, characteristic of a disordered high pressure phase II, is observed. The concerted framework distortion and guest network disordering accommodates the increased hydration level while maintaining the seven-fold coordination environment of the potassium cations to framework oxygen atoms and water molecules. We have thus established the atomistic details of a guest-host order-disorder transition under pressure-induced hydration conditions in a zeolite with GIS-framework and compared it to other zeolites during pressure-induced hydration. We find that the structural changes mediated by the extra framework cations and their coordination environment under PIH conditions are at the core of these different mechanisms and are driving the changes in the ellipticity of pore openings, order-disorder and disorder-order transitions and framework distortions.

Keywords: zeolite crystal chemistry, high-pressure chemistry, synchrotron powder diffraction

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Lattice dynamics in incommensurate elemental crystals at high pressure

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In recent years, surprisingly complex crystal structures have been discovered in the elements at high pressures. Incommensurately modulated structures and incommensurate host-guest composite structures have been observed in various elements across the periodic table, e.g., Rb, Ba, Sc, Te, P, and I. While considerable progress has been made in determining the detailed crystal structures of these complex phases, the mechanisms of their formation and stability are not yet fully understood. Experimental data on the lattice dynamics of the complex phases will be a key ingredient to address this question, and inelastic x-ray scattering (IXS) spectroscopy is the technique of choice to study phonons throughout the Brillouin zone on samples in diamond anvil high-pressure cells. IXS experiments were performed on single crystals of the incommensurate-composite phases Rb-IV and Ba-IV as well as the incommensurately modulated phase Te-III. As a unique feature of incommensurate composite systems, two LA-like phonon branches are observed in both Rb and Ba along the direction of incommensurability, which are attributed to separate LA-type lattice vibrations in the host and guest subsystems. The host and guest sound velocities have been determined as a function of