

Germany, ²TU Braunschweig, Institut fuer Werkzeugmaschinen und Fertigungstechnik, Langer Kamp 19b, Braunschweig, 38106, Germany, E-mail: katharina.rolfs@hmi.de

Magnetic Shape memory alloys are materials that can potentially substitute giant magnetostrictive systems and piezoelectrical ceramics in actuating devices due to the large magnetically induced strains. It also opens the door to a myriad of other industrial applications. Because of their relatively high operational temperature and the low magnetic fields needed to induce macroscopic strains, Ni-Mn-Ga-single crystals are one of the most common alloys for actuators based on the magnetic shape memory effect. Since the Bridgeman-technique for single-crystal growth is not able to cope with the high vapour-pressure of manganese, a recently developed technique called SLARE (Slag Remelting And Encapsulation) was used for a reliable and repeatable growth of homogeneous single crystals of known composition and low porosity. Using this new method, it is now possible to grow single crystals such as Ni_{49.7}Mn_{29.3}Ga₂₁ of tetragonal martensitic structure (5M) exhibiting a magnetic field induced strain of more than 4% below 170 mT. Since this effect occurs only in the ferromagnetic modulated (5M and 7M) martensitic structures, the application of these materials is still limited by the phase-transition temperature from martensite to austenite, which is now about 65°C in Ni-Mn-Ga. In order to augment the working temperature further, Co-doped Ni-Mn-Ga single crystals have been grown successfully. Up to now a possible working temperature of approximately 120°C has been achieved in Ni_{45.1}Co_{4.9}Mn_{31.9}Ga_{19.1} showing a stress induced (7.5MPa) strain of 1.5%. The stress-strain-analysis and the crystallographic characterization of these promising materials will be discussed here in detail.

Keywords: shape-memory alloys, single crystals growth, alloy development

MS.55.1

Acta Cryst. (2008). A64, C97

Structure of nanomaterials via electron multiple scattering

Michel A Van Hove

City University of Hong Kong, Physics and Materials Science, 83 Tat Chee Avenue, Kowloon Tong, Hong Kong, none, 12345, Hong Kong SAR, E-mail: vanhove@cityu.edu.hk

We have extended to nanostructures the basic theoretical capabilities of surface structure determination by low energy electron diffraction (LEED), by adopting a non-periodic cluster approach and substantially accelerating the computation time for complex structures. Conventional LEED computation times scale as the square or the cube of the number of atoms N whose positions are to be fit to experimental data. In our new method, called NanoLEED, that scaling is reduced to $N \log N$, allowing the solution of much more complex structures, including nanostructures. We describe the application of the new method to an ordered array of buckyballs adsorbed on a Cu(111) surface and to individual silicon nanowires. In the former case, existing experimental approaches can be used since the sample is a periodic extended surface. In the latter case of individual nanostructures, new experimental approaches have been proposed, such as LEED with a convergent beam [1] and LEED with an STM tip as source [2]. The computational method can be readily applied to other structural techniques such as photoelectron diffraction and x-ray absorption fine structure.

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Funded in part by RGC Grant No. CityU1/02C and CityU Grant No. 9610059.

Keywords: electron scattering, multiple scattering, nanocrystals

MS.55.2

Acta Cryst. (2008). A64, C97

Distinguishing chirality using electron diffraction

Carol J Hirschmugl, Luke Burkholder, Sara Chamberlin, Hin Chuck Poon, Dilano Saldin, Wilfred Tysoe

University of Wisconsin-Milwaukee, Department of Physics, 1900 E Kenwood Blvd, Milwaukee, WI, 53211, USA, E-mail: cjhirsch@uwm.edu

Adsorption of either R- or S-2-butanol chirally modifies a Pd(111). Enantioselectivity has been confirmed by adsorbing either R- or S-propylene oxide as a probe molecule and measuring the resulting coverage of the propylene oxide on the templated surface. This work reveals that low energy electron diffraction I/V curves are different for the R- and S- 2-butanol adsorbates, indicating that in contrast to x-ray diffraction, electron scattering is enantiodifferentiating. A Delay Line Detector Low Energy Electron Diffraction (DLD-LEED) system using a minimal electron dose to collect a series of LEED images as a function of energy has been used to examine the hydrocarbon adsorbate structures for S- and R-2-butanol. Total electron doses of approximately 10^7 electrons are small enough that less than 1% of the adsorbates interact with and are potentially destroyed by the electron beam during the entire collection time of the experiment. The LEED data show that the 2nd order diffraction spots ($\{2,-1\}$ and $\{-1,2\}$) exhibit an asymmetry in the I/V curve that is dependent on the chirality of the adsorbed molecule. This difference disappears for a racemic mixture of adsorbed 2-butanol.

Keywords: chiral recognition, electron diffraction techniques, surface studies

MS.55.3

Acta Cryst. (2008). A64, C97-98

Surface enrichment layers in pressure sensitive adhesive films

Alexander Diethert¹, Stephan V. Roth², Peter Muller-Buschbaum¹

¹TU München, Physik-Department LS E13, James-Franck-Str. 1, Garching, Bayern, 85748, Germany, ²HASYLAB at DESY, Notkestr. 85, Hamburg, 22603, Germany, E-mail: diethert@ph.tum.de

Pressure sensitive adhesives (PSA) are used for many different applications, such as for example adhesive foils or binding materials. A prominent class of PSA films is based on statistical copolymers. Typically, two or three different monomers are combined in the statistical copolymer to balance the different requests of the PSA. The adhesive properties of the PSA films are mainly determined by surface-near regions. However, detailed information about surface structures of such adhesive films is still missing. In the presented work we focus on PSA model systems of statistical copolymers consisting of two different types of monomers. On average our polymer chains are composed of 90% poly(ethyl hexylacrylate) and of 10% of a second monomer which is referred to as the minority component. Different types of monomers are used for the minority component, such as polystyrene, poly(methyl methacrylate) or

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

MS.55.4

Acta Cryst. (2008). A64, C98

Coordination effects in magnetic nanostructures

Carlo Carbone

Consiglio Nazionale delle Ricerche, Istituto di Struttura della Materia, Area Science Park Basovizza, Trieste, Italy, 34012, Italy, E-mail : carlo.carbone@ism.cnr.it

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

MS.55.5

Acta Cryst. (2008). A64, C98

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

Elizabeta Holub-Krappe¹, Cecilia Andersson², Masako Sakamaki³, Takehisa Konishi³, Takashi Fujikawa³, Hermann H. Rossner¹, Biplab Sanyal², Olle Eriksson², Lars Nordstrom², Jonathan Hunter Dunn⁴, Andreas Persson², Olof Karis², Dimitri Arvanitis²

¹Hahn-Meitner-Institut Berlin GmbH, Magnetism, SF2, Glienicker Str. 100, Berlin, Berlin, D-14109, Germany, ²Department of Physics, Uppsala University, Box 530, SE - 751 21 Uppsala, Sweden, ³Graduate School of Advanced Integration Science, Chiba University, 1-33 Yayoi-cho, Inage, Chiba 263-8522, Japan, ⁴MAX-lab, Lund University, Box 118, SE - 221 00 Lund, Sweden, E-mail: holub-krappe@hmi.de

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

MS.56.1

Acta Cryst. (2008). A64, C98-99

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

Yejun Feng^{1,2}

¹Argonne National Laboratory, Advanced Photon Source, 431E-002, 9700 S. Cass Ave., Argonne, IL, 60439, USA, ²The James Franck Institute, University of Chicago, GCIS-ESB47, 929 E. 57th St., Chicago, IL 60637, USA, E-mail: yejun@aps.anl.gov

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