

MA 8 Surface Magnetism

Time: Monday 15:00–17:15

Room: HSZ 103

MA 8.1 Mon 15:00 HSZ 103

The magnetic surface of a non-magnetic bulk material: $\text{YCo}_2(111)$ — ●JOSEF REDINGER¹, SERGI KHMELEVSKYI¹, PETER MOHN¹, and MICHAEL WEINERT² — ¹Inst. f. Allgemeine Physik, Vienna University of Technology, Getreidemarkt 9/134, A-1060 Vienna, Austria — ²Department of Physics, University of Wisconsin - Milwaukee, P.O. Box 413, Milwaukee, WI 53201, USA

A material with a magnetic surface and non-magnetic bulk would be highly desirable for technological applications since thin films of such a material would provide a natural magnetic multilayer with perfect matching of the electronic potentials at the magnetic/nonmagnetic interface. Using full-potential DFT calculations, we predict the existence of a stable magnetic (111) surface of the intermetallic compound YCo_2 which is nonmagnetic in the bulk with large magnetic moments in the topmost Co layer for both Y- and Co-terminated (111) surfaces. The magnetism does not extend beyond two Co layers, and despite a rather large contraction of the top Co-Y interlayer distance which tends to suppress magnetism, we find only a slightly reduced surface moment as compared to an ideal bulk truncated surface. The Y-terminated surface shows rather moderate interlayer relaxations, while intralayer relaxations are negligible for both terminations. The $\text{YCo}_2(111)$ surface matches perfectly to $\text{Cu}(111)$ thus facilitating the use of magnetically dead Cu cap layers, which will not kill the Co moments at the interface, according to our DFT results.

[1] S. Khmelevskyi, P. Mohn, J. Redinger, and M. Weinert, Phys. Rev. Lett. 94,146403 (2005)

MA 8.2 Mon 15:15 HSZ 103

Polarised Synchrotron Radiation and Angle-Resolved Photoemission for Spin Resolution on Valence Band States without Mott Detectors — ●MATTIA MULAZZI^{1,2}, MICHAEL HOCHSTRASSER³, IVANA VOBORNIK², JUN FUJII², MARTINA CORSO⁴, JÜRIG OSTERWALDER⁴, and GIORGIO ROSSI^{1,2} — ¹Department of Physics, University of Modena, Modena, Italy — ²INFN-TASC, Trieste, Italy — ³Laboratorium für Festkörperphysik, ETH Zürich, Zürich, Switzerland — ⁴Physik-Institut, Universität Zürich, Zürich, Switzerland

Magnetic dichroism in core-level photoemission proved to be a very powerful technique to investigate the properties of magnetic crystals. To equivalent experiments on the valence bands less efforts have been devoted because of the intrinsic complexity of the electron states. In this work we report on angle-resolved photoemission data taken with polarised synchrotron light on the $\text{Ni}(111)$ valence band. At particular k -vectors $\text{Ni}(111)$ shows sp states spin split by the exchange interaction. Momentum distribution curves have been measured as a function of the azimuthal emission angle, of the photon energy and polarisation and of the magnetisation state of the crystal to detect a signature of the sp states spin in a spin-integrated experiment. As soon as the photon polarisation or energy are changed, matrix elements intervene mixing to the purely magnetic effects. A comparison of data to calculated spectra obtained from a layer-KKR computational scheme resulted necessary to disentangle the two phenomena giving a better understanding of the magnetic dichroism in valence band and the $\text{Ni}(111)$ sp states spin polarisation without a time-consuming Mott scattering experiment.

MA 8.3 Mon 15:30 HSZ 103

XMCD at O K edge of Fe, Co, and Ni films grown with O surfactant — ●C. SORG¹, N. PONPANDIAN¹, M. BERNIEN¹, J. KURDE¹, K. BABERSCHKE¹, R. Q. WU², and H. WENDE¹ — ¹Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — ²Department of Physics and Astronomy, University of California, Irvine, California 92697, USA

We have grown ultrathin ferromagnetic films of Fe, Co, and Ni with oxygen as a surfactant on $\text{Cu}(100)$ and studied the systematics of their near edge X-ray absorption fine structure (NEXAFS) and X-ray magnetic circular dichroism (XMCD) at the O K edge [1,2]. It was shown earlier that using O as a surfactant improves the growth of these films toward a more layer-by-layer one [3]. Angular-dependent NEXAFS measurements at the O K edge give final evidence that the O does not form a bulk-like oxide with the $3d$ ferromagnet, and the O atoms stay on top of the growing film. The spectral features of the NEXAFS are identified with the help of density functional calculations. Due to the hybridization with the ferromagnet, the O acquires an induced magnetic moment that

can be probed by XMCD at the O K edge. The calculations reproduce the experimental spectra very well and yield spin and orbital moments of the ferromagnetic films as well as the induced moments of the oxygen surfactant [2]. – Supported by BMBF (05 KS4 KEB 5).

[1] C. Sorg *et al.*, Surf. Sci. **565**, 197 (2004).

[2] C. Sorg *et al.*, Phys. Rev. B, submitted (2005).

[3] R. Nünthel *et al.*, Surf. Sci. **531**, 53 (2003); *ibid.* **566-568**, 100 (2004).

MA 8.4 Mon 15:45 HSZ 103

Magnetization and neutron reflectivity of AuFe films — ●V. N. GLADILIN^{1,2}, V. M. FOMIN^{1,2,3}, J. T. DEVREESE^{1,3}, K. TEMST⁴, and C. VAN HAESDONCK⁴ — ¹TFVS, Departement Fysica, Universiteit Antwerpen, B-2610 Antwerpen, Belgium — ²Department of Theoretical Physics, State University of Moldova, MD-2009 Kishinev, Moldova — ³Department of Semiconductor Physics, TU Eindhoven, NL-5600 MB Eindhoven, The Netherlands — ⁴Laboratorium voor Vaste-Stoffysica en Magnetisme, Katholieke Universiteit Leuven, B-3001 Leuven, Belgium

We examine the effect of surface-induced anisotropy on the impurity-spin magnetization in spherical grains of dilute AuFe alloys. The strength of the surface-induced anisotropy is analysed as a function of the ratio between the elastic mean free path for conduction electrons and the radius of a grain. Based on our results for the impurity-spin magnetization, we calculate polarised-neutron reflectivity of AuFe films, which consist of closely packed spherical grains. We show that microstructure of a film has a crucial effect on the temperature-dependent spin asymmetry in the polarised-neutron reflectivity. This work has been supported by the Concerted Action (GOA) and the Interuniversity Attraction Poles (IAP) research programmes, and also by the Fund for Scientific Research – Flanders (FWO projects G.0306.00, G.0274.01, G.0435.03, and WOG WO.035.04N).

MA 8.5 Mon 16:00 HSZ 103

Magnetization reorientation in Au/Co: in-situ prepared ultrathin films — ●D. ARVANITIS¹, C. ANDERSSON¹, T. KONISHI², E. HOLUB-KRAPPE³, O. KARIS¹, and H. MALETTA³ — ¹Department of Physics, Uppsala University, Uppsala, Sweden — ²Department of Chemistry, Chiba University, Inage, Chiba, Japan — ³Hahn-Meitner-Institut, Berlin, Germany

We present X-ray Magnetic Circular Dichroism (XMCD) results to characterize the Spin Reorientation Transition (SRT) in ultra-thin in-situ prepared epitaxial Au/Co sandwich structures. The samples are prepared on an epitaxial $\text{Au}(111)$ layer grown in-situ on a $\text{W}(110)$ single crystal. We have investigated modifications in magnetic properties induced both by varying the Co film thickness (2-4 atomic layers) and thickness of the Au cap (0 to 5 atomic layers). For our in-situ samples, the SRT upon Au capping, at 300K, takes place around 4 atomic layers in contrast to related samples prepared ex-situ [1]. We present a novel phase diagram for the SRT for our in-situ grown films. An in-plane easy direction is observed for the whole investigated thickness range for the in-situ prepared Co films without cap, in contrast to work on in-situ $\text{Co}/\text{Au}(111)$ [2]. Around 4 atomic layers Co, the addition of a small amount of a Au cap induces the system to exhibit a stable remanence both with an in-plane and an out-of-plane easy direction.

[1] R. Sellmann, H. Fritzsche, H. Maletta *et al.* Phys. Rev. B **64**, 054418/1 (2001)

[2] R. Allenspach, M. Stampanoni, A. Bischof, Phys. Rev. Lett. **65**, 3344 (1990)

MA 8.6 Mon 16:15 HSZ 103

Coordination effects in low-dimensional Fe-Pt alloys — ●AXEL ENDERS, JAN HONOLKA, KLAUS KUHNKE, VIOLETTA SESSI, DIEGO REPETTO, and KLAUS KERN — Max-Planck-Institut fuer Festkoerperforschung, Heisenbergstrasse 1, D-70569 Stuttgart

FePt alloys are in the focus of extensive research due to their remarkably large magnetic anisotropy. Our results on atomically thin FePt monolayers demonstrate that a large anisotropy is achieved also in nanostructures which do not exhibit the often-discussed L10 structure. The key for large anisotropy values rather seems to be the alloying of iron with a constituent that (i) is magnetically polarizable and (ii) exhibits large spin-orbit coupling, such as Pt. To support this we have performed XMCD measurements on Fe-Pt nanostructures with varying Fe-Fe and

Fe-Pt coordination. The investigated structures include Fe impurities, Fe chains, Fe/Pt surface alloy and Fe/Pt bulk alloy on Pt substrates. As a general trend, we observe that Fe-Pt coordination stabilizes the magnetic order, while Fe-Fe coordination decreases the net magnetization significantly. The latter may be attributed to a low-spin state or even antiferromagnetism in small Fe clusters on Pt. The magnetic anisotropy and orbital magnetic moments are compared for all structures.

MA 8.7 Mon 16:30 HSZ 103

The influence of step edges and strain on the domain wall width

— •WULF WULFHEKEL, SIMONA BODEA, and JÜRGEN KIRSCHNER —
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The influence of substrate steps and epitaxial strain on magnetic domain walls in thin Fe films was investigated by means of spin polarized scanning tunneling spectroscopy. Domain walls in a 2 ML film grown on a W(001) substrate were imaged. The domain wall width is reduced when the wall is located at a substrate step edge. This is explained by the atomic arrangement at the step edges and the influence on the ferromagnetic exchange and magnetic anisotropy. Measurements of the width of domain walls in 4 ML Fe films indicate a reduced exchange constant compared to bulk Fe. This is related in parts to the reduced dimensionality and the huge strain of 10% in the Fe films.

MA 8.8 Mon 16:45 HSZ 103

Structural and electronic properties of pseudomorphic $\text{Cr}_{1-x}\text{Fe}_x$ -submonolayers on W(110)

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Submonolayer coverages of $\text{Cr}_{1-x}\text{Fe}_x$ -random-alloys have been investigated using low energy electron diffraction (LEED), scanning tunneling spectroscopy (STS) and Kerr-magnetometry. The Curie-temperatures of the alloys strongly depend on the composition and vary surprisingly similar to the bulk behavior. We observe a maximum of T_C at $x = 0.95$.

Characteristic peaks in the STS spectra, indicating unoccupied surface states, show up at constant energy values independent on the composition. Assuming a *rigid-band*-model, the Fermi-energy should decrease with respect to the *3d*-states for increasing Cr concentration. But this behavior was not observed. Thus the rigid-band model fails. However, with the assumption that the *4s*-states are shifted above E_F the observation of a nearly composition-independent electronic structure can be tentatively explained.

We compare the results obtained here with previous results for $\text{Fe}_x\text{Mn}_{1-x}/\text{W}(110)$ submonolayers [1].

[1] M. Pratzner and H.J. Elmers, Phys.Rev.B **69**,134418(2004).

MA 8.9 Mon 17:00 HSZ 103

Probing surface magnetism using nonlinear optics: an *ab initio* study of Fe/W(110)

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The nonlinear optical response of a structurally optimized Fe/W(110) thin film is investigated numerically using *ab initio* methods. The thin films consist of a monolayer of Fe on top of four monolayers of W, with different directions of the magnetization in the Fe layer. The calculation is based on eigenstates obtained using the full-potential linearised augmented plane-wave method, converged self-consistently to an accuracy better than $10 \mu\text{Ry}$, including the spin-orbit interaction. The magnetic ground state shows an easy axis in the $\bar{1}\bar{1}0$ -direction, in agreement with experiment. From the eigenstates we are able to calculate the magneto-optical transition matrix elements, the nonlinear optical susceptibility, and the second-harmonic response.