# O 72: [MA] Joint Session "Surface Magnetism III" (jointly with O)

Time: Thursday 15:15–19:15 Location: BH 243

O 72.1 Thu 15:15 BH 243

**Ultimate limit of electron-spin precession upon reflection in ferromagnetic films** — A. Hallal[1], T. Berdot[1], P. Dey[1], L. Tati Bismaths[1], L. Joly[1], A. Bourzami[2], F. Scheurer[1], H. Bulou[1], •J. Henk[3], M. Alouani[1], and W. Weber[1] — [1]Institut de Physique et Chimie des Matériaux de Strasbourg, France — [2]Université Ferhat-Abbas, Sétif, Algeria — [3]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

We report the discovery of 180° electron-spin precession in spin-polarized electron-reflection experiments on Fe films on Ag(001) [1], the largest possible precession angle in a single electron reflection. Both experiments as a function of Fe film thickness and *ab initio* calculations show that the appearance of this ultimate spin precession depends with utmost sensitivity on the relaxation of the Fe surface layers during growth. Similar spin precession is also predicted for other ferromagnetic films.

[1] A.Hallal *et al.*, Phys. Rev. Lett. **107** (2011) 087203.

O 72.2 Thu 15:30 BH 243

**High resolution electron energy loss spectroscopic studies of surface spin waves in ultrathin Co films on Cu(001)** — •Rajeswari Jayaraman[1], Harald Ibach[1], Antonio Tonino Costa[2], and Claus Michael Schneider[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Departamento de Ciências Exatas, Universidade Federal de Lavras, 37200-000 Lavras, Minas Gerais, Brazil

Electron energy loss spectroscopy has become a valuable tool for studies of the dispersion of spin waves at ferromagnetic surfaces. Using our recently developed high resolution spectrometer [1] we have extended a previous study [2] of the surface spin waves of fcc cobalt films deposited on Cu(001) along the [011] direction to lower wave vectors $k_{\|}$ and lower spin wave energies. Spin waves are resolved down to $k_{\|} = 0.2\text{Å}^{-1}$ and spin wave energies of 15meV. For $k_{\|} = 0.2-0.35\text{Å}^{-1}$ spectra with resolution of 7meV exhibit a noticeable contribution of bulk spin waves, in agreement with theoretical calculations. We have furthermore studied the dispersion along the [001] direction. In agreement with theory [3] we find that the spin wave dispersion is nearly isotropic in this system even at higher wave vectors.

[1] H. Ibach et al., to be published.

[2] R. Vollmer et al., Phys. Rev. Lett. 91, 147201 (2003).

[3] A.T. Costa et al., Phys. Rev. B 69, 64413 (2004); A.T. Costa et al., Phys. Rev. B 70, 054406 (2004).

O 72.3 Thu 15:45 BH 243

**Ultrafast Magnetization Dynamics of Gadolinium and Terbium Studied by XUV Photoelectron Spectroscopy** — •Martin Teichmann[1,2], Kristian Döbrich[1,2], Björn Frietsch[1,2], Cornelius Gahl[1,2], Robert Carley[1,2], Olaf Schwarzkopf[3], Philippe Wernet[3], and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Straße 2a, 12489 Berlin — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin — [3]Helmholtz-Zentrum für Materialien und Energie GmbH, Albert-Einstein-Straße 15, 12489 Berlin

Recent results from IR-pump-XUV-probe angle-resolved photoelectron spectroscopy (ARPES) experiments on the ultrafast demagnetization of thin films of Gd(0001) and Tb(0001) on W(110) will be presented. Following excitation by an intense IR pulse, ARPES with 35 eV photons allows us to directly probe the response of the exchange-split valance band. As a signature of ultrafast demagnetization by the IR pulse, we see a rapid reduction of the exchange-splitting in the valence band of both metals. However, due to its larger spin-lattice coupling, the response of terbium to laser excitation is far stronger than gadolinium. We also observe significant differences between the responses of the minority and majority bands in the first picosecond, both within and between the two metals. This ultrafast response is in contrast to quasi-equilibrium thermal demagnetization, and reveals a spin dependence to the exchange coupling between the valence and 4f states responsible for magnetic ordering. Laser excitation drives the system out of magnetic equilibrium on the picosecond timescale.

O 72.4 Thu 16:00 BH 243

**Structural aspects of magnetic coupling in a bilayer CoO(111) on Ir(100)** — Florian Mittendorfer[1], Raimund Podloucky[2], and •Josef Redinger[1] — [1]Inst. of Applied Physics, Vienna University of Technology, Vienna, Austria — [2]Inst. of Physical Chemistry, University of Vienna, Vienna, Austria

Experimentally, stoichiometric CoO is found to form a (111)-like hexagonal c(10x2) bilayer on the square fcc Ir(100) surface [1]. Besides lateral displacements and vertical bucklings two distinct local building blocks can be detected: hexagonal BN-like almost co-planar Co-O fragments and NaCl-type O atoms above Co triangles. Consequently, different magnetic couplings for the different arrangements should be expected, which will be further modified by the coupling to the non-magnetic substrate. We have performed DFT and DFT+U calculations for the proposed c(10x2) CoO(111)/Ir(100) structure and structural variants and also for the NaCl (RS) and Wurtzite (WZ) type bulk phases. Quite interestingly for the bulk phases PBE and even HSE predict the WZ to be the stable one, a trend which could only be reversed in PBE+U calculations for high values of U. Furthermore ferromagnetic coupling for bulk WZ CoO is found to be energetically much closer to the antiferromagnetic groundstate as compared to RS CoO. For the bilayer CoO(111)/Ir(100) systems this translates into a rather complex magnetic arrangement of ferro and antiferromagnetc couplings, which could be easily modified by small changes to the geometrical structures as determined by the CoO/Ir interface.

[1] C. Ebensperger et al., Phys Rev. B81, 235405 (2010).

O 72.5 Thu 16:15 BH 243

**Interfacial uniaxial anisotropy and magnetization reversal of Fe/$BaTiO_3$(001) layers** — •Vasili Hari Babu[1], Remya Kunjuveettil Govind[2], Joachim Gräfe[1], Martin Welke[1], Karl-Michael Schindler[2], and Reinhard Denecke[1] — [1]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany

Multiferroics, consisting of both ferroelectric and ferromagnetic phases, have attracted scientific and technological interest due to the magnetoelectric coupling between the phases. In these heterostructures, the growth and magnetic anisotropy of the ferromagnetic phase are to be known to exploit the sizeable magnetoelectric effects. In the present work, Fe films were grown up to 24 *ML* thickness on a ferroelectric $BaTiO_3$(001) substrate by electron beam evaporation in an ultra high vacuum chamber and the determination of the magnetic properties was carried out by using *in-situ* magneto-optic Kerr effect. The layers were seen to have onset of ferromagnetic ordering at 6 *ML* thickness and the layers up to 12 *ML* thick were seen to exhibit uniaxial magnetic anisotropy (UMA) in the Fe[110] direction. However, the magnetization reversal of layers above 16 *ML* thick was seen to exhibit a growing cubic anisotropy along with the UMA from the fact that the growth of Fe(10) unit cell is 45° rotated to the $BaTiO_3$(10) direction in order to reduce the lattice mismatch. The competition between the uniaxial (aided by the interface) and cubic anisotropies of these layers is explained by accounting the quadratic magneto-optic Kerr effects.

O 72.6 Thu 16:30 BH 243

**Electric-field induced phase transition in Fe/Ni(111)** — •Lukas Gerhard, Moritz Peter, and Wulf Wulfhekel — Physikalisches Institut, Karlsruher Institut für Technologie (KIT), Germany

It is known that both the crystallographic and the magnetic structure of Fe thin films exhibit a rich phase diagram. As has been found recently, this can be exploited to trigger a phase transition in 2 ML thick Fe films by magento electric coupling (MEC) [1]. In order to show that the phenomenon is not limited to this particular system, we studied 1 ML Fe films on a Ni(111) substrate. In atomically resolved scanning tunneling microscopy (STM) images two different crystallographic structures were revealed: Fcc and hcp domains coexist and show slightly different local densities of states. Indeed these domains can be switched by the application of very high electric fields. The induced crystallographic phase transition is studied with atomic resolution showing the lateral displacement of every Fe atom. The dynamic behaviour of the observed transition shows the same characteristics as the MEC in Fe/Cu(111) and can be explained by electric field induced lattice relaxations. A full understanding of the magnetism in

this system requires additional theoretical efforts. [1] L. Gerhard et al. Magnetoelectric coupling at metal surfaces. Nat. Nano 5, 792-797 (2010)

O 72.7 Thu 16:45 BH 243

**Enhanced magnetoelastic coupling of Fe layers on the NiO/Ag(001)** — •Anita Dhaka, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

Magnetoelastic (ME) coupling is the driving force for magnetostriction of bulk samples. The ME coupling coefficients $B_1$ and $B_2$ determine the magnetostriction $\lambda_{100}$ and $\lambda_{111}$, respectively, of cubic systems. They also determine the impact of lattice strain on the magnetic anisotropy. Therefore their experimental determination is of utmost importance for the understanding of magnetic anisotropy of epitaxially strained monolayers [1]. We have performed *in-situ* ME stress measurements on Fe monolayers on epitaxially grown NiO/Ag(001) to investigate the effect of an antiferromagnetic (AFM) buffer layer on the magnetoelasticity of ferromagnetic (FM) monolayers. Here, we measured the ME coupling coefficient $B_2$ of 6 monolayer (ML) Fe, which is unexpectedly large. We find $B_2 = -19.6 \pm 1.6$ MJ/m$^3$, which differs in both magnitude and sign from the bulk value of $+7.83$ MJ/m$^3$ [1]. For the deposition of 6 ML Fe on Ag(001) we measure $B_2 = +2 \pm 0.6$ MJ/m$^3$, which is almost a factor of four smaller than the bulk value. Notably, the induced strain in the Fe film on both substrates is comparable. This suggests that the FM-AFM interface plays an important role for the enhanced $B_2$ of Fe on NiO.

[1] D. Sander, Rep. Prog. Phys. 62, 809 (1999).

O 72.8 Thu 17:00 BH 243

**Growth mode and atomic structure of MnSi thin films on the Si(111) surface** — •Benjamin Geisler[1], Peter Kratzer[1], Takayuki Suzuki[2,3], Theresa Lutz[2], Giovanni Costantini[2,4], and Klaus Kern[2,5] — [1]Fakultät für Physik and Center for Nanointegration, Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [3]Department of Electronics Engineering and Computer Science, Fukuoka University, Fukuoka 814-0180, Japan — [4]Department of Chemistry, University of Warwick, Coventry, CV4 7AL, United Kingdom — [5]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Thin films of MnSi, epitaxially grown on Si(111), are interesting in the field of spin injection into semiconductors. However, due to the complexity of the material, little is known about the film atomic structure and its dependence on the growth conditions. We performed DFT calculations for thin films of MnSi on Si(111) in their ground state crystal structure (B20) to analyze experimental STM images which recently revealed the coexistence of different surface terminations. We give an explanation for the atomic structure behind this observation and present evidence that the film structure depends on the growth protocol (codeposition vs. reactive epitaxy). Furthermore, our calculations indicate an increased magnetic moment of the films due to the biaxial strain induced by the substrate and a preference of ferromagnetic alignment over antiferromagnetic orderings. This makes the material promising for applications in Si-based spintronics.

**15 min. break**

O 72.9 Thu 17:30 BH 243

**Surface morphology and atomic structure of $Fe_3Si$ on GaAs(001) and GaAs(110) and magnetic correlations** — •Sani Noor[1], Igor Barsukov[2], M. Samet Özkan[1], Lina Elbers[1], Nikita Melnichak[2], Benjamin Geisler[3], Jürgen Lindner[2], Peter Kratzer[3], and Ulrich Köhler[1] — [1]Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum — [2]Experimentalphysik - AG Farle, Universität Duisburg-Essen — [3]Fakultät für Physik and Center for Nanointegration (CeNIDE), Universität Duisburg-Essen

The system $Fe_3Si$/GaAs is a FM/SC combination that possesses properties such as a low lattice mismatch, high thermal stability and half-metallic behaviour that make it an interesting candidate for spintronic devices.

In this contribution we present STM studies of stoichiometric $Fe_3Si$ layers grown epitaxially on GaAs(001) and GaAs(110) and compare the structural findings with the magnetic behaviour. From MOKE, SQUID and FMR measurements the magnetic moments as well as the magnetic anisotropies could be determined as a function of the layer thicknesses. Furthermore, we find a transition from superparamagnetic behaviour to ferromagnetic behaviour at a thickness of 3 ML. In accordance with theoretical calculations an enhanced magnetic moment can be observed for thicknesses below 20 ML. We also compare STM simulations of the $Fe_3Si$ surface with the experimental filled and empty state images.

O 72.10 Thu 17:45 BH 243

**Interplay between magnetic anisotropy and quantum-well states in thin magnetic films** — •Tamene Dasa, Pavel Ignatiev, and Valeriy Stepanyuk — Max-Planck-Institut für Mikrostrukturphysik Weinberg 2, D-06120 Halle, Germany

In this work the magnetic properties of thin magnetic films on non magnetic substrate have been investigated. The main focus is on the interplay between the magnetic anisotropy (MA) and the spin-polarized qauntum-well states arising in such films. The study is performed in the framework of the Density Functional Theory (DFT) by means of the VASP code and the LSDA for the exchange-correlation. We consider Co and Fe films, with vertical size varying from 1 to 6 monolayers, on Pt(001) surface. The Pt substrate is expected to provide high MA.[1] Our results demonstrate that the magnetic anisotropy energy (MAE) and the easy axis direction can be altered by changing the thickness of the film. This effect is explained in terms of the spin-polarized quantum-well states within the film. We also show the possibility to tune the MAE by means of capping the magnetic film by non-magnetic material.

[1] P. Gambardella, S. Rusponi, M. Veronese, S. S Dhesi, C. Grazioli, A. Dallmeyer, I. Cabiria, R. Zeller, P. H. Dederichs, K. Kern, C. Carbone, and H. Brune, Science **300**, 1130 (2003).

[2] M. Tsujikawa, A. Hosokaw and Tatsuki Oda, Phys. Rev. B **77**, 054413 (2008).

O 72.11 Thu 18:00 BH 243

**Effect of the external electric field on surface states** — •Pavel Ignatiev, Oleg Brovko, and Valeri Stepanyuk — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We present an *ab initio* study of surface states exposed to the external electric field (EEF). We consider two examples: the Shockley-type surface state on Cu(111) and spin-polarized surface states arising on Co nanoislands. Using the KKR method supplemented with a possibility to account for the EEF, we demonstrate that the EEF affects both energetics and intensities of surface states. Our results on Cu(111) are compared with recent STS studies on the Stark shift of the Cu(111) Shockley surface state.[1] For spin-polarized surface states on a Co bilayer on Cu(111), we show that the spin-selective screening of the EEF by evanescent vacuum surface states tails leads to a possibility of reversing the sign of the surface states spin polarization.[2] Field-induced variations of the majority and the minority surface states band structures change significantly standing-wave patterns [3] of the spin-polarized electrons opening, thus, another way to locally switch spin-polarization of confined surface states. The effect of the electric field on magnetism of the Co bilayer is characterized also in terms of the effective magnetoelectric coefficient.[4]

[1] L. Limot *et al.*, Phys. Rev. Lett. **91**, 196801 (2003); J. Kröger *et al.*, Phys. Rev. B **70**, 033401 (2004).

[2] P. A. Ignatiev, V. S. Stepanyuk, Phys. Rev. B **84**, 075421 (2011).

[3] H. Oka *et al*, Science **327**, 843 (2010).

[4] C.-G. Duan *et al.*, Phys. Rev. Lett. **101**, 137201 (2008).

O 72.12 Thu 18:15 BH 243

**Quantum Spin Holography with Surface State Electrons** — •Oleg O. Brovko[1,2] and Valeri S. Stepanyuk[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

Recently Moon and coworkers have shown that information can be stored in a fermionic state of a two-dimensional electron gas and have dubbed the proposed concept quantum holographic encoding [1]. They have constructed molecular holograms of CO molecules on a Cu(111) surface, hosting a Shockley-type surface state (SS) [2]. Interference of electron waves scattered at the molecules led to the formation of an electron density pattern representing an information page [1]. This page has then been read out with an STM. It has been also shown that using the innate energy dispersion of SS electrons one can not only project the hologram in two spatial degrees of freedom but also stack them one on top the other in the energy dimension.

In our contribution we expand the concept and show that the spin of the electron can also act as a new dimension for information storage. If the molecules or atoms used in creation of a hologram are magnetic, then the scattering of surface state electrons becomes spin-dependent, allowing one to store different information pages in different spin channels. As an example we demonstrate the possibility of simultaneous encoding of two different information pages with electrons of the same energy but opposite spins.

[1] C.R. Moon et al., Nature Nano. 4, 167 (2009)
[2] W. Shockley, Phys. Rev. 56, 317 (1939)

O 72.13 Thu 18:30 BH 243

**First-principles investigation of energy– and impurity–dependent electron focusing effect** — •Mohammed Bouhassoune, Peter H. Dederichs, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

It has been shown recently that the electronic signature of subsurface impurities can be revealed using Scanning Tunneling Spectroscopy (STS) [1,2]. A single impurity buried below the surface induces anisotropic spatial oscillations of the charge density due to a focused coherent interference of scattered electrons. These oscillations whose strength is determined by the shape of the host Fermi surface can be observed at the surface even if the impurity is far below the substrate. Using the full-potential Korringa-Kohn-Rostoker Green-function (KKR-GF) method, we investigate the energy dependent scattering of electrons at several magnetic and non-magnetic buried impurities below the Cu(100) surface. This allows a real-space mapping of the constant energy surfaces of the host material and a possible characterization of the impurity through the analysis of the induced phase shifts of the electron-density oscillations.

This work is supported by the HGF-YIG Programme FunSiLab – Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] A. Weismann et al., Science **323**, 1190 (2009).
[2] S. Lounis *et al.*, Phys. Rev. B **83**, 035427 (2011) and references therein.

O 72.14 Thu 18:45 BH 243

**Spin-dependent two-electron emission from ferromagnetic Fe(001)** — •Jürgen Kirschner[1], Frank O. Schumann[1], Carsten Winkler[1], Franz Giebels[2], Herbert Gollisch[2], and Roland Feder[2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle — [2]Theoretische Festkörperphysik, Universität Duisburg-Essen, 47048 Duisburg

We present a joint experimental and theoretical study of correlated electron pair emission from a ferromagnetic Fe(001) surface induced by spin-polarized low-energy electrons [1]. Spin-dependent angular and energy distributions of the emitted pairs have been measured and calculated. They are analyzed with the aid of the spin-, momentum-, symmetry-, and layer-resolved valence electron density of states, which we obtained by an ab-initio density functional theory calculation. The observed spectra are found to arise almost completely from only three surface parallel atomic layers. Momentum distributions for parallel spins of the emitted electrons exhibit an exchange-correlation hole, which is larger than the correlation hole in the antiparallel spin case. By comparing experimental antiparallel-spin pair spectra with their theoretical counterparts we determine an effective screening strength of the Coulomb interaction in the surface region.

[1] F. Giebels, H. Gollisch, R. Feder, F.O. Schumann, C. Winkler, and J. Kirschner, Phys. Rev. B 84, 165421 (2011).

O 72.15 Thu 19:00 BH 243

**Extending the two-dimensional electron spin-filter to a larger range of scattering energies and angles** — •D. Kutnyakhov[1], K. Medjanik[1], S.A. Nepijko[1], H.J. Elmers[1], G. Schönhense[1], C. Tusche[2], J. Kirschner[2], F. Giebels[3], H. Gollisch[3], and R. Feder[3] — [1]Inst. f. Physik, Univ. Mainz — [2]MPI f. Mikrostrukturphysik, Halle — [3]Theor. Festkörperphysik, Univ. Duisburg-Essen

In continuation of recent work on the novel imaging spin-filter technique based on electron diffraction from W(001) in the specular (00)-LEED spot [1,2], we studied the scattering energy (E) and angle of incidence (theta)-landscape of the spin sensitivity S, and reflectivity $I/I_0$. The setup includes a spin-polarized GaAs electron source and a delayline detector for spatially-resolving detection. Intensities, spin-orbit-induced asymmetries and figures of merit have been calculated by means of a relativistic layer KKR SPLEED code [3]. We assumed a 6 % inward relaxation of the topmost layer. The quasi-particle potential input for the SPLEED calculations was obtained by computing the ab-initio ground state electronic structure (FLAPW) and secondly augmenting the resulting potential by a complex self-energy correction. E-theta-behaviour studies open a path to an increased angular acceptance and energy range of the approach, thus increasing the performance of the multichannel spin-filter for electron spectroscopy [2].

Funded by DFG (Scho341/9 and TR 49), graduate school MAINZ.

[1] C. Tusche et al., APL 99 (2011) 032505; [2] M. Kolbe et al., PRL 107 (2011) 207601; [3] R. Feder in Polarized Electrons in Surface Physics, ed. by R. Feder (World Scientific, Singapore, 1985).