MA 13: Surface Magnetism

Time: Tuesday 10:30–13:15 Location: EB 301

MA 13.1 Tue 10:30 EB 301

Advances in Magnetic Exchange Force Microscopy — •Schwarz Alexander, Kaiser Uwe, Schmidt Rene, and Wiesendanger Roland — Department Physik, Institut für Angewandte Physik, Universität Hamburg, Jungíusstr. 11, 20355 Hamburg

Recently, the feasibility of magnetic exchange force microscopy (MExFM), which allows to visualize magnetic structures with atomic resolution, has been demonstrated [1]. This novel technique utilizes a force microscopy set-up to detect the short-ranged magnetic exchange interaction between two atomic magnetic moments (spins) residing on an atomically sharp tip as well as on the probed surface. Atomically resolved data obtained with an iron coated tip on two very different antiferromagnetic systems are compared: (i) a 3D insulator with localized spins that are coupled via superexchange and (ii) a 2D metallic bandferromagnet with delocalized spins coupled via itinerant exchange. In (i) latter case, a direct exchange between tip and sample spins at small separations seems to be necessary to observe a magnetic signal. For system (ii) the magnetic signal appears to be stronger and detectable at larger separations. Both systems exhibit a peculiar interplay of chemical and magnetic interactions, because they are approximately of the same range.

[1] U. Kaiser, A. Schwarz, R. Wiesendanger, Nature **4**46, 522 (2007).

MA 13.2 Tue 10:45 EB 301

Ab initio calculation of symmetric and antisymmetric exchange parameters — •Marcus Heide, Gustav Bihlmayer, and Stefan Blügel — Institut für Festk"orperforschung (IFF), Forschungszentrum Jülich

A simple approximation to the energy of a spin configuration is the classical Heisenberg model $E = \sum_{i,j} J_{i,j}\, \mathbf{S}_i^\dagger\, \mathbf{S}_j$. It's exchange integrals $J_{i,j}$ are dominated by non-relativistic effects. Staying within a bilinear approximation but accounting for spin-orbit coupling effects, the model can be generalized by $E = \sum_{i,j} \mathbf{S}_i^\dagger\, \mathsf{M}_{i,j}\, \mathbf{S}_j$ with the 3×3 matrices $\mathsf{M}_{i,j}$ [1]. This matrices contain terms describing the symmetric and antisymmetric (Dzyaloshinskii-Moriya) exchange as well as the magnetocrystalline anisotropy.

In this talk, we focus on thin magnetic surface films of hexagonal geometry and estimate the matrices $\mathsf{M}_{i,j}$ from first principles. Thereby, we employ spin-spiral calculations in order to obtain the exchange terms. The resulting ground states are discussed within our model ansatz.

[1] T. Moriya, Phys. Rev. **120**, 91 (1960)

MA 13.3 Tue 11:00 EB 301

Dzyaloshinskii-Moriya interaction driven non-collinear magnetic order of a Mn monolayer on W(001) — •Paolo Ferriani[1], Elena Vedmedenko[1], Kirsten von Bergmann[1], Stefan Heinze[1], Marcus Heide[2], Gustav Bihlmayer[2], Matthias Bode[1], Andre Kubetzka[1], Roland Wiesendanger[1], and Stefan Blügel[2] — [1]Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

The Dzyaloshinskii-Moriya (DM) interaction, arising from inversion symmetry breaking, has been found to play a crucial role at nanostructure surfaces, as recently established by the discovery of chiral magnetic order in ultrathin films [1]. Such interaction, favouring non-collinear magnetism, competes with the Heisenberg exchange and the magnetic anisotropy, leading to a complex magnetic phase space [2] that is so far largely unexplored. Here, we investigate the magnetic state of one monolayer Mn/W(001), based on density functional theory and Monte Carlo calculations. Using the full-potential linearized augmented plane wave method, we find that the DM interaction stabilizes a spin-spiral state on the nanometer scale. Monte Carlo simulations of the domain boundary between spirals propagating along equivalent crystallographic directions show the formation of intriguing labyrinth structures. The theoretical results are in agreement with spin-polarized scanning tunneling microscopy measurements.

[1] M. Bode *et al.*, Nature **447**, 190 (2007).
[2] Rößler *et al.*, Nature **442**, 797 (2006).

MA 13.4 Tue 11:15 EB 301

Giant positive magneto-crystalline anisotropy in ferromagnetic Mn/W(001) overlayer. — Martin Ondračeк, Alexander Shick, •František Máca, and Tomas Jungwirth — Institute of Physics ASCR, Prague, Czech Republic

Proposal of the ferromagnetic (FM) ground state for Mn monatomic overlayer on W(001) is reported recently by Ferriani *et al.* [1] on the basis of first-principles calculations. We study the magneto-crystalline anisotropy (MAE), spin (M_S) and orbital (M_L) magnetic moments, and tunneling anisotropic magneto-resistance (TAMR) of FM-Mn/W(001). The anisotropic properties of Mn/W(001) were investigated making use of the relativistic version of the FP-LAPW method [2], in which SO coupling is included in a self-consistent second-variational procedure. The magnetic force theorem was used to evaluate the MAE and the DOS anisotropy.For the Mn atom, out-of-plane $M_S = 3.18\mu_B$ and $M_L = 0.09\mu_B$ are calculated. There is a strong induced W-interface $M_S = -0.34\mu_B$ and $M_L = -0.06\mu_B$. The spin and orbital polarizations of W are quickly decaying away from the interface, showing slow oscillations. When the magnetization is rotated in-plane, there is no anisotropy in M_S, and a pronounced reduction of in-plane M_L. Accordingly, the very big positive MAE of 5.6 meVper Mn-atom is calculated, which is shown to originate from the W contribution. In addition, the TAMR is estimated from the densities of states anisotropy. [1] Ferriani P., Heinze, S., Bihlmayer, G., Blügel, S., Phys. Rev. **B 72** (2005), 024452. [2] A.B. Shick, D.L. Novikov, and A.J. Freeman, Phys. Rev. B **56**,R14259 (1997).

MA 13.5 Tue 11:30 EB 301

Ab-initio simulation of magnetic exchange force microscopy of antiferromagnetic Fe/W(001) — •Cesar Lazo[1], Vasile Caciuc[2], Hendrik Hölscher[3], and Stefan Heinze[1] — [1]Institute of Applied Physics, University of Hamburg, Hamburg, Germany — [2]Institute of Physics, University of Münster, Germany — [3]Center for Nanotechnology, University of Münster, Germany

Magnetic exchange force microscopy (MExFM) is a promising new technique to perform magnetic imaging with atomic resolution by measuring the magnetic exchange force between a magnetically coated tip and a magnetic sample [1]. Here, we apply density functional theory using the full-potential linearized augmented plane wave (FP-LAPW) method to investigate the exchange forces on the antiferromagnetic monolayer Fe on W(001) [2]. We use an Fe cluster as a tip model and include relaxations of the cluster and the surface. Interestingly, relaxation effects of tip and sample depend sensitively on the local magnetic configuration. Therefore, relaxations play a crucial role for the magnetic signal. In particular, the onset of the exchange forces is shifted to larger distances, which facilitates their experimental observation. Based on the calculated force-distance curves we simulate MExFM images which display a competition of chemical and magnetic forces.

[1] U. Kaiser et al., Nature 446, 522 (2007).
[2] A. Kubetzka et al., Phys. Rev. Lett. 94, 087204 (2005).

MA 13.6 Tue 11:45 EB 301

High wave vector spin waves in 1 ML Fe/W(110) — •Jacek Prokop, Yu Zhang, Wen Xin Tang, Ioan Tudosa, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We report on a first observation of the high wave vector spin wave (SW) excitations in the ferromagnetic Fe monolayer (ML) epitaxially grown on a W(110) single crystal. Using a spin-polarized electron energy loss spectroscopy (SPEELS) we measured a spin wave dispersion along the [001] direction. The ML Fe was deposited at room temperature (RT), and annealed at 900 K in ultrahigh vacuum (UHV) condition. The SPEELS measurements were performed at 120 K. The SW excitations show up as fine unique features emerging from an elastic peak shoulder in the minority electron spectrum. The measured asymmetry for the Fe ML magnon peaks achieves 30 %. The magnons in the iron ML are much softer than that in the bulk Fe, and those in the 2 ML Fe/W(110) film [1]. We show that the energies of the SW excitations in the Fe ML are also lower than the surface mode of the bcc Fe(110) surface, and the SW are strongly damped. The obtained results will be discussed and compared with the existing calculations performed within the itinerant electron theory.

[1] W. X. Tang, Y. Zhang, I. Tudosa, J. Prokop, M. Etzkorn, and J. Kirschner, Phys. Rev. Lett. 99, 087202 (2007).

MA 13.7 Tue 12:00 EB 301

Unique playground for non-collinear magnetism : Fe monolayers on hexagonal transition-metal surfaces — •Börn Hardrat, Paolo Ferriani, and Stefan Heinze — Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany

Recently, the complexity of magnetic order even in simple systems such as single monolayer (ML) thick magnetic films on non-magnetic substrates has been dramatically demonstrated by the discovery of a spin-spiral state for a Mn ML on W(110) [1] and a nanoscale magnetic structure for an Fe ML on Ir(111) [2].

Here, we use density functional theory calculations based on the full-potential linearized augmented plane wave (FLAPW) method to systematically study the magnetic order of an Fe ML on hexagonal hcp (0001) and fcc (111) surfaces of 4*d*- and 5*d*-TMs. We demonstrate that due to substrate *d*-band filling the exchange coupling changes gradually from antiferromagnetic (AFM) on Tc, Ru, Re, and Os to ferromagnetic (FM) on Rh, Ir, Pd, Os and Pt. On Ru and Re the AFM coupling leads to a non-collinear Néel ground state due to topological frustration of exchange interaction. On Ru, Rh and Ir, the nearest-neighbor exchange coupling is small and exchange beyond nearest-neighbors, higher order spin interactions, and anisotropic exchange interaction compete making these systems a playground for intriguing magnetic order.

[1] M. Bode *et al.*, Nature **447**, 190 (2007).
[2] K. von Bergmann *et al.*, PRL **96**, 167203 (2006).

MA 13.8 Tue 12:15 EB 301

Orbital magnetic moment of single Co atom on Pt(111) surface - a view from correlated band theory — •Alexander Shick[1] and Alexander Lichtenstein[2] — [1]Institute of Physics ASCR, Na Slovance 2, Prague, Czech Republic — [2]University of Hamburg, Jungiusstrasse 9, 20355 Hamburg

The electronic and magnetic character of Co adatom on the Pt(111) surface is investigated. The relativistic version of the correlated band theory LSDA+U method (including spin-orbit coupling) is employed to induce the orbital polarization. It is shown that with a reasonable choice of Coulomb-U, LSDA+U calculations give the orbital magnetic moment of Co adatom in a good agreement with experimental XMCD data (P. Gambardella *et al.*, Science 300 (2003) 1130). Both the electron correlation induced orbital polarization and the structural relaxation play an essential role in the orbital moment formation. Microscopic origins of the orbital moment enhancement are discussed.

MA 13.9 Tue 12:30 EB 301

Magnetic Anisotropy of a single Fe atom on Pt(111) — •Tobias Schuh[1], Timofey Balashov[1], Albert F. Takacs[1], Arthur Ernst[2], Sergey Ostanin[2], Jürgen Henk[2], Patrick Bruno[2], Toshio Miyamachi[3], Shigemasa Suga[3], and Wulf Wulfhekel[1] — [1]Physikalisches Institut, Universität Karlsruhe (TH), Wolfgang- Gaede Str. 1, 76131 Karlsruhe — [2]MPI für Mikrostrukturphysik, Weinweg 2, 06108 Halle — [3]Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan

The storage of data in modern hard disks relies on the stability of the magnetization of magnetic bits. Reducing the size of the bits allows higher storage density. The smallest bit can be realized by a single atom and its stability by the magnetic anisotropy of the atom.

We used a scanning tunneling microscope to image single Fe atoms on Pt(111) at 4 K. With inelastic tunneling spectroscopy the spin excitations of individual Fe atoms were measured. The excitations were detected in the second derivative of the tunneling current exhibiting a peak and a dip symmetric with respect to the Fermi energy. From the position of the extrema the excitation energy was determined. Assuming a spin of $S = 1\hbar$ for the Fe atom, the excitation energy is found to be identical to the uniaxial magnetic anisotropy.

We determined the magnetic anisotropy to 5.7±0.1 meV per atom in good agreement to XMCD measurements of single Co atoms on Pt(111) [1]. The experimental energy is compared with theoretical calculations.

[1] P. Gambardella *et al.*, *Science* **300** 1130 (2003)

MA 13.10 Tue 12:45 EB 301

Differences in growth and magnetism between thin Fe films on vicinal and flat Au(111) — •Tobias Allmers and Markus Donath — Physics Institute, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

In this contribution we report on differences in growth behavior and magnetic properties of Fe films deposited on vicinal (v-) and flat Au(111). The different growth mode results in a different magnetic behavior: We found that the transition from out-of-plane to in-plane magnetization as a function of film thickness is delayed for the system Fe/v-Au(111) with respect to Fe/Au(111). Furthermore, we found no distinguished easy in-plane magnetization direction for Fe/Au(111), while the easy in-plane magnetization direction for Fe/v-Au(111) is perpendicular to the step edges. In addition, the spin-dependent electronic structure below and above the Fermi level was investigated with respect to the symmetry character and the sensitivity towards adsorbates of the respective spectral features.

MA 13.11 Tue 13:00 EB 301

Quantitative determination of spin-dependent quasiparticle renormalization in ferromagnetic 3d metals — •Jaime Sánchez-barriga, Andrei Varykhalov, Jörg Fink, Oliver Rader, Hermann Dürr, and Wolfgang Eberhardt — Bessy GmbH, Albert Einstein str. 15, D-12489, Berlin, Germany

Spin dependent low-energy electronic excitations in 3d ferromagnets are of special interest due to the need of a microscopic understanding of the electronic structure of solids. Low-energy electrons (or holes) become dressed by a cloud of excitations resulting in quasiparticles of a finite lifetime and a different effective mass. These type of excitations have been studied by many theoretical methods, and it has been found that because of many body effects no sharp quasiparticle peaks exist for binding energies larger than 2 eV. Interestingly, it has been shown that strong correlation effects could particularly affect majority spin electrons, leading to a pronounced damping of quasiparticles at binding energies around 2 eV and above. In order to give an experimental corroboration to these findings, we have performed a systematic study of the spin-dependent quasiparticle lifetime and band structure of ferromagnetic 3d transition metal surfaces by means of spin and angle-resolved photoemission spectroscopy. On hcp Co(0001), fcc Ni(111) and bcc Fe(110), we have found a more pronounced renormalization of the majority spin quasiparticle spectral weight going from Ni to Co which are both strong ferromagnets. For Fe, a weak ferromagnet, such a process becomes more prominent in the minority channel.