MA 45: Spin Structures at Surfaces and in thin films I (Skyrmions)

Time: Thursday 15:00–18:30 Location: BEY 118

MA 45.1 Thu 15:00 BEY 118

fcc-Fe monolayer on Ir(111): Atomic-scale meron-antimeron spin-texture predicted from a multi-scale study based on an realistic *ab initio* spin model — •David Siegfried Georg Bauer, Nicolai Kiselev, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

This research is work in progress and we hope to present here the final answer of the magnetic structure for the Fe/Ir(111) system. We are using a multi-scale approach, employing a classical spin Hamiltonian containing Heisenberg (EX), four-spin (FS), and Dzyaloshinskii-Moriya (DM) interaction as well as magnetic anisotropy with newly fitted exchange parameters obtained from *ab initio* calculations of Ref. [1].
We found a new class of magnetic patterns consisting of staggered meron-antimeron pairs within a supercell of 128 atoms, containing 9 meron-antimeron pairs and 18 topological defects. We carefully checked the shape and size of the supercell, which is commensurate with the underlying magnetic lattice. The magnetic structure is in very good agreement to the experimental SP-STM data [1]. We explain this structure by an interplay between the EX, FS and DM interaction, where the FS interaction plays a key role making this structure energetically favorable in comparison to a skyrmion lattice. Due to the local topological charges of the (anti-)meron of $Q = (-)1/2$, the electron may pick up a Berry phase when transversing through such a magnetic structure giving rise to interesting transport properties.
[1] S. Heinze *et al.*, Nature Phys. **7**, 713 (2011).

MA 45.2 Thu 15:15 BEY 118

Tailoring magnetic skyrmions in ultra-thin transition-metal films — •Bertrand Dupé, Markus Hoffmann, Charles Paillard, and Stefan Heinze — Institue of Theoretical Physics and Astrophysics, University of Kiel, 24098 Kiel, Germany

Skyrmions in magnetic materials offer attractive perspectives for future spintronic applications [1] since they are topologically stabilized spin structures on the nanometer scale which can be manipulated at low electric current densities [2,3]. Recently, it has been discovered that due to the broken inversion symmetry at surfaces magnetic skyrmion lattices can occur in ultra-thin transition metal films [4,5]. Here, we present an understanding of skyrmions in such systems based on first-principles electronic structure theory. We determine the magnetic interactions for ultra-thin films composed of Pd and Fe on the Ir(111) surface using density functional theory and explain the occurrence of skyrmion phases in an external magnetic field using Monte-Carlo simulations. Our simulations not only confirm the succession of phases recently reported in experiments [5] but also demonstrate the possibility of tailoring skyrmion properties at transition-metal interfaces [6].

[1] J. Sampaio, *et al* Nature Nanotech. **8**, 839 (2013). [2] F. Jonietz, *et al* Science **330**, 1648 (2010). [3] X. Z. Yu, N. Kanazawa, *et al* Nature Comm. **3**, 988 (2012). [4] S. Heinze, *et al* Nature Phys. **7**, 713 (2011). [5] N. Romming, *et al* Science **341**, 636 (2013). [6] B. Dupé, *et al* submitted.

MA 45.3 Thu 15:30 BEY 118

Temperature-driven phase transition of Fe/Ir(111) nanoskyrmions — •Stefan Krause, Andreas Sonntag, Jan Hermenau, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg

Skyrmions are topologically protected field configurations with particle-like properties. They are in the focus of many ongoing investigations due to their potential application for future spintronic devices. Using spin-polarized scanning tunneling microscopy (SP-STM) at low temperature ($T = 11$ K), a lattice of nanoskyrmions has been shown to be the ground state of the one-atomic-layer thick Fe/Ir(111) surface [1].

In our recent SP-STM studies we investigated the influence of temperature onto the Fe/Ir(111) nanoskyrmionic lattice. The experiments reveal that the lattice is stable against thermal agitation up to $T \approx 27.4$ K. Further elevating T to 28.0 K results in a fading of the magnetic SP-STM contrast, indicating a phase transition into the paramagnetic state. By repeatedly varying T we elaborate a very sharp phase transition at $T \approx 27.7$ K. At second monolayer Fe step edges the skyrmionic lattice is found to persist even to higher T, which is attributed to pinning.

The experimental results will be presented and discussed in terms of magnetic corrugation amplitude of the skyrmion lattice and pinning decay length.

[1] S. Heinze *et al.*, Nat. Phys. **7**, 713 (2011).

MA 45.4 Thu 15:45 BEY 118

Exotic topologically nontrivial spin structures in systems with competing Dzyaloshinskii-Moriya interaction and four-spin interaction — •Nikolai S. Kiselev, David S. G. Bauer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Systems of low dimensionality such as monatomic chains, nano-islands and monolayers exhibit unique properties different from bulk materials. In particular, due to the surface/interface induced changes of the electronic properties, monolayers of transition metals show unusual magnetic properties. For instance, the ground state of the Fe/Ir(111) [1] system corresponds to a complex previously unknown spin structure, which we identified as a staggered lattice of chiral meron-animeron pairs. The spin structure in such systems arises due to the interplay of three main energy contributions: Heisenberg exchange, Dzyaloshinskii-Moriya interaction, and four-spin interaction (FSI). We present a three-dimensional magnetic phase diagram (PD) in terms of the applied magnetic field, four-spin interaction coupling constant, and temperature. In this PD we identified the area of existence of the spiral state and the hexagonal lattice of nano skyrmions, which can be stabilized at zero field. We explain mechanism of their stabilization. Generalization of our model explains the emergence of the spiral state and skyrmions in Pd/Fe/Ir(111) [2].

[1] S. Heinze et al., Nature Phys. 7, 713 (2011).
[2] N. Romming et al., Science 341, 636 (2013).

MA 45.5 Thu 16:00 BEY 118

Non-collinear spin structure in an Fe monolayer on Ir(001) — •Markus Hoffmann, Bertrand Dupé, Paolo Ferriani, and Stefan Heinze — Institut für Theoretische Physik und Astrophysik, Universität Kiel, 24098 Kiel

Recently, complex magnetic ground states have been reported for a number of transition-metal nanostructures on surfaces [1-4]. The driving force behind these non-collinear spin structures is a competition of exchange, Dzyaloshinskii-Moriya (DM) and higher-order spin interactions. Here, we present a first-principles study of the magnetic properties of an Fe monolayer on Ir(001) based on density-functional theory using the projector augmented wave method as implemented in the VASP code. After mapping our total energy calculations to an extended Heisenberg model we perform Monte-Carlo simulations. We find that a complex non-collinear spin structure can be stabilized by higher-order exchange interactions. Its low total energy is confirmed by subsequent DFT calculations. Finally, we present simulated spin-polarized scanning tunneling microscopy images which allow to verify the proposed spin structure experimentally.

[1] P. Ferriani *et al.*, Physical Review Letters **101**, 027201 (2008).
[2] Y. Yoshida *et al.*, Physical Review B **85**, 155406 (2012).
[3] M. Menzel *et al.*, Physical Review Letters **108**, 197204 (2012).
[4] S. Heinze *et al.*, Nature Physics **7**, 713 (2011).

MA 45.6 Thu 16:15 BEY 118

In situ conversion electron Mössbauer spectroscopy on ultrathin Fe(100)/Ir(100) films — •Sergey Makarov[1,2], Werner Keune[1,2], Heiko Wende[1], and Jürgen Kirschner[2] — [1]Fakultät für Physik und CeNIDE, Universität Duisburg-Essen — [2]Max-Planck-Institut für Mikrostrukturphysik Halle

In the present work we apply ^{57}Fe conversion electron Mössbauer spectroscopy for the study of magnetic order in uncoated three- and four-atomic monolayers (ML) thick epitaxial ^{57}Fe(100) ultrathin films grown in ultrahigh vacuum by molecular - beam epitaxy on the Ir(100) surface with the (5x1)Hex reconstruction. The spectra were taken in situ in UHV in zero external magnetic field at 30 K using a channeltron electron detector.

These spectra of 3 and 4 ML ^{57}Fe on Ir(100)-(5x1)Hex reveal magnetic order even at 30 K. Surprisingly, the measured CEM spectra indicate two inequivalent ^{57}Fe sites. Moreover, for 3 ML ^{57}Fe we obtain the average angle between the hyperfine field direction and γ-radiation, which shows a strong out-of-plane component of Fe spin orientation. In contrast, a preferred in-plane Fe spin alignment for 4 ML ^{57}Fe/Ir(100)-(5x1)Hex was observed.

15 min. break

MA 45.7 Thu 16:45 BEY 118

The influence of oxygen adsorption on the magnetic structure of the iron monolayer on the Ir(001) surface — •Frantisek Maca[1], Josef Kudrnovsky[1], Vaclav Drchal[1], and Josef Redinger[2] — [1]Institute of Physics ASCR, Prague, Czech Republic — [2]Institute of General Physics TU Vienna, Vienna, Austria

We present an ab initio study of the electronic structure and magnetic order of one Fe monolayer on the Ir(001) surface covered by adsorbed oxygen and hydrogen. We show that the adsorption of oxygen (and also of the hydrogen) leads to the p(2x1) antiferromagnetic order. The p(2x1)-ordering is weakened by decreasing oxygen coverage and changes into complex magnetic ground state for the oxygen free case. This result was obtained by two complementary approaches, namely using the total energy evaluations for limited number of magnetic configurations and by a disordered local moment analysis. Based on the calculated magnetic ground states, we also estimate theoretically the spin-polarized scanning tunneling images using a simple Tersoff-Hamann model.

F. Máca, J. Kudrnovský, V. Drchal, and J. Redinger, Phys. Rev. B 88, 045423 (2013).

MA 45.8 Thu 17:00 BEY 118

New mechanism for Skyrmion phase stabilization in multilayers of transition metals — •Ashis Kumar Nandy, Nikolai Kiselev, David Bauer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Previously, Skyrmions have been experimentally found in bulk B20 materials such as MnSi[1], or layers of FeCoSi [2]. Recently, Skyrmions which are observed in an atomic scale multilayer of transition metals as in Pd/Fe/Ir(111)[3] exist at an applied magnetic field of $\sim$ 1 T. The skyrmion size is about $\sim$ 1 - 10 nm. Here we present a multi-scale model based on ab initio calculations and atomistic spin dynamic simulation which predict the existence of a skyrmionic phase in transition metal monolayers e.g. Mn/W(110) or Fe/Ir(111) at high magnetic field. Theoretically predicted Skyrmions have a much higher stability range in an applied magnetic field and much smaller sizes of about 1 nm. We provide a description for the complex phases occurring in such systems and present a magnetic phase diagram for some real compounds. The stability of found solutions are discussed in details.

We propose a new mechanism based on an interplay between internal and surface/interface induced interactions in transition metal multilayers, which can allow one to stabilize a lattice of skyrmions and isolated skyrmions even at zero magnetic field by adjusting only thicknesses and number of layers in multilayers. [1] S. Mühlbauer *et al.*, Science **323**, 915 (2009). [2] X. Z. Yu *et al.*, Nature **465**, 901 (2010). [3] N. Romming *et al.*, Science **341**, 636 (2013).

MA 45.9 Thu 17:15 BEY 118

MnGe grown as a thin film - a new aspirant in skyrmion research — •Josefin Engelke[1], Dirk Menzel[1], and Vadim Dyadkin[2] — [1]IPKM, TU Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany — [2]Swiss-Norwegian Beamlines at the ESRF, Grenoble, 38000, France

Since the discovery of skyrmions in MnSi, there has been a lot of research in the field of the magnetic B20 alloys. Especially the growth of thin films is of great interest, because the skyrmion phase is enlarged compared to bulk material [1,2]. While most of the compounds exhibit a very low ordering temperature, MnGe offers magnetic order at much higher temperatures, which brings it closer to application in future spintronic devices.

We have grown MnGe as a thin film on Si(111) substrates by MBE [3]. The films have been structually characterized by RHEED, AFM and XRD. These techniques give evidence that MnGe forms in the cubic B20 crystal structure as islands exhibiting a very smooth surface. A magnetic characterization reveals that the ordering temperature of MnGe thin films is slightly enhanced compared to bulk material. The properties of the helical magnetic structure obtained from magnetization and magnetoresistivity measurements are compared with films of the related compound MnSi. The much larger Dzyaloshinskii-Moriya interaction in MnGe results in a higher rigidness of the spin helix.

References: [1] J. Engelke et al., J. Phys. Soc. Japn. 81, 124709 (2012). [2] M. N. Wilson et al., Phys. Rev. B 86, 144420 (2012). [3] J. Engelke et al., J. Phys.: Condens. Matter 25, 472201 (2013).

MA 45.10 Thu 17:30 BEY 118

Creation and annihilation of skyrmions in ultrathin magnetic films — •Julian Hagemeister, Robert Wieser, Elena Vedmedenko, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg

Recently, the possibility of a selective manipulation of skyrmion structures has been demonstrated experimentally [1]. While the feasibility of the skyrmion-manipulation has been discussed for several systems [2], the time scale of the switching behavior of skyrmions and the energy barrier of this process is unknown up to now.

Here, we present a theoretical description of the thermal and field dependent stability of skyrmions obtained from classical Monte-Carlo simulations within the Heisenberg model for the example of a Pd monolayer on Fe/Ir(111) [1]. The skyrmions are stabilized by a ferromagnetic exchange coupling, the Dzyaloshinskii-Moriya-interaction and the Zeeman energy. The switching mechanism between the ferromagnetic and the skyrmionic state via an activated transition of the energy barrier between these two phases is studied. The field dependence of the life-times is discussed. Furthermore, the forced creation of a skyrmion within a ferromagnetic phase by a targeted spin manipulation is investigated.

[1] N. Romming, C. Hanneken, M. Menzel, J. E. Bickel, B. Wolter, K. von Bergmann, A. Kubetzka, and Roland Wiesendanger, (2013). Science 341, 636-639. [2] S.-Z. Lin, C. Reichhardt, and A. Saxena, (2013). Appl. Phys. Lett. 102, 222405.

MA 45.11 Thu 17:45 BEY 118

Skyrmion magnetic structure of an ordered FePt monolayer deposited on Pt(111) — •Svitlana Polesya, Sergiy Mankovsky, Sven Bornemann, Jan Minar, and Hubert Ebert — Dept. Chemie/Physikalische Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Deutschland

The effect of the Dzyaloshinsky-Moriya interaction on the magnetic structure of an ordered FePt monolayer deposited on Pt (111) surface has been investigated[1]. All exchange interactions are obtained by means of first-principles calculations, using the spin-polarized relativistic Korringa-Kohn-Rostoker multiple scattering formalism. The interplay of relativistic exchange coupling interactions leads to a helimagnetic (HM) structure at normal conditions for $T = 0$ K. An applied magnetic field, however, creates a so-called Skyrmion structure, which is formed into a Skyrmion lattice at a certain value of the magnetic field. A T-B phase diagram for FePt/Pt(111) has been obtained performing Monte Carlo simulations based on the extended Heisenberg model.

[1] S. Polesya, S. Mankovsky, S. Bornemann, J. Minár, H. Ebert, arXiv:1310.5681

MA 45.12 Thu 18:00 BEY 118

Skyrmion states in triangular-lattice Heisenberg antiferromagnet with frustrated interactions — •Andrey Leonov and Maxim Mostovoy — Zernike Institute for Advanced Materials, University of Groningen, Groningen, 9700AB, The Netherlands

In geometrically frustrated magnets with the triangular lattice, the interplay between nearest- and next-nearest neighbor interactions can stabilize a variety of interesting multi-q phases including the skyrmion crystal state. The spin structure of these skyrmions is somewhat different from that of skyrmions induced in magnets with a non-centrosymmetric lattice by the Dzyaloshinskii-Moriya (DM) interaction, which has lead to difference in static and dynamic properties of these two types of skyrmions. In particular, the DM skyrmions repel each other, whereas the skyrmions on the triangular lattice show the long-ranged attraction that leads to the formation of metastable skyrmion clusters and may stabilize the skyrmion liquid state. In addition, the skyrmions in frustrated systems have more low-energy degrees of freedom and can carry the topological charge and chirality of either sign for a fixed external magnetic field. We applied Monte Carlo simulations to study the rich magnetic field phase diagram of a frustrated triangular antiferromagnet with a uniaxial anisotropy. Using the Landau-Lifshitz-Gilbert equation, we also studied dynamical properties of isolated skyrmions, skyrmion pairs and skyrmion crystals, such as the excitation of collective modes of these systems with time-dependent external magnetic fields and currents.

MA 45.13 Thu 18:15 BEY 118

The role of cubic and exchange anisotropies in the thermodynamical stability of skyrmions and half-skyrmions in cubic helimagnets — •Andrey Leonov[1] and Ulrich K. Rössler[2] — [1]Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — [2]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

In non-centrosymmetric chiral magnets, *isotropic* Dzyaloshinskii-Moriya interactions induce long-range 1-dimensional (cones and helicoids) and 2-dimensional ($\pm\pi$-skyrmions and $\pi/2$-skyrmions) homochiral modulations of the magnetization [1]. In this contribution we investigate the role of small anisotropic forces as cubic anisotropy and anisotropic exchange in suppression of the conical phase and the thermodynamical stability of skyrmions [2]. We also consider reorientational effect of cubic anisotropy on the propagation direction of helicoids and axes of skyrmions along certain crystal directions. The constructed T-H phase diagrams hold existence regions for different modulated and homogeneous phases separated by first- and second-order transition lines. The results demonstrate that a plethora of different precursor phenomena, modulated mesophases, and reorientation transitions may arise in cubic helimagnets near magnetic ordering depending on very weak magnetic couplings. [1] U. K. Rößler et al., J. of Phys.: Conf. Ser. 303, 012105 (2011); [2] A. Leonov, Ph.D thesis, Dresden University of Technology, Dresden (2012).