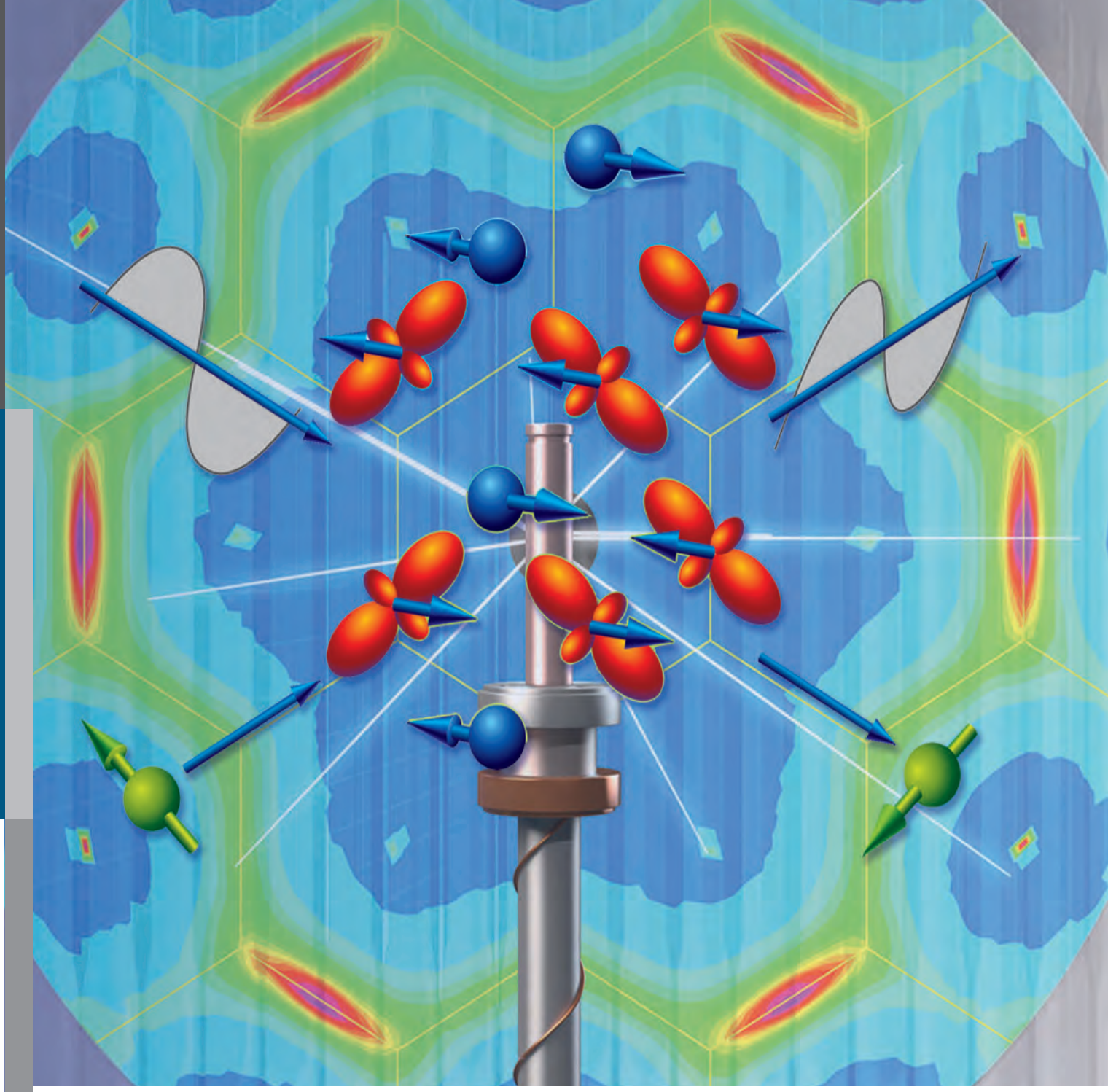


Member of the Helmholtz Association

JCNS Workshop 2013

Trends and Perspectives in Neutron Scattering: Magnetism and Correlated Electron Systems

Program and Abstracts

7 – 10 Oct. 2013, Tutzing **www.fz-juelich.de/jcns/JCNS-Workshop2013**

Jülich Centre for Neutron Science

Heinz Maier-Leibnitz Zentrum

JÜLICH FORSCHUNGSZENTRUM

Dear colleagues,

Neutron scattering has proven to be a key method for achieving deep insight into the physics associated with magnetic phenomena and correlated electrons. Our basic understanding of crucially important topics such as the magnetic structure of complex materials in bulk, thin films or nanoparticles, the mechanism behind magnetic phenomena and superconductivity, spin dynamics in highly correlated electron systems etc. depend on and benefit immensely from research with neutrons.

The workshop will bring experts together to address the following topics:

- **Magnetic Nanoparticles and Nanocrystals**
- **Molecular Magnets**
- **Highly Correlated Transition Metal Chalcogenides**
- **Unconventional Superconductors**
- **Magnetoelectrics, Multiferroics**
- **Frustrated and Complex Spin Systems**
- **Interface Effects in Heterostructures**
- **Materials for Energy Conversion and Storage**

During the next days about 40 invited and contributed presentations will be given and exciting posters will add additional information in the mentioned topics. We would like to believe that this workshop at a gorgeous site at the Starnberger See will advance the field and we are looking forward to fruitful discussions and to a stimulating exchange of knowledge.

Scientific Organizing Committee

Thomas Brückel Yixi Su

Presentation Schedule

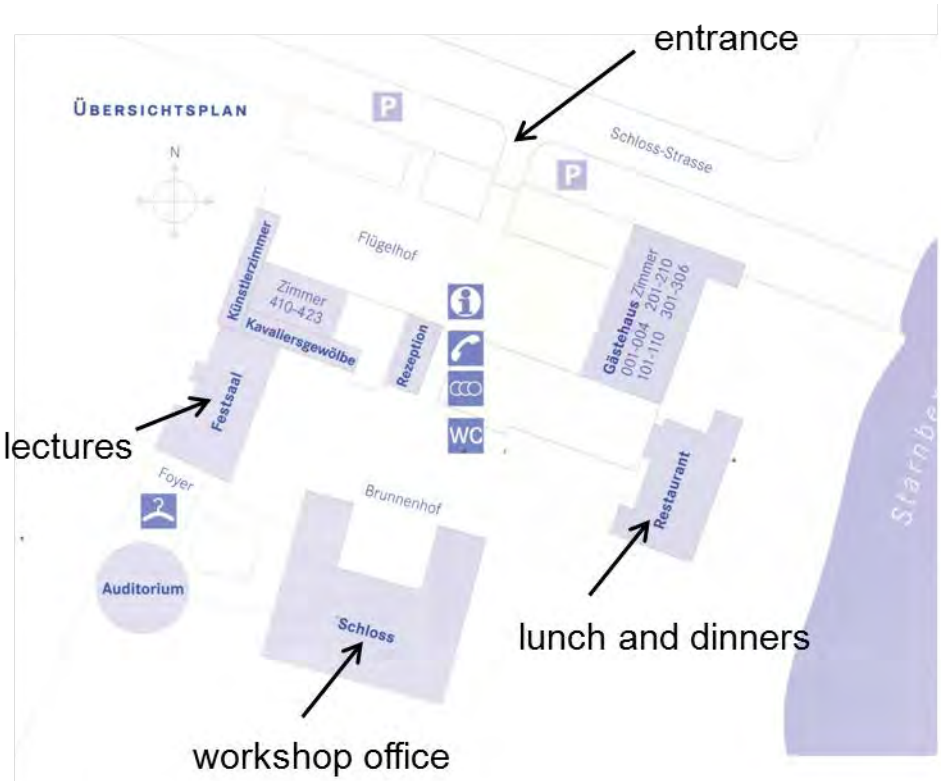
Program JCNS Workshop 2013 "Trends and Perspectives in Neutron Scattering: Magnetism and Correlated Electron Systems"

Monday, 7 October 2013		Tuesday, 8 October 2013		Wednesday, 9 October 2013		Thursday, 10 October 2013	
10:00	Registration	09:00	Gaulin	09:00	Bibes	09:00	Wiedenmann
		09:30	Bech Christensen	09:30	Fontcuberta	09:30	Michels
		09:50	Chakrabarty	10:00	Bernhard	10:00	Disch
		10:10	Häußler	10:30	Pavlenko	10:30	Petracic
		10:30	Coffee break	10:50	Coffee break	10:50	Coffee break
		11:00	Cermak	11:30	Brück	11:20	Kenzelmann
		11:20	Nemkovskiy	12:00	Hermann	11:50	Angst
		11:40	Sazonov	12:30	Voigt	12:20	Closing remarks
12:15	Lunch	12:00	Fu	12:50	Clementyev	12:30	Lunch
		12:20	Ioffe	13:10	Lunch		
13:15	Workshop Opening	13:00	Lunch				
13:30	Triscone	14:00	Gegenwart	14:30	Excursion		
14:00	Tonnerre	14:30	Inosov				
14:30	Röhlsberger	15:00	Demirdis		Bus tour to the Murnau Museum		
15:00	Lauter	15:20	Xiao				
15:30	Coffee break	15:40	Nandi				
16:00	Chapon	16:00	Coffee break				
16:30	Petricek	16:30	Schmalian	18:00	Workshop Dinner "Griesbräu" in Murnau		
17:00	Frontzek	17:00	Su				
17:20	Brandl	17:30	Hiess				
17:40	Nair	18:00	Poster Session				
18:30	Dinner	19:30	Dinner				

as of 2013-08-29

Evangelische Akademie Tutzing

Site Map



JCNS Workshop 2013

"Trends and Perspectives in Neutron Scattering: Magnetism and Correlated Electron Systems"

October 7-10, 2013, Tutzing

Program

Monday, October 7, 2013

13:15 Opening of the workshop and welcome

Interface Effects in Heterostructures

1 13:30 J.-M. Triscone, DPMC, University of Geneva, France (invited)
2-dimensional electron gases in oxide heterostructures

2 14:00 Jean-Marc Tonnerre, Institut Néel, CNRS and Université Joseph Fourier Grenoble, France (invited)
Depth-resolved magnetic profile in Fe ultrathin films on vicinal Ag substrate close to spin reorientation transition

3 14:30 Ralf Röhlsberger (invited)
Photon polarization precession spectroscopy: A new technique for the study of magnetic dynamics with x-rays

4 15:00 Valeria Lauter, Oak Ridge National Laboratory, USA (invited)
Interfacially-coupled epitaxial ferromagnetic oxide heterostructures studied by polarized neutron reflectometry

15:30 Coffee Break

Frustrated and Complex Spin Systems

5 16:00 Laurent Chapon, Institut Laue Langevin, Grenoble, France (invited)
tbd

6 16:30 Václav Petříček, Institute of Physics ASCR v.v.i., Prague, Czech Republic (invited)
How can we study magnetic structures with Jana2006?

7 17:00 Matthias Frontzek, Paul Scherrer Institut, Villigen, Switzerland
The multiferroic, geometric frustrated $CuCrO_2$ compound: interlayer exchange and domain formation

8 17:20 Georg Brandl, Heinz Maier-Leibnitz Zentrum (MLZ) and Physik-department E21, Technische Universität München, Garching, Germany
Investigation of helimagnon excitations in single-domain MnSi with the new triple-axis option on the spectrometer MIRA at the FRM II

9 17:40 Harikrishnan Nair, JCNS 2/PGI 4, Scattering Methods, Forschungszentrum Jülich, Jülich, Germany
The true magnetic ground state of frustrated A-site spinels: An approach using polarized neutrons

18:30 Dinner

Tuesday, October 8, 2013

Frustrated and Complex Spin Systems

10 9:00 Bruce D. Gaulin, McMaster University, Hamilton, Canada (invited)
Effective spin ½ Hamiltonians in XY pyrochlores and ground state selection via order-by-disorder in $Er_2Ti_2O_7$

11 9:30 Nils Bech Christensen, Technical University Denmark, Denmark
The case for magnon decay in the organic square lattice, spin ½ Heisenberg antiferromagnet $(5CAP)_2CuCl_4$

12 9:50 T. Chakarabarty, IIT Bombay, Powai Mumbay, India
BaV_3O_8: A possible Majumdar-Ghosh system with s=1/2

13 10:10 Wolfgang Häußler, Heinz Maier-Leibnitz Zentrum (MLZ) and Physik-department E21, Technische Universität München, Garching, Germany
Relaxation in the re-entrant spin glass $Fe_{14.5}Cr_{85.5}$

10:30 Coffee Break

Frustrated and Complex Spin Systems (continued)

14 11:00 Petr Čermák, Forschungszentrum Jülich, JCNS, Outstation at MLZ, Garching, Germany
Recent development in "218" Rh, Pd and Pt based heavy fermion compounds

15 11:20 Kirill Nemkovski, Forschungszentrum Jülich, JCNS at MLZ, Garching, Germany
Interplay of low-energy phonons and magnetic excitations in Kondo insulator YbB_{12}: complementary neutron/synchrotron study

16 11:40 Andrew P. Szonov, RWTH Aachen, JCNS Outstation at MLZ, Garching, Germany
Low-temperature magnetic structure of the pyrochlore spin liquid $Tb_2Ti_2O_7$ under magnetic field H || [111]

17 12:00 Zhendong Fu, Forschungszentrum Jülich, JCNS at MLZ, Garching, Germany
Coexistence of novel magnetic orders and spin-glass-like phase in pyrochlore antiferromagnet $Na_3Co(CO_3)_2Cl$

18 12:20 Alexander Ioffe, Forschungszentrum Jülich, JCNS at MLZ, Garching, Germany
The JCNS instrument suite – an excellent set to investigate magnetic phenomena

13:10 Lunch

Unconventional Superconductors

19 14:00 Philipp Gegenwart, Georg-August-Universität Göttingen, Germany (invited)
Eu-based iron pnictide superconductors

20 14:30 Dmytro Inosov, Max-Planck-Institut für Festkörperforschung, Stuttgart, and Technische Universität Dresden, Dresden, Germany (invited)
Peculiar magnetism of iron pnictides aside from superconductivity

21 15:00 Sultan Demirdis, Forschungszentrum Jülich, JCNS at MLZ, Garching, Germany
Electron irradiation of iron-based superconductors

22 15:20 Y. Xiao, Jülich Centre for Neutron Science and Peter Grünberg Institut, JARA-FIT, Forschungszentrum Jülich, Jülich, Germany
Magnetic anisotropic energy gap and low-energy spin wave excitation in the antiferromagnetic block phase of $K_2Fe_4Se_5$

23 15:40 S. Nandi, Jülich Centre for Neutron Science and Peter Grünberg Institut, JARA-FIT, Forschungszentrum Jülich, Jülich, Germany
Understanding the magnetism in $K_{0.8}Fe_{1.6}Se_2$

16:00 Coffee Break

24 16:30 Jörg Schmalian, Karlsruhe Institute of Technology, Germany (invited)
Nematic fluctuations and unconventional magneto-elastic coupling in iron based superconductors

25 17:00 Yixi Su, Forschungszentrum Jülich, JCNS at MLZ, Garching, Germany
Magnetic anisotropy of low-energy spin excitations in iron pnictide superconductors

26 17:30 Arno Hiess, European Spallation Source, Lund, Sweden
Temperature and doping dependence of the spin dynamics in the cubic superconductor $U_{(1-x)}Th_xBe_{13}$

18:00 **Postersession**

19:30 Dinner

Wednesday, October 9, 2013

Interface Effects in Heterostructures

27 9:00 Manuel Bibes, Unité Mixte de Physique CNRS/Thales, Palaiseau, France, (invited)
Putting a strain on $BiFeO_3$

28 9:30 Josep Fontcuberta, Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Bellaterra, Catalonia, Spain (invited)
Engineering electronic occupancy at surfaces and interfaces of transition metal oxides

29 10:00 Christian Bernhard, University of Fribourg, Switzerland (invited)
The magnetic proximity effect in cuprate-high T_c/manganite multilayers studied by polarized neutron reflectometry and resonant x-ray techniques

30 10:30 Natalia Pavlenko, University of Augsburg, and Max-Planck-Institute of Solid State Physics, Stuttgart, Germany
Nanoscale magnetism and electronic phase separation at titanate interfaces

10:50 Coffee Break

Materials for Energy Conversion and Storage

31 11:30 Ekkes Brück, Delft University of Technology, The Netherlands (invited)
Magnetocaloric materials for cooling applications near room temperature

32 12:00 Raphael P. Hermann, Jülich Centre for Neutron Science and Peter Grünberg Institut, JARA-FIT, Forschungszentrum Jülich, Jülich, Germany (invited)
Lattice dynamics in thermoelectric skutterudites

33 12:30 Jörg Voigt, Jülich Centre for Neutron Science and Peter Grünberg Institut, JARA-FIT, Forschungszentrum Jülich, Jülich, Germany
Anisotropy of the magneto-caloric effect in single crystalline $MnFe_4Si_3$

34 12:50 Evgeny Clementyev, Institute for Nuclear Research RAS, Moscow, Russia
Volume collapse and valence instabilities in CeNi

13:10 Lunch

14:30 Excursion to the Schloss-Museum Murnau

18:00 Workshop dinner in the "Griesbräu" in Murnau

Thursday, October 10, 2013

Magnetic Nanoparticles and Nanocrystals

35 9:00 Albrecht Wiedenmann, Institut Laue Langevin, Grenoble, France (invited)
Magnetic nanomaterials studied by innovative small angle neutron scattering techniques

36 9:30 Andreas Michels, University of Luxembourg, Luxembourg (invited)
Magnetic SANS on nanomagnets

37 10:00 Sabrina Disch, Institut Laue Langevin, Grenoble, France (invited)
Polarized (GI)SANS by iron oxide nanocubes and their assemblies

38 10:30 Oleg Petracic, Jülich Centre for Neutron Science and Peter Grünberg Institut, JARA-FIT, Forschungszentrum Jülich, Jülich, Germany
Structural and magnetic correlations of self-assembled nanoparticle superlattices

10:50 Coffee Break

Magnetoelectrics and Multiferroics

39 11:20 Michel Kenzelmann, Paul Scherrer Institut, Villigen, Switzerland (invited)
tbd

40 11:50 Manuel Angst, Jülich Centre for Neutron Science and Peter Grünberg Institut, JARA-FIT, Forschungszentrum Jülich, Jülich, Germany
Neutron scattering on Rare Earth Ferrites

12:20 **Closing remarks, end of the workshop**

12:30 Lunch

Poster Presentations

2013-1
Alice Klapper, JCNS-2/PGI-4, Forschungszentrum Jülich, Jülich, Germany
Structural and magnetic properties of FePt@MnO heterodimer nanoparticles and their self-assembly

2013-2
Nicolò Violini, Jülich Centre for Neutron Science, Forschungszentrum Jülich, Jülich, Germany
T-REX: A Time-of-flight Reciprocal space Explorer for the future ESS source

2013-3
Artem Feoktystov, Jülich Centre for Neutron Science at MLZ, Forschungszentrum Jülich, Garching, Germany
Detailed SANS contrast variation in toluene-based Co ferrofluid

2013-4
Pavlo Portnichenko, Institut für Festkörperphysik, TU Dresden, Dresden, Germany
Disperse magnon excitations in $Ca_3Co_2O_6$

2013-5
Robert J. Aldus, Jülich Centre for Neutron Science at MLZ, Forschungszentrum Jülich, Garching, Germany
The magnetic properties of $Nd_2Sn_2O_7$, a candidate of quantum spin liquid, at temperatures as low as 2 K

2013-6
Milan Klicpera, Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic
Structural and electronic properties of $CeCuAl_3$ single crystal and vibron states in $Ce(Cu,Al)_4$ compounds

2013-7
Vinod Kumar, Department of Physics, National Institute of Technology, Hamirpur (H.P.), India
Magnetic properties of $LaCo_{1-x}Ni_xO_3$ (x=0, 0.1, 0.2, 0.4)

2013-8
Johannes Reim, Jülich Centre for Neutron Science JCNS-2 and Peter Grünberg Institut PGI-4, Forschungszentrum Jülich, Jülich, Germany
Long range incommensurable spin ordering in a swedenborgite compound

2013-9
Kirill Nemkovski, Forschungszentrum Jülich, JCNS at MLZ, Garching, Germany
DNS – a versatile diffuse neutron scattering spectrometer with polarization analysis at FRM II: towards enhanced count rate and extended Q-range

2013-10
Wentao Jin, Jülich Centre for Neutron Science JCNS-2 and Peter Grünberg Institut PGI-4, JARA-FIT, Forschungszentrum Jülich, Jülich, Germany
Field-induced spin reorientation in $EuFe_2(As_{0.85}P_{0.15})_2$ revealed by resonant magnetic x-ray scattering

2013-11
Martin Meven, Institut für Kristallographie, RWTH Aachen and JCNS at MLZ, Forschungszentrum Jülich, Garching, Germany
Single crystal diffraction studies on new magnetic and superconducting compounds with HEiDi

2013-12
Koji Kaneko, Quantum Beam Science Directorate, Japan Atomic Energy Agency, Ibaraki, Japan
Presence of chiral character in the spin resonance of the unconventional superconductor $CeCoIn_5$

2013-13
Dmitry Trunov, NRC "Kurchatov Institute", Department of condensed matter physics, Moscow, Russia
Magnetic excitation in intermediate-valence $EuCu_2Si_2$

2013-14
Karin Schmalzl, Jülich Centre for Neutron Science, Forschungszentrum Jülich, Outstation at ILL, Grenoble, France
Effects of magnetic order and lattice dynamics in $CuCrS_2$

2013-15
Vladimir Hutanu, Institut für Kristallographie, RWTH Aachen and JCNS at MLZ, Forschungszentrum Jülich, Garching, Germany
Detailed investigation of magnetic structure in peculiar multiferroic $Ba_2CoGe_2O_7$

2013-16
Sabine Pütter, Forschungszentrum Jülich, JCNS at MLZ, Garching, Germany
Fabrication of transition metal oxide thin films by molecular beam epitaxy: New offer for users of the Heinz Maier-Leibnitz Zentrum at the FRM II

2013-17
Markus Waschk, Jülich Centre for Neutron Science JCNS-2 and Peter Grünberg Institut PGI-4, JARA-FIT, Forschungszentrum Jülich, Jülich, Germany
Interface induced magnetism in $[LaMnO_3/SrMnO_3]_N$ heterostructures

2013-18
Markus Schmitz, Jülich Centre for Neutron Science JCNS-2 and Peter Grünberg Institut PGI-4, JARA-FIT, Forschungszentrum Jülich, Jülich, Germany
Electrically induced magnetic transition at the LSMO/BTO interface

JCNS Workshop 2013

Trends and Perspectives in Neutron Scattering:

Magnetism and Correlated Electron Systems

Abstracts

Status: 09-09-2013

2-dimensional electron gases in oxide heterostructures

A. FÊTE, D. LI, D. STORNAIOULO, S. GARIGLIO, M. GABAY*, and **J.-M. TRISCONE**

DPMC, University of Geneva, 24 quai E.-Ansermet, 1211 Geneva 4, Switzerland
*Laboratoire de Physique des Solides, Université de Paris Sud, 91405 Orsay, Cedex, France

Oxide materials display within the same family of compounds a variety of exciting electronic properties ranging from ferroelectricity to ferromagnetism and superconductivity. These systems are often characterized by strong electronic correlations, complex phase diagrams and competing ground states. This competition makes these materials very sensitive to external parameters such as pressure or magnetic field. An interface, which naturally breaks inversion symmetry, is a major perturbation and one may thus expect that electronic systems with unusual properties can be generated at oxide interfaces. A striking example is the interface between $LaAlO_3$ and $SrTiO_3$, two good band *insulators*, which was found in 2004 to be conducting [1], and, in some doping range, superconducting with a maximum critical temperature of about 200 mK [2]. The characteristics observed in the normal and superconducting states are consistent with a two-dimensional electronic system.
In this presentation, I will briefly motivate the search for novel properties at oxide interfaces before to focus on the 2-dimensional electron gas observed in at the $LaAlO_3/SrTiO_3$ interface. The thickness of the electron gas is found to be a few nanometers at low temperatures. This electron gas with low electronic density, typically 5 10^{13} electrons/cm^2, and naturally sandwiched between two insulators is ideal for performing electric field effect experiments allowing the carrier density to be tuned. I will discuss the origin of the electron gas [3]; field effect experiments and the phase diagram of the system [4]; superconductivity and the role of spin orbit [5,6]; and if time allows the physics of high mobility samples that display Shubnikov de Haas oscillations [7].

[1] A. Ohtomo, H. Y. Hwang, Nature **427**, 423 (2004).
[2] N. Reyren, S. Thiel, A. D. Caviglia, L. Fitting Kourkoutis, G. Hammerl, C. Richter, C. W. Schneider, T. Kopp, A.-S. Ruetschi, D. Jaccard, M. Gabay, D. A. Muller, J.-M. Triscone and J. Mannhart, Science **317**, 1196 (2007).
[3] M.L. Reinle-Schmitt, C. Cancellieri, D. Li, D. Fontaine, S. Gariglio, M. Medarde, E. Pomjakushina, C.W. Schneider, Ph. Ghosez, J.-M. Triscone, and P.R. Willmott, Nature Communications, **3**, 932 (2012).
[4] A. Caviglia, S. Gariglio, N. Reyren, D. Jaccard, T. Schneider, M. Gabay, S. Thiel, G. Hammerl, J. Mannhart, and J.-M. Triscone, Nature **456**, 624 (2008).
[5] A.D. Caviglia, M. Gabay, S. Gariglio, N. Reyren, C. Cancellieri, and J.-M. Triscone, Physical Review **104**, 126803 (2010).
[6] A. Fête, S. Gariglio, A. D. Caviglia, M. Gabay, J.-M. Triscone, Physical Review B (RC) **86**, 201105 (2012).
[7] A.D. Caviglia, S. Gariglio, C. Cancellieri, B. Sacépé, A.Fête, N. Reyren, M. Gabay, A.F. Morpurgo, J.-M. Triscone, Physical Review Letters **105**, 236802 (2010).

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Depth-resolved magnetic profile in Fe ultrathin films on vicinal Ag substrate close to spin reorientation transition

Emmanuelle JAL[1], Maciej DABROWSKI[2], **Jean-Marc TONNERRE**[1], Marek PRZYBYLSKI[2,3], Nicolas JAOUEN[4], Stéphane GRENIER[1], Jürgen KIRSCHNER[2,5]

[1]Institut Néel, CNRS and Université Joseph Fourier, Grenoble, France
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[3]Academic Centre of Materials and Nanotechnology and Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland
[4]Synchrotron SOLEIL, Saint-Aubin, Gif-sur-Yvette, France
[5]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

In this presentation, we discuss the sensitivity of soft x-ray resonant magnetic reflectivity to probe the depth dependence of the amplitude and orientation of the magnetization in ultrathin films [1]. The interface effects and their extension across Fe layers deposited on a Ag(116) vicinal surface and coated with Au are investigated. Below 5 monolayers (ML) the anisotropy is out-of-plane. Above 5ML, a spin reorientation transition takes place and, at low temperature, the system exhibits an oscillation of the in-plane magnetic anisotropy from along to perpendicular to the steps, originating from quantum well states in Fe Films [2]. Moreover, a competition between magnetocrystalline anisotropy and magnetic shape anisotropy tilts the magnetization from the surface plane toward the terrace plane when the magnetization is oriented perpendicular to the step edges [3]. We will focus on the distribution of the out-of-plane magnetic component. The measurements were carried out at SEXTANTS beam line at synchrotron SOLEIL in the vicinity of the L_3 Fe edge at 20K under an in-plane applied magnetic field and in remanence. The rotation of the magnetization can be directly observed through the change of the angular dependence of the asymmetry $(I^+-I^-)/(I^++I^-)$ where I^+ and I^- are the reflectivity curves collected for opposite circular polarization states. The signal at low angles is related to the longitudinal in-plane component (perpendicular to the steps) and, at large angles, to the out-of-plane one. The analysis of various configurations of acquisition allows us to probe the detail of the magnetization throughout layers of different thickness (wedge sample). While, for thicknesses below 5ML, the data can be fitted with a homogeneous magnetization in amplitude and orientation, above, it is required to consider an inhomogeneous distribution across the layer for the magnetization amplitude [4] as well as for the orientation of the magnetization yielding a non-collinear structure.

[1] J.-M. Tonnerre, M. Przybylski, M. Ragheb, F. Yildiz, H. C. N. Tolentino, L. Ortega, and J. Kirschner, Phys. Rev. B **84**, 100407(R) (2011).
[2] J. Li, M. Przybylski, F. Yildiz, X. D. Ma, and Y. Z. Wu, Phys. Rev. Lett. **102**, 207206 (2009).
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[4] E. Jal, M. Dabrowski, J.-M. Tonnerre, M. Przybylski, S. Grenier, N. Jaouen, and J. Kirschner, Phys. Rev. B **87**, 224418 (2013).

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October 7, 2013, 14:30h Interface Effects in Heterostructures

Photon polarization precession spectroscopy: A new technique for the study of magnetic dynamics with x-rays

Ralf RÖHLSBERGER

Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Inelastic scattering reveals the dynamical properties of condensed matter by analysing the energy difference between incoming and outgoing particles like neutrons and photons. Typically, the energy resolution is determined (and limited) by the energy spread of the incoming particles, thus further bandwidth reduction to achieve the ultimate energy resolution goes at the expense of the signal to noise ratio. A very elegant decoupling of the energy resolution from the band width of the probing particles has been achieved in the method of neutron spin echo (NSE) spectroscopy. Effectively being a time of flight method, the NSE technique relies on the finite rest mass of the neutron. For that reason this technique does not seem to be transferable to photons, although it would be highly desirable. Here I introduce the concept of a new resonant x-ray scattering method that should allow to probe magnetic excitations (i.e. spinwaves) in condensed matter. Similar to NSE, its energy resolution is decoupled from and thus independent of the energy bandwidth of the incident radiation. It relies on encoding the energy transfer in the inelastic scattering process in the photon polarization rather than the photon energy.

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Interfacially-coupled epitaxial ferromagnetic oxide heterostructures studied by polarized neutron reflectometry

Valeria LAUTER

Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, USA

Oxide heterostructures show novel properties arising from reconstruction at the interface. In this paper I will present recent results obtained on the Magnetism Reflectometer at SNS in collaboration with several groups.

Although the antiferromagnetic interfacial coupling has been established in the $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) / $SrRuO_3$ (SRO) bilayers [1] and superlattices [2], the key issues regarding the spin structure of SRO biasing layer formed during the cooling process and its crucial effect on the biased LSMO magnetization reversal have remained unclear. Here we report the spin structure of an exchange-biased ferromagnetic oxide heterostructure, $La_{0.67}Sr_{0.33}MnO_3$ / $SrRuO_3$, through magnetization and polarized neutron reflectometry measurements. We reveal that the magnetization reversal process of the $La_{0.67}Sr_{0.33}MnO_3$ biased layer critically depends on the frozen-in spin structure of the $SrRuO_3$ biasing layer during the cooling process. Furthermore, we observe unexpected double-shifted hysteresis loops of the biased layer that originate from the formation of lateral 180^o magnetic domains within the biasing layer, a new mechanism not found in conventional exchange-bias systems [3]. This study sets an example of intriguing interfacial phenomena and illustrates the importance of interfacial coupling in complex oxide heterostructures.

The unique properties of perovskite TMOs are often controlled by the minute deviations of structure from ideal, including octahedral tilts that couple to the exchange integrals and band width, and collective Jahn-Teller deformations of octahedral networks. We investigated lanthanum strontium cobaltite thin films epitaxially grown on substrates of different symmetry. The $La_{1-x}Sr_xCoO_3$ materials show a rich phase diagram ranging from a spin glass with $x<0.18$ to strong ferromagnetic behavior at $x>0.3$ where polarized neutron reflectometry revealed a strong difference in magnetic properties in identical LSCO films grown on different $La_{0.30}Sr_{0.70}Al_{0.65}Ta_{0.35}O_3$ (LSAT) and $NdGaO_3$ substrates [4, 5].

Research at Oak Ridge National Laboratory's Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

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[3] X. Ke, L. J. Belenky, V. Lauter et al., PRL **110**, 237201 (2013).
[4] Y.-M. Kim, J. He, M. D. Biegalski, H. Ambaye, V. Lauter et al., Nature Materials, **11**, 888-894 (2012).
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How can we study magnetic structures with Jana2006?

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Recently it has been shown that a direct use of Shubnikov (magnetic) space and superspace groups facilitates work with non-modulated as well as with modulated magnetic structures and simplifies algorithms for handling their diffraction data [1]. The basic idea lies in the application of the magnetic and nuclear symmetry not only during data processing (merging symmetry related reflections for single crystal data or reducing generated reflections to independent ones for powder) but also in calculation of magnetic structure factors. For incommensurately modulated magnetic structures this approach may be especially beneficial [2], for instance in analyzing multiferroic phases.
In the lecture we shall explain implementation of the new concept in the program Jana2006[3] and we shall demonstrate how different magnetic models can be derived from the representation analysis of the paramagnetic phase [4]. For analysis of magnetic symmetry Jana2006 offers an interactive list of Shubnikov space or superspace groups as follows from the individual irreps. The corresponding magnetic structure model can be visualized in the VESTA program [5]. For similar but more detailed analysis Jana2006 can also connect to the recently developed program ISODISTORT [6] and use its results.
Utilization of the magnetic and nuclear symmetry leads to better stability of the refinement. Jana2006 offers simultaneous refinement against different diffraction experiments including commensurate and incommensurate phases and allows for combination of powder and single crystal data. This opens manifold possibilities for refinement of modulated magnetic structures from various experiments and also possibility to calculate nuclear and magnetic structures together. Another advantage of the new approach consists in a logical way how to twin domains can be described.

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The multiferroic, geometric frustrated $CuCrO_2$ compound: interlayer exchange and domain formation

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Multiferroic materials have become of interest for their unusual low-temperature properties in general and in particular for the observation that their magnetic structure can be modified through an electric field and their electric polarization can be adjusted through a magnetic field. The most promising candidates for a controllable multiferroic have been found among the materials with inherent geometric magnetic frustration.

Among these, the delafossite $CuCrO_2$, which crystallizes in the rhombohedral *R*-3*m* space group, is a multiferroic compound with an apparent strong coupling of spin and charge. In contrast to other multiferroic compounds $CuCrO_2$ shows a spontaneous electric polarization upon antiferromagnetic ordering without an accompanying structural phase transition. The spin-charge coupling in the delafossites has been discussed within the frame of the *p-d* hybridization model, first introduced by Taka-hisa Arima [1]. However, so far only the multiferroic delafossites are known examples for this spin-charge coupling mechanism and its properties are therefore still to be fully characterized.

In my contribution, I'll present a detailed study on $CuCrO_2$ single crystals using neutron diffraction [2] and spectroscopy [3] as well as electric polarization measurements up to 60 T in pulsed magnetic fields. Based on our studies, I will show a revised magnetic structure model and present a model Hamiltonian including in-plane next-next nearest neighbor and inter-layer exchange interaction. I will stress the importance of the latter for the multiferroic properties and briefly discuss it alone breaks inversion symmetry. Furthermore, neutron diffraction in applied electric fields helped us to clarify the domain distribution in the field cooled state which necessitates a re-interpretation of macroscopic measurements.

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Investigation of helimagnon excitations in single-domain MnSi with the new triple-axis option on the spectrometer MIRA at the FRM-II

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The weak chiral helimagnet MnSi has attracted considerable interest due to its unusually rich magnetic phase diagram. In zero field below $T_c \approx 28.5$ K, a helical state is found composed of four magnetic domains oriented along the cubic <111> directions with a propagation vector $|k| = 0.035$ Å^{-1}. A comprehensive theory of the collective magnetic excitations of the helimagnetic state, predicting so-called helimagnons has been developed by Belitz et al. [1]. The results were confirmed by Janoschek et al. [2]. Based on the fundamental magnon of the underlying ferromagnet, which can be induced by applying a field $B > 0.6$ T, it features multiple strongly-coupled helimagnon bands that emerge as a universal characteristic of systems with chiral interactions.

In practice, the presence of many helimagnon bands – due to the large number of Brillouin zones involved – makes it difficult to resolve individual helimagnons [1], although the data was found to be in excellent agreement with the theory. To extract directly the dispersion of the various dispersion branches, we have induced a single-domain **k**-state in MnSi using a weak magnetic field, thus decreasing the number of observable helimagons and increasing the intensity of the measurable helimagnons by a factor of four. Helimagnons were measured along several **q** directions, using the new triple-axis option of the spectrometer MIRA at the FRM-II. In this contribution, we will give a short overview of the features of the triple-axis option, and present the first measurements of helimagnons in single-domain MnSi.

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The true magnetic ground state of frustrated A-site spinels: An approach using polarized neutrons

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The *diamond-lattice antiferromagnet A*-site spinels MAl_2O_4 (*M* =Mn, Fe, Co) with competing nearest- and next-nearest-neighbour interactions (J_1 and J_2, respectively) can realize *"spiral spin liquid"* state through proper tuning of J_2/J_1 [1]. $CoAl_2O_4$ have been studied previously with focus on spin liquid state but the short-range order and the spin dynamics have been interpreted in terms of spin glass state [2], kinetically arrested domains [3] or spin liquid state [4]. We investigate the physics of *A*-site spinels by studying *M* = Mn, Fe on the left of Co in periodic table and *M* = Ni on the right. Combining magnetometry and polarized neutron scattering we provide a better approach to the true magnetic ground state of these frustrated magnets. Our studies at the polarized diffuse scattering spectrometer, DNS, FRM II show that short-range spin correlations coexist with long-range antiferromagnetism ($T_N \sim 42$ K) in $MnAl_2O_4$ while in $FeAl_2O_4$, only short-range spin correlations exist till 4 K. Extending our studies to $NiAl_2O_4$ single crystal, we find evidence for the "*spiral spin liquid*" state through magnetic diffuse neutron scattering cross-sections in the (*hhl*) planes which match very well with reverse Monte Carlo simulations as well as to the predictions by a J_1-J_2 meanfield model. Inelastic neutron scattering experiments at IN12, ILL show signatures of emergent excitations out of the "*spiral spin liquid*" state. Our results on $S = 1$ $NiAl_2O_4$ points towards exciting scenarios in frustrated magnetism especially since the importance of quantum fluctuations in these systems is suggested [5].

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Effective spin ½ Hamiltonians in XY pyrochlores and ground state selection via order-by-disorder in $Er_2Ti_2O_7$

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Inelastic neutron scattering measurements have allowed a detailed and robust understanding of the microscopic spin Hamiltonian in the XY pyrochlore magnets $Yb_2Ti_2O_7$ [1] and $Er_2Ti_2O_7$ [2]. These materials display net ferromagnetic and antiferromagnetic Curie-Weiss constants, respectively. Both also possess ground state crystal field doublets which are well separated from their corresponding excited states, leading to an effective spin ½ description for the corresponding Yb^{3+} and Er^{3+} moments.

Our measurements on $Er_2Ti_2O_7$, in particular, solve a long-standing problem as to why the particular ground state spin structure of this material is realized through a continuous phase transition [2,3]. The characteristics of this ground state selection, through the Order-by-Quantum Disorder (ObQD) mechanism will be discussed, along with discussion of the ObQD spin wave gap which is a necessary consequence.

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The case for magnon decay in the organic square lattice, spin ½ Heisenberg antiferromagnet $(5CAP)_2CuCl_4$

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I will discuss the case for spontaneous magnon decay in square lattice Heisenberg antiferromagnets for magnetic fields near the saturation field. Initially predicted by Zhitomirsky and Chernyshev [1], experimental evidence for magnon decay in the classical spin 5/2 system $Ba_2MnGe_2O_7$ was subsequently reported by Masuda and collaborators [2]. Our efforts have gone towards establishing its occurrence in the experimentally more cumbersome quantum limit, s=1/2, in the quasi two-dimensional organic $(5CAP)_2CuCl_4$ [3,4]. With exchange interactions of order 0.1 meV, the saturation field in $(5CAP)_2CuCl_4$ is easily accessible. The experimental part of the presentation will feature a combination of time-of-flight and triple axis neutron scattering experiments, and will highlight the difficulties encountered in trying to establish magnon decay in weakly scattering, low-exchange systems.

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BaV_3O_8: A possible Majumdar-Ghosh system with s=1/2

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BaV_3O_8 contains both magnetic V^{4+}(s=1/2) ions and non-magnetic V^{5+}(s=0) ions. The V^{4+} ions are arranged in a coupled Majumdar-Ghosh chain like network. Our magnetic susceptibility χ(T) data fit well with the Curie-Weiss formula in the temperature range of 80-300K and it yields a Curie constant C= 0.39 cm3K/mole-V^4+ and an antiferromagnetic Weiss temperature θ = -26K. The χ(T) curve shows a broad maximum at T ≈ 25K indicative of short-range order (SRO) and an anomaly corresponding to long-range order (LRO) at T_N ~ 6K. The value of the 'frustration index' ($f=|\theta/T_N| \sim 5$) suggests that the system is moderately frustrated. Above the LRO temperature the experimental magnetic susceptibility data match well with the coupled Majumdar-Ghosh chain model[1] with the ratio of the nnn (next-nearest neighbor) to nn (nearest neighbor) magnetic coupling α = 2 and $Jnnn/k_B$ = 40K. In a mean-field approach when considering the inter-chain interactions, we obtain the total inter-chain coupling to be about 16K. The LRO anomaly at T_N is also observe in the specific heat Cp (T) data and is not sensitive to an applied magnetic field up to 90 kOe. A ^{51}V NMR signal corresponding to the non-magnetic vanadium was observed. Anomalies at 6K were observed in the variation with temperature of the ^{51}V NMR linewidth and in the spin-lattice relaxation rate $1/T_1$, indicating that they are sensitive to the LRO onset and fluctuations at the magnetic V sites. The existence of two components (one short and another long) is observed in the spin-spin relaxation rate $1/T_2$ data in the vicinity of T_N. The shorter component seems to be intimately connected with the magnetically ordered state. We suggest that both magnetically ordered and non-long range ordered (non-LRO) regions coexist in this compound below the long range ordering temperature.

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Relaxation in the re-entrant spin glass $Fe_{14.5}Cr_{85.5}$

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Spin glasses show frustrated magnetic interactions due to competing exchange interactions and, thus, possess no magnetic long-range order. Typically spin glass phase transitions occur at temperatures below 60K. Whether the phase transition takes place from a paramagnetic phase or from a magnetically ordered structure, e.g. (anti-) ferromagnetic phases, it is distinguished between diluted and re-entrant spin glasses, respectively. In re-entrant spin glasses clusters of magnetic order coexist with the magnetic amorphous spin glass phase. In the spin glass phase slow decay processes on large time scales occur because of the occurrence of many local minima in the energy landscape of the magnetic states.

In this contribution we show experimental results of the observation of the relaxation processes during the phase transition in the re-entrant spin glass $Fe_{14.5}Cr_{85.5}$ by means of the neutron spin echo method. The intermediate scattering function at different temperatures around the antiferromagnetic to spin glass phase transition temperature of about 26 K were measured. The fit of the general spin glass relaxation equation based on the Weron model [1] shows, that the relaxation processes in such samples may be governed by different contributions of hierarchical ordered and parallel spin interactions compared to diluted spin glasses.

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Recent development in "218" Rh, Pd and Pt based heavy fermion compounds

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Intermetallic compounds $R_2T\text{In}_8$ (R = rare earth, T = transition metal), commonly called "218" because of stoichiometry, are structurally related to a class of well-known Ce-based heavy-fermions like CeCoIn_5 or CeRhIn_5. They are located between fully 3D-compound CeIn_3 and quasi-2D "115" superconductors, which makes them ideal candidates to study structural dimensionality effects on various properties. Recent development in this field showed that it is possible to grow compounds with T = Pd [1] or Pt [2] with "218" stoichiometry. Therefore further study of "218" compounds is desired since it was little bit overlooked relative to more known "115" compounds.

We are interested in evaluation of magnetic structures and crystal field effects along the series of Rh based "218" compounds for various rare-earth elements. The single crystals of compounds with R = Nd, Tb, Dy, Ho, Er, Tm were successfully grown. Results of bulk measurements (specific heat, susceptibility) together with magnetic structures determined from several neutron experiments (D10, IN3, VIVALDI, CYCLOPS at ILL and an experiment in applied magnetic field on E4 at HZB) are presented. Evolution of all these properties was compared to those of their Ce_2RhIn_8 counterpart and also to our results of INS experiment.

Final part of the presentation is devoted to an overview of recently discovered compounds based on Pd and Pt [3].

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Interplay of low-energy phonons and magnetic excitations in Kondo insulator YbB_{12}: complementary neutron/synchrotron study

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Peculiarities in the lattice dynamics of the Kondo insulator YbB_{12} have been studied by means of inelastic neutron and x-ray scattering. Selected phonon modes were traced above and below the characteristic temperature $T^* \sim 50$ K, which corresponds to the opening of the gap in the electron density of states along with a transformation of the magnetic excitation spectrum. The intensities of some low-energy modes exhibit an anomalous temperature dependence for $\boldsymbol{q}$ vectors close to the Brillouin zone boundary. This effect is thought to arise from a coupling with magnetic excitations of the same symmetry, which exist at nearby energies. It is argued that this magneto-vibrational coupling could be responsible for the steep temperature crossover existing in YbB_{12} between the low-temperature (Kondo insulator) and high-temperature (incoherent spin-fluctuation) regimes.

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Low-temperature magnetic structure of the pyrochlore spin liquid $Tb_2Ti_2O_7$ under magnetic field $\boldsymbol{H}$ || [111]

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Initial experiments performed on $Tb_2Ti_2O_7$ suggested a classical spin-liquid behavior, akin to a cooperative paramagnet where strongly correlated magnetic moments fluctuate down to 50 mK at least [1]. However, the exact reason why it behaves as a spin liquid remains a matter of debate after more than 12 years of investigation.

It was suggested that, unlike spin ices, the crystal field scheme of $Tb_2Ti_2O_7$ allows the admixture of excited crystal field levels into the ground state doublet, leading the name "quantum spin ice" [2]. However, for $\boldsymbol{H}$ || [111] the quantum spin-ice model predicts a magnetization plateau [3], which was not observed experimentally [4]. Alternatively, we proposed a symmetry breaking as the source of the magnetic fluctuations in the ground state, yielding a two-singlet ground state for the Tb ion [5].

Here, we have studied the field-induced magnetic structures of $Tb_2Ti_2O_7$ by single-crystal neutron diffraction under a field applied along the [111] local anisotropy axis, up to $H = 12$ T and down to $T = 40$ mK. We collected a hundred magnetic Bragg peaks for each field and temperature value and refined the magnetic structures with $\boldsymbol{k} = 0$ propagation vector by performing a symmetry analysis. We observe a gradual reorientation of the Tb magnetic moments towards the field direction, close to a "3-in, 1-out / 1-in, 3-out" spin structure in the whole field range 0.05-12 T; this invalidates both the magnetization plateau and the "all-in, all-out" spin structures previously proposed [4]. We also perform a quantitative comparison with mean-field calculations and we propose the presence of a low-temperature dynamic symmetry breaking of the local trigonal symmetry, akin to a dynamic Jahn-Teller effect, i.e. preserving the overall cubic symmetry.

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Coexistence of novel magnetic orders and spin-glass-like phase in pyrochlore antiferromagnet $Na_3Co(CO_3)_2Cl$

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We present comprehensive investigations on a pyrochlore antiferromagnet $Na_3Co(CO_3)_2Cl$ [1]. The field dependence of the DC susceptibility follows the Almeida-Thouless line, suggesting a spin-glass-like phase transition. The AC susceptibility measurements determine the glassy transition temperature to be 4.5 K and reveal a frequency-independent peak at 17 K. The temperature dependence of the specific heat shows a sharp peak at 1.5 K and a broad hump at around 5 K, which are attributed to a long-range magnetic phase transition and a spin-glass-like freezing process, respectively. The $Na_3Co(CO_3)_2Cl$ sample proves to be chemically ordered since no obvious site disorder has been detected by means of neutron diffraction. The diffuse neutron scattering with polarization analysis reveals short-range spin correlations characterized by dominating antiferromagnetic coupling between nearest neighbors and weak ferromagnetic coupling between next nearest neighbors. The long-range magnetic order below 1.5 K is evidenced by the magnetic reflections observed at 50 mK and can be well explained with an all-in-all-out spin configuration. Inelastic neutron scattering of $Na_3Co(CO_3)_2Cl$ exhibits spin-wave-like excitations at 3.7 K, indicating that the spin-glass-like transition at T_g = 4.5 K is not a conventional spin glass transition. The possibility of a chiral spin glass scenario for this transition is checked by means of Hall effect measurements. The peak observed in magnetic susceptibility at 17 K is attributed to the onset of an intermediate partially-ordered phase transition, qualitatively consistent with the theoretical predictions.

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Eu-based iron pnictide superconductors

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$EuFe_2As_2$ based iron-pnictide superconductors display a unique interplay of Eu 4f moments with structural, magnetic and superconducting properties. The talk reviews recent experiments on the phase diagram, electronic nematicity and magnetoelastic coupling in $EuFe_2(As_{1-x}P_x)_2$ single crystals [1-6].

Work in collaboration with S. Zapf, M. Dressel, H.-A. Krug von Nidda, J. Fink, and Y. Xiao.

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Peculiar magnetism of iron pnictides aside from superconductivity

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Layered iron-pnictide compounds received a lot of attention in recent years as unconventional high-temperature superconductors. Yet, here I would like to focus instead on their magnetic properties, which are not any less exciting and likely lie at the foundation of the microscopic mechanisms underlying superconductivity. We have investigated the magnetic dynamics of different iron-arsenide parent compounds [1] and that of non-superconducting Mn-substituted Ba-122 material, $Ba(Fe_{1-x}Mn_x)_2As_2$ [2, 3], by inelastic neutron scattering and other complementary techniques. The effects of magnetic anisotropy, the role of magnetic impurities in stabilizing peculiar magnetic states, and the possibility of studying the enigmatic spin-nematic order of iron pnictides above T_N will be discussed in this presentation.

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October 8, 2013, 15:00h Unconventional Superconductors

Electron irradiation of iron-based superconductors

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While chemical heterogeneity and subsequent spatial variations of the superconducting parameters, as well as crystalline disorder on the scale of several dozen nm determine strong vortex pinning in iron-based superconductors at low fields [1,2,3], at higher magnetic fields the critical current density J_c is determined by quasi-particle scattering in the vortex cores. The latter leads to the mean-free path variation pinning mechanism due to the local fluctuations of the dopant atom distribution. Plausibly, the relevant scatterers are the dopant atoms themselves. In order to test this hypothesis, we study the evolution of vortex pinning and creep in $Ba(Fe_{1-x}Co_x)_2As_2$ as function of dopant concentration x, using the magneto-optical imaging technique and Hall probe array magnetometry. We also study the surface resistance as a function of temperature for single crystalline $Ba(Fe_{1-x}Co_x)_2As_2$ across the phase diagram, using the cavity perturbation method. In order to test this premise irradiation of Co, Ni and P-doped 122-type iron-based compounds with high-energy 2.5 MeV electrons is performed for several doping levels of the materials and to different doses. Such irradiation introduces atomic sized point-like defects. In all cases, the differential magneto-optical technique is used to reveal large-scale disorder, to discard single crystals with pathological defects, and to select use single crystals with a spatially homogenous distribution of T_c .Following irradiation it appears that the critical temperature Tc shows a similar depression for all studied materials. The weak collective contribution to *Jc* in Co-doped is found to clearly increase. Moreover this contribution appears after irradiation of the P-doped compound in which it was previously absent. This allows one to confirm the role of atomic point-like pins as scatterers in Ni and Co-doped compounds, as well as the hypothesis that these defects are at the origin of the weak collective pinning contribution to *Jc* at larger fields.

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Magnetic anisotropic energy gap and low-energy spin wave excitation in the antiferromagnetic block phase of $K_2Fe_4Se_5$

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Neutron scattering experiments were performed to investigate magnetic order and magnetic excitations in ternary iron chalcogenide $K_2Fe_4Se_5$. The formation of a superlattice structure below 580 K together with the decoupling between the Fe-vacancy order-disorder transition and the antiferromagnetic order transition appears to be a common feature in the $A_2Fe_4Se_5$ family. The study of spin dynamics of $K_2Fe_4Se_5$ reveals two distinct energy gaps at the magnetic Brillouin zone center, which indicates the presence of magnetic anisotropy and the decrease of local symmetry due to electronic and orbital anisotropy. The low-energy spin wave excitations of $K_2Fe_4Se_5$ can be properly described by linear spin wave theory within a Heisenberg model. Compared to iron pnictides, $K_2Fe_4Se_5$ exhibits a more two-dimensional magnetism as characterized by large differences not only between out-of-plane and in-plane spin wave velocities, but also between out-of-plane and in-plane exchange interactions [1].

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Understanding magnetism in $K_{0.8}Fe_{1.6}Se_2$

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The discovery of iron-based superconductors [1] a few years ago has stimulated tremendous research interests worldwide in unconventional high-T_C superconductivity. The new excitement in this field has been generated very recently due to the discovery of the new superconducting compound $K_xFe_{2-y}Se_2$ with T_C above 30 K [2]. Using polarized neutrons, we have determined magnetization distribution in $K_{0.8}Fe_{1.6}Se_2$. Magnetic structure factors derived from the polarization dependence of the intensities of the Bragg reflections were used to make a maximum-entropy reconstruction of the distribution projected on the [110] plane. The reconstruction shows clearly that more than 96 % magnetization is confined to the region around the iron atoms and that the magnetization associated with either Se or K atoms is less than 5 %. The distribution of magnetization around the Fe atom is only slightly nonspherical with a shape extended in the [001] directions in the projection. Details of the form factor modeling shows that the electrons which give rise to the paramagnetic susceptibility are confined to the Fe atoms and their distribution suggests that they occupy 3d t_{2g}-type orbitals with 80% in those of xy/yz symmetry. Orbital moment contributes significantly to the total paramagnetic moment of Fe.

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October 8, 2013, 16:30h Unconventional Superconductors

Nematic fluctuations and unconventional magneto-elastic coupling in iron based superconductors

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We demonstrate how emergent nematic order and nematic fluctuations, that are shown to be of magnetic origin, affect several macroscopic properties of both the normal and superconducting states of the iron pnictides. Due to its magnetic origin, long-range nematic order enhances magnetic fluctuations, leaving distinctive signatures that affect elastic and inelastic neutron scattering experiments and the NMR spin-lattice relaxation rate. We show that due to the magneto-elastic coupling, nematic fluctuations soften the shear modulus in the normal state, but harden it in the superconducting state. In the nematic phase, electrons are scattered by magnetic fluctuations that are anisotropic in momentum space, giving rise to a resistivity anisotropy whose sign changes between electron-doped and hole-doped compounds. Finally, we argue that T_c in the iron pnictides might be enhanced due to nematic fluctuations of magnetic origin.

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Magnetic anisotropy of low-energy spin excitations in iron pnictide superconductors

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It has been well documented that below T_C low-energy spin dynamics of iron based superconductors is dominated by a collective excitation centered at the Fermi surface nesting wavevector (½, ½, 0), known as the spin resonance mode. Recent observations of an apparent magnetic anisotropy just below the resonance energy on both hole- and electron-doped iron pnictide superconductors [1-2], via longitudinal polarization analysis of inelastic neutron scattering, have stimulated strong debates about the nature of this anisotropic low-energy mode. Further investigations on optimally electron-doped $Ba(Fe_{1-x}Co_x)_2As_2$ superconductor (T_C=24.5 K) carried out at the polarized triple-axis spectrometer IN22 will be presented. Our results will be discussed in the context of possible connections of this peculiar excitation mode to quantum critical point (QCP), nematicity and orbital ordering.

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Temperature and Doping Dependence of the Spin Dynamics in the Cubic Superconductor $U_{(1-x)}Th_xBe_{13}$

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Recently several rare-earth- and actinide-based unconventional superconductors have been (re-) investigated by inelastic neutron scattering (INS) revealing details of the microscopic momentum- and energy-dependent spin dynamics in the normal and the superconducting state. In several compounds the change in the spin dynamics on entering the superconducting state allowed identifying the symmetry of the superconducting order parameter. Most of these superconductors, for which magnetic fluctuations are discussed to be relevant for superconductivity, show a layered crystal structure. Contrary to those, UBe_{13} is an actinide-based heavy-fermion superconductor (T_c = 0.85 K, γ > 1J/molK^2) with a cubic crystal structure. A large single crystal of the cubic 5f superconductors UBe_{13} (Tc = 0.85 K) has been investigated by high-resolution cold neutron three-axis spectroscopy on PANDA at FRM2, Germany, and IN14 at ILL, France.

In agreement with previous experiments, we observed longitudinally polarized spin dynamics building up below $T \sim 50$K. The energy dependence of the normal state response can be modeled superimposing a quasi-elastic (QE) contribution with a Lorentzian line-shape and an inelastic contribution. The QE signal is consistent with fluctuations established in previous experiments on powder samples and linked to anomalies in the specific heat, from which a Kondo temperature T_K = 20 K has been deduced. The inelastic contribution shows a maximum at ΔE = 0.55 meV probably related with the observed Schottky-like anomaly in bulk measurements around T = 2 K which is supposed involving few magnetic moments only.

Our data taken in the superconducting state shows a shift of spectral weight to higher energies with respect to the normal state, which indicates the opening of a *superconducting* gap is reflected in the *spin* dynamics. The observed shift in UBe_{13} coincides with the inelastic contribution already present in the normal state, similar to the observation of a pseudogap phase in under-doped copper-based high-T_c-superconductors.

Looking at the $U_{(1-x)}Th_xBe_{13}$ phase diagram, the temperature of this T = 2 K Schottky-like anomaly decreases with doping. This resembles again the copper-based high-T_c-superconductors, for which the pseudogap temperature decreases with doping. The anomaly vanishes at the concentration with highest Tc. With such a scenario in mind, we are currently investigating the energy scales of optimally doped $U_{1-x}Th_xBe_{13}$ with x = 0.035. Preliminary INS results will be presented and compared to our findings for the pure UBe_{13} compound.

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October 9, 2013, 9:00h Interface Effects in Heterostructures

Putting a strain on $BiFeO_3$

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The strong coupling of ferroic orders (elastic, electric and magnetic) with the various structural degrees of freedom (notably polar and antiferrodistortive) provides multiferroic $BiFeO_3$ with very rich phase diagrams, as well as with a highly tunable, multifunctional character. Applied to $BiFeO_3$ thin films, epitaxial strain engineering reveals various unexpected features as well as novel multifunctional phases with enhanced properties and application potential. Combining advanced characterization techniques (X-ray and neutron diffraction, Mössbauer spectroscopy and piezoresponse force microscopy) and ab initio calculations, we have established that in $BiFeO_3$ strain anomalously drives the Curie temperature down [1]. This sheds light on the interplay between polar and oxygen tilting instabilities but also reveals the possibility to strain-drive the magnetic and ferroelectric transition temperatures close together, offering an original approach to achieve enhanced magnetoelectric responses [2]. The competition between both structural stabilities is also illustrated by the weak influence of strain on polarization [3]. Finally, we will show how Mossbauer and Raman spectroscopy data can reveal strain-driven changes in the spin arrangements and excitations [4].

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October 9, 2013, 9:30h Interface Effects in Heterostructures

Engineering electronic occupancy at surfaces and interfaces of transition metal oxides

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Electron occupancy of 3d- and 4d-orbitals of transition metal is determined by the total number of electrons in the 3/4-d-shell and by the energies of the five 3/4-d-orbitals. At free surfaces or at interfaces between dissimilar oxides in epitaxial heterostructures, there is an inherent breaking of symmetry that may produce charge redistribution that could ultimately lead to emerging properties.

It will be shown that the symmetry breaking at the free surfaces of transition metal oxides produces a preferential occupation of out-of-plane $3z^2$-r^2 that add and combine with any existing strain effect to determine the electronic properties of these surfaces [1]. Examples will include 3d-Mn and 4d-Ru ions in $AMnO_3$ and $ARuO_3$ perovskites.

Next, the occurrence of electronic reconstructions at the interface between (110) and (111) $SrTiO_3$ single crystals and several oxides will be addressed. It will be show that, under the appropriate conditions, a highly mobile 2D electron gas can be obtained. Interestingly enough, this achievement does not require crystalline interfaces but amorphous capping layer can also be used [2]. These findings may not only contribute to disclose the ultimate origin of these charge redistribution but also to pave the way to integrate these oxides on silicon platforms.

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October 9, 2013, 10:00h Interface Effects in Heterostructures

The magnetic proximity effect in cuprate-high T_c/manganite multilayers studied by polarized neutron reflectometry and resonant x-ray techniques

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Artificially grown multilayers of superconductors and ferromagnets are a fascinating playground to study the interaction between competing orders. Usually the focus is on the proximity-effect-induced modification of the superconducting order parameter and the resulting complex quantum phenomena. For multilayers from cuprate high T_c superconductors and ferromagnetic manganites there exists a corresponding magnetic proximity effect that gives rise to an induced ferromagnetic moment in the superconductor and a suppression (or modulation) of the ferromagnetic order in the ferromagnet [1-4]. In my talk I will show how polarized neutron reflectometry (PNR) in combination with resonant X-ray absorption and reflection measurements can be used to establish the intrinsic nature of this magnetic proximity effect and to explore its modification in the superconducting state [3-5].

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October 9, 2013, 10:30h Interface Effects in Heterostructures

Nanoscale magnetism and electronic phase separation at titanate interfaces

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Breaking the translation or inversion symmetry at surfaces and interfaces may lead to the formation of new charge, spin and orbital electronic states which are different than the bulk states. The emergence of these states is particularly relevant for oxides where the balance of competing interactions and the resulting stable electronic phase crucially depend on the local oxidation state near the interface. A prominent example is the interface of $LaAlO_3/SrTiO_3$ (LAO/STO), which exhibits a two-dimensional electron liquid state and undergoes a transition into a superconducting state below 0.2 K. Depending on growth conditions LAO/STO has also been found to display pronounced magnetotransport effects indicating the existence of local moments. Recently, even a coexistence of ferromagnetism and superconductivity has been reported, possibly due to an electronic phase separation within the interface.

Using a combination of density functional and field theoretical methods, we analyze the magnetic state of the LAO/STO interfaces and STO surfaces and provide evidence that it is caused by the spin polarization of Ti 3d interface electrons and depends strongly on the oxidation state of the interfaces/surfaces [1-2]. We show that oxygen vacancies induce a complex multiorbital reconstruction which involves a lowering of the local symmetry and an inversion of t_{2g} and e_g orbitals resulting in the occupation of the e_g orbitals of Ti atoms neighboring the O vacancy. In contrast to stoichiometric nonmagnetic LAO/STO, the vacancy-induced orbital reconstruction generates a two-dimensional interface magnetic state not observed in bulk $SrTiO_3$. This allows for the notion that areas with increased density of oxygen vacancies produce ferromagnetic puddles and account for the previous observation of a superparamagnetic behavior in the superconducting state. We analyze the electronic phase separation at the LAO/STO interface and find anomalous enhancement of the critical size of the magnetic regions upon the increase of the degree of oxygen reduction at titanate interfaces. We also discuss the related mechanisms of the interface ferromagnetic order and peculiarities of magnon spectrum in the context of nanoscale neutron scattering experiments.

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October 9, 2013, 11:30h Materials for Energy Conversion and Storage

Magnetocaloric materials for cooling applications near room temperature

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The efficient coupling between lattice degrees of freedom and spin degrees of freedom in magnetic materials can be used for refrigeration. This coupling is enhanced in materials exhibiting the giant magnetocaloric effect. The coexistence of strong and weak magnetism in alternate atomic layers has recently been shown to be a tool to design new materials[1]. The weak magnetism of Fe layers (disappearance of local magnetic moments at the Curie temperature) is responsible for a strong coupling with the crystal lattice while the strong magnetism in adjacent Mn-layers ensures Curie temperatures high enough to enable operation at and above room temperature. Varying the composition on these magnetic sublattices gives a handle to tune the working temperature and to achieve a strong reduction of the undesired thermal hysteresis. In this way we design novel materials based on abundantly available elements with properties matched to the requirements of an efficient refrigeration cycle.
A typical example of this class of materials is $(Mn, Fe)_2(P, Si)$ crystallizing in the hexagonal Fe_2P type of structure. Because the X-ray scattering-crossection of Mn and Fe and P and Si are very similar, neutron scattering is an indispensible tool for studying this type of materials. With neutron scattering we can simultaneously probe the crystallographic and magnetic structure of these novel materials.

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October 9, 2013, 12:00h Materials for Energy Conversion and Storage

Lattice dynamics in thermoelectric skutterudites

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Thermoelectric materials used for cooling in Peltier elements or for energy harvesting in waste heat recovery systems find a use in still rare niche application areas, because of the modest efficiency in currently used materials. A good thermoelectric material must exhibit a large electric conductivity and simultaneously a poor thermal conductivity. An increase in efficiency thus requires both a decrease of the lattice heat conductivity and proper optimization of the electronic properties *e.g.* by doping.

The $YbFe_4Sb_{12}$ filled skutterudite is an interesting model system with relatively low thermal conductivity. Inelastic scattering relates the low thermal conductivity observed in this material to the rattling of Yb guest atoms in the skutterudite cages. As the dynamics of these rattlers reduce the phonon mean free path, the lattice thermal conductivity is reduced. Interestingly, an anomalous temperature dependence of the elastic constants, with a rapid decrease in the c_{11} and c_{44} elastic constants at ~50 K is observed. The origin of this decrease was investigated with several methods and related to Yb valence change [1]. Results on this material and on related materials for solid state thermal energy conversion will be presented.

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October 9, 2013, 12:30h Materials for Energy Conversion and Storage

Anisotropy of the magneto-caloric effect in single crystalline $MnFe_4Si_3$

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Magnetic refrigeration for domestic home applications offers a huge potential to increase the energy efficiency of cooling devices. This requires cheap, abundant and non-toxic materials. $MnFe_4Si_3$, which orders ferromagnetically close to room temperature, exhibits a modestly large magneto-caloric effect (MCE). Based on powder data for the macroscopic and structural properties, the effect has been attributed to comparably large localized magnetic moments on the Mn ions with comparably large magnetic moments [1,2].

We have re-investigated the macroscopic properties of single crystals grown by the Czochralski method. Samples show a distinct behavior of the magnetic and resistive properties, depending on whether an external magnetic field is employed parallel or perpendicular to the hexagonal *c*-direction. According to earlier investigations, the space group symmetry for the compound is $P6_3/mcm$. However, our neutron single crystal investigations indicate a higher degree of Mn/Fe order than described in the literature leading to a reduction of the space group symmetry to P3. Preliminary results from resonant ultra sound spectroscopy and neutron powder diffraction imply a close relation between changes in the lattice at ~ 300 K and the magnetic phase transition at 305 K.

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Volume collapse and valence instabilities in CeNi

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The metastable CeNi phase has been studied by means of neutron and X-Ray diffraction, magnetic measurements and X-Ray absorption spectroscopy (XANES and EXAFS). The sample was synthesized at high pressure (9 GPa) and high temperature. The measurements were performed on the neutron source IBR-2 (JINR, Dubna) and on the synchrotron Sibir-2 (NRC "KI", Moscow).

The ground state formation in Ce-based intermetallics is a result of a complex interplay of the RKKY exchange interaction, the 4f electrons hybridization and the crystal field interaction. CeNi is an intermediate valence compound with a nonmagnetic ground state. This compound exhibits anomalous behavior of many physical properties including the first-order structural phase transition and well-defined coherent effects in the magnetic spectral response.

A dramatic volume collapse by 22% has been observed in intermetallic CeNi (to be compared with the well-known γ-α collapse in FCC cerium by about 15%). The crystal structure of the volume-collapsed CeNi phase was determined by both neutron and X-ray diffraction. Metastable CeNi belongs to the Zintl-phase crystal structures with a space group Fd3m (№227), Ce and Ni positions (8a): (0 0 0) and (8b): (½ ½ ½), respectively, and the lattice spacing a = 6.4807 Å.

Compared to the "parent" orthorhombic phase of CeNi the metastable phase and isostructural high-pressure phase of CeNi demonstrate much higher degree of the 4*f* electron delocalization and one of the highest deviations of Ce valence from the 3+ state. According to the temperature dependence of the specific heat the Sommerfeld coefficient in metastable CeNi is 9.5 mJ/(mol K^2) which is pretty low for an intermediate valence compound.

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Magnetic Nanomaterials Studied by Innovative Small Angle Neutron Scattering Techniques

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The potential of new techniques for Small Angle Neutron Scattering (SANS) is illustrated by investigations on magnetic nanomaterials. Polarised neutrons have been used as a special type of contrast variation for magnetic systems where low magnetic contrasts had to be analysed beside strong nuclear contributions or vice versa. Pulsed time-resolved SANS techniques have been developed which allow the investigation of the dynamic response to an external excitation with microsecond time resolution. Ordering and relaxation processes of particle moments have been investigated in magnetic colloids, in a solid Cu-Co alloy, and in a soft metallic glass in response to an oscillating magnetic field. For conventional stroboscopic SANS with a continuous neutron flux the accessible time scale is limited to some milliseconds. The time resolution can be substantially improved by the pulsed frame overlap TISANE technique which is currently implemented at the SANS instruments of HZB and ILL. The frequency dependence of the anisotropic SANS pattern in oscillating magnetic fields has been measured up to 7000 Hz, which is nearly two orders of magnitude faster than the limit for continuous stroboscopic techniques. The data have been analysed in terms of Debye-like dynamics of the particle moments with characteristic relaxation times in the order of 30-100 μs. Changes of nanostructure in response to a periodic stimulus have never been observed before in this time range by neutron techniques. This capability is expected to greatly extend the scope of SANS studies to a wide range of materials.

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October 10, 2013, 9:30h Magnetic Nanoparticles and Nanocrystals

Magnetic SANS on nanomagnets

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Small-angle neutron scattering (SANS) is a very powerful technique for the investigation of magnetic nanostructures, since it provides information from within the *bulk* of a material and on a length scale between a few nanometers and a few hundred of nanometers (~ 1-300 nm) [1]. However, up to now, SANS was almost exclusively utilized with an unpolarized or a polarized incident neutron beam (denoted as SANSPOL), and an analysis of the spin state of the neutron after the scattering process is frequently not performed. Due to recent progress in the development of efficient ^{3}He spin filters, it has only now become possible to perform routinely longitudinal (one-dimensional) neutron-polarization analysis (so-called POLARIS), for instance, at the instruments D22 and D33 at the ILL. In the first part of the talk we discuss recent POLARIS data on nanocrystalline ferromagnets, in particular, we report on the observation of a cross-shaped angular anisotropy in the non-spin-flip SANS cross section, only observable by means of POLARIS [2]. In a second example we present unpolarized magnetic SANS data of a Nd-Fe-B nanocomposite permanent magnet [3]. Here, we have studied the magnetization-reversal process by computing the autocorrelation function of the spin misalignment, which provides information on the characteristic size of spin inhomogeneities in the material. In the last part of the talk we demonstrate how numerical micromagnetics can be used in order to compute the magnetic SANS of nanocomposites [4-6]. In contrast to neutron experiments, in which one generally measures only a weighted sum of the Fourier components of the magnetization, this approach allows one to study the behavior of the individual contributions to the cross section. The micromagnetic procedure furnishes unique and fundamental information regarding the magnetic microstructure and corresponding magnetic scattering from nanomagnets.

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October 10, 2013, 10:00h Magnetic Nanoparticles and Nanocrystals

Polarized (GI)SANS by iron oxide nanocubes and their assemblies

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The physical properties of magnetic nanoparticles are intensely investigated for both fundamental and technological reasons. A broad interest is attributed to their manifold possible applications in magnetic data storage, magnetic imaging, or biomedical applications [1,2]. With regard to these applications, the main aspects of fundamental interest include the magnetic anisotropy and the related magnetization distribution in individual nanoparticles as well as interparticle interactions and collective properties in assemblies of nanoparticles.

Shape-anisotropic nanoparticles are strong candidates for investigation of increased magnetic anisotropy and dipolar interactions. The influence of nanoparticle shape on the degree of surface spin disorder has recently been reported [3]. Mesocrystals obtained through oriented self-assembly of shape anisotropic nanoparticles display a rich shape-induced structural diversity [4,5]. Their oriented arrangement is crucial for investigation of the directional and collective magnetic properties.

In this contribution, we will present a combined polarized SANS and GISANS study by iron oxide nanocubes and their assemblies. For the non-interacting nanoparticles, the spatial magnetization distribution and in particular the influence of particle size on surface spin disorder is determined using polarized SANS. Polarized GISANS measurements on mesocrystals of the same samples give insight into the magnetic correlations in interacting nanoparticles.

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Structural and magnetic correlations of self-assembled nanoparticle superlattices

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Nanoparticle superlattices can be considered as novel type of materials with controllable electronic, optical and magnetic properties. Their building blocks are nanoparticles (or 'nanocrystals') from a metallic, metal-oxide, or semiconducting material or hybrid between different materials [1]. I will report about the structural and magnetic properties of 2- or 3-dimensional 'superlattices' of magnetic nanoparticles. Depending on the substrate and the self-assembly technique we can fabricate either 'superlattice films' showing various growth modes as known from classical thin films or 3d mesocrystals [2-5]. The lateral ordering is quantified using electron microscopy and grazing incidence small angle X-ray scattering (GISAXS) [4,5]. The magnetic behavior and correlations are investigated by magnetometry, polarized neutron reflectometry (PNR) and grazing incidence small-angle neutron scattering (GISANS) [5].

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Neutron scattering on Rare Earth Ferrites

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Magnetoelectric multiferroics have a large applications potential and often involve complex phase competitions. Among different possible mechanisms of multiferroicity, ferroelectricity originating from charge ordering (CO) is particularly intriguing because it potentially combines large electric polarizations with strong magnetoelectric couplings – but example materials where this is realized are very difficult to find.

After $LuFe_2O_4$ had been proposed to be a multiferroic due to ferroelectricity originating from Fe^{2+}/Fe^{3+} CO below 320 K in 2005 [1], this material has become the generally accepted prototypical example of this mechanism and rare earth ferrites RFe_2O_4 have correspondingly attracted increasing attention [2]. In addition to the supposed multiferroicity, these materials are also interesting as potential model systems of frustrated Ising spin metamagnetism. Neutron diffraction to solve the spin structure, and indirectly the CO, on high-quality single crystals of $LuFe_2O_4$ [3] and more recently $YbFe_2O_4$ and YFe_2O_4 will be discussed. $LuFe_2O_4$ and $YbFe_2O_4$, which have similar ionic radii of the rare earth, have the same spin and charge structures affected by geometrical frustration – the charge order is not ferroelectric [3]. YFe_2O_4 has different, more complex, spin and charge structures.

The origin of the complex spin-charge order indicated by diffraction is still an open question [2]. To understand this origin, the determination of phonons and magnetic excitations will be helpful. A first experiment with inelastic neutron scattering on a large $LuFe_2O_4$ crystal will also be presented

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Posters

Poster 2013-01

Structural and magnetic properties of FePt@MnO heterodimer nanoparticles and their self-assembly

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On the length scale of few nanometers, surface effects are not negligible and therefore play an important role for the magnetic behavior of nanoparticles. In this work we investigate the magnetic properties of so-called FePt@MnO heterodimer nanoparticles, which consist of two exchange-coupled spherical nanoparticles, i.e. a ferromagnetic FePt and an antiferromagnetic MnO particle.

The dimer nanoparticles have been precharacterized with respect to their structural properties via small angle x-ray scattering (SAXS) and a form factor model for particles consisting of two spherical subunits could be verified. The magnetic properties dependent on the size of the nanoparticles have been investigated with ZFC and FC measurements, using SQUID magnetometry.

SANS technique with polarization was used to investigate the magnetic form factor of the single particles. For the MnO nanoparticles a magnetic scattering contribution has not been observed, whereas the FePt particles exhibit a clear nuclear-magnetic cross term at low temperatures. For investigation of the internal spin structure of MnO diffuse neutron scattering was used. The influence of the FePt on the antiferromagnetic ordering was observed by determination of the magnetic lattice constant.

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Poster 2013-02

T-REX: A Time-of-flight Reciprocal space Explorer for the future ESS source

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Within the ESS Design Update Phase program funded by the German Federal Ministry of Education and Research, we investigate the performance of a suite of time-of-flight spectrometers at the future ESS long pulse source. Here we present the current state-of-the-art in the study of a bispectral spectrometer concept and describe the main aspects of the conceptual design. The instrument promises the applicability to a wide manifold of scientific research activities: magnetism, strongly correlated electron materials, disordered systems, functional materials, soft-matter and biophysics. Grace to the large neutron flux it will implement time-of-flight spectroscopy with Polarization Analysis as a standard tool, e. g. for studying the effect of confinement on the magnetic excitations in nano-particles or to uniquely derive the vibrational hydrogen excitations in soft matter through separation of the nuclear spin incoherent scattering.
The instrument is supposed to accept neutrons generated both at the cold moderator and the thermal pre-moderator, by making use of a super-mirror extraction system. The chopper system is specifically designed to make an efficient use of the flux provided by the source, by means of a combination of the poly-chromatic operation methods: Repetition Rate Multiplication (RRM) and Wavelength Frame Multiplication. It is integrated with a specially developed pulse suppression chopper that enables variable acquisition time frames, by means of selective pulse suppression of the sub-pulses generated by the resolution defining choppers.
The secondary spectrometer features a wide area detector, yielding a dynamic range that extends from $1\text{meV} < E_i < 100\text{meV}$ and $0.05\ \text{Å}^{-1} < Q < 10\ \text{Å}^{-1}$, thus exploring a wide range of the reciprocal space. The energy resolution can be adapted by quantized variation of the commensurate chopper frequencies, within the limits imposed by the secondary path uncertainty. Simulations performed by means of ray-tracing methods showed that the elastic energy resolution (FWHM) varies in the range from 1.2% to 3% at 5meV and from 5% to 15% at 82 meV, thus providing flexible trading of resolution for flux.
The instrument is specifically designed to allow the use of polarized neutrons and exploit the XYZ polarization analysis, by means of the so-called MAGIC Pastis coil layout. A prototype is under construction for the TOPAS spectrometer at the FRM II, which uses a wide-angle banana shaped ^{3}He Neutron Spin Filter cell to cover a large range of scattering angle, both in horizontal and vertical direction.

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Poster 2013-03

Detailed SANS contrast variation on toluene-based Co ferrofluid

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Contrast variation is a powerful technique [1], which is widely applied for studies of complex systems in small-angle neutron scattering experiments. The advantage of H/D substitution in the solvent without change in its chemical properties makes it possible to study such many-component systems in detail. In case of polydisperse systems one has to consider averaging of the scattering intensity over the particle size distribution. Thus, the direct modeling of the scattering intensities requires a certain number of free parameters, which can give the researcher a wrong result. The developed approach of contrast variation for polydisperse systems [2] allows researcher to obtain parameters, which can be later fixed in the model. A successful application of the approach in contrast variation on iron oxide magnetic fluids can be found in [3, 4].

In the present work we report about the contrast variation study of cobalt ferrofluid based on toluene with oleoyl sarcosine coating. The initial magnetic fluid (1.2 vol. % of Co) was diluted with toluene in the ratio 1:5. Several contrasts were prepared so that the amount of deuterated toluene in the solvent varied in the range 0-85%. The corresponding buffer solutions were prepared and used for background subtraction. Structural parameters of the nanoparticles were precisely obtained and used for further modeling of the scattering curves.

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Poster 2013-04

Dispersive magnon excitations in $Ca_3Co_2O_6$

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The geometrically frustrated trigonal cobaltate $Ca_3Co_2O_6$ is considered to be a model system for a one-dimensional Ising-like antiferromagnet [1]. Its crystal structure represents a hexagonal arrangement of one-dimensional chains, which consist of alternating nonmagnetic CoO_6 octahedra and CoO_6 trigonal prisms with a large magnetic moment. Spin-orbit coupling results in large single-ion anisotropy of the order of 70 meV, leading to an Ising-type character of magnetism in this system.

We have employed inelastic neutron scattering (INS) on a large mosaic of $Ca_3Co_2O_6$ single crystals to study the spectrum of low-energy magnetic excitations in this material. Based on the earlier powder data [2], it was suggested that such excitations are limited to a number of non-dispersive crystal-field-type lines. In our experiment, however, we demonstrate the presence of at least one magnon branch with a clear dispersion along the chain direction. It is characterized by a large spin gap of ~26 meV and a band width of ~5 meV. From the measured magnon dispersion, we could unambiguously determine the out-of-plane exchange constant and the magneto-crystalline anisotropy for this system.

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Poster 2013-05

The magnetic properties of $Nd_2Sn_2O_7$, a candidate of quantum spin liquid, at temperatures as low as 2 K

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The rare earth pyrochlores $R_2M_2O_7$ where *R* is a rare-earth ion and *M* is a transition metal ion have been the subjects of intense research over the last two decade with the the discoveries of novel magnetic behaviour such as spin ice [1] co-operative paramagnets, Berry Phase behaviour and more recently magnetic monopoles and magnetic current. Most experimental data on oxide pyrochlores has been collected on the rare-earth titanates with large 4f magnetic moments and interpreted classically. This vastness of this work is generally because the samples can be synthesised into large single crystals and the complex low-temperature states found in samples like $Tb_2Ti_2O_7$, $Ho_2Ti_2O_7$ and $Dy_2Ti_2O_7$.

We present neutron scattering, magnetic susceptibility and specific heat capacity results which fully characterise the magnetic properties of the pyrochlore $Nd_2Sn_2O_7$ at temperatures at least as low as 1.8 K. We find that no transition to a magnetically ordered state is visible in zero field down to 2 K using neutron scattering, but that in magnetic field the Nd moments can be polarized easily. A refinement of the resultant neutron scattering pattern suggests some strong single ion anisotropy in the system implying a possible exotic ground state. Our susceptibility measurements show a transition to an ordered state at approximately 1 K which exhibits interesting field dependent characteristics. An experiment at ANSTO is planned which will explore the neutron scattering pattern below the magnetic transition with the aim of establishing the nature of the transition and the low temperature state.

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Poster 2013-06

Structural and electronic properties of $CeCuAl_3$ single crystal and vibron states in $Ce(Cu,Al)_4$ compounds

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Strong electron-phonon interaction leads to the forrmation of vibron quasi-bound states in several studied Ce-based materials, e.g. $CeAl_2$ [2], $CePd_2Al_2$ [3] or recently $CeCuAl_3$ [4]. The additional peak observed in energy spectra of these compounds is satisfactory described by vibron theory [1]. Presented study is focused on $CeCuAl_3$ compound, where the magnetic structure as well as propagation vector are not known. Moreover, the structure type, in which this compound crystallizes, is not determined unambiguously. We present the thorough study of crystal structure as well as electronic properties by means of magnetization, specific heat and electrical resistivity measurements.

The tetragonal $BaNiSn_3$-type crystal structure was determined unambiguously as the structure of $CeCuAl_3$. Moreover, we found structural phase transition around 300°C. The phase transition changes the structure parameters only, the crystal structure is preserved. Electronic properties investigation reveals antiferromagnetic order below 2.5 K and magnetization easy axis along [100] direction. We expect the magnetic moments oriented perpendicular to the c-axis. Relatively strong ferromagnetic correlations are present in this compound as well as anisotropic Kondo interaction.

$Ce(Cu,Al)_4$ compounds, where the substitution of Cu by Al (in $CeCuAl_3$) causes the change of magnetic order from antiferromagnetic to ferromagnetic one, were investigated with respect to the presence/absence of vibron states and theirs development by inelastic neutron scattering measurements. An analysis of our inelastic data will be presented based on the vibron model.

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Poster 2013-07

Magnetic properties of $LaCo_{1-x}Ni_xO_3$ (x = 0, 0.1, 0.2, 0.4)

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We report here the magnetization studies of the rare earth cobaltite $LaCo_{1-x}Ni_xO_3$ (x = 0, 0.1, 0.2, 0.4) synthesized using conventional solid state reaction method. X-ray diffraction followed by reitveld refinement confirms the single phase rhombohedral structure with $R\bar{3}c$ space group for all the samples. A homovalent +3 state and spin state transition of Co^{+3} has been observed upon Ni substitution in x-ray absorption measurements at Co and Ni K-edge. Thermally driven spin state transition has been found to disappear with Ni substitution. Below a certain low temperature, samples with x = 0, 0.1, show paramagnetic to antiferromagnetic transition but the sample with x = 0.2, 0.4 shows paramagnetic to spin glass transition. Coexistence of AFM-FM phases has also been revealed in isothermal magnetization measurements at low temperature. The overall magnetic behaviour has been explained on the basis of change in crystal field, orbital ordering and various magnetic interactions between transition metal networks.

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Poster 2013-08

Long range incommensurable spin ordering in a swedenborgite compound

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The new swedenborgite compound family ($P6_3mc$)[1] displays similarly to the pyrochlores a highly frustrated network of tetrahedrally coordinated magnetic ions. However, its broken inversion symmetry raises further the complexity of ordering due to non-vanishing Dzyaloshinski-Moriya interactions. Recently investigated materials of this family show various signs for unusual geometric frustration [2–5]. In compounds with magnetic Co and Fe ions, where single crystals are available like the $CaBaCo_2Fe_2O_7$, we observed an antiferromagnetic ordering below $T_N \approx 160K$, which, turned out to be rather complex. Diffuse neutron scattering at DNS (FRM II Munich) has shown that the magnetic spins order in a three times larger supercell. A particular intriguing result was the chiral interference observed as an asymmetry of the magnetic Bragg intensities.

Further powder diffraction experiments with higher resolution at POWGEN (SNS Oak Ridge) have revealed unexpected and interesting features of additional satellite peaks close to the main magnetic peaks, with a propagation vector $\tau = 0.016 Å^{-1}$ corresponding to a long periodicity of ≈400Å, which could be modeled with three magnetic satellite peaks located along the edges of the structural Brillouin zone surrounding the main magnetic ones.

Single crystal diffraction data from MORPHEUS (SINQ Villigen) and BIODIFF (FRM II Munich) shows quite peculiar agreements and differences.

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Poster 2013-09

DNS – a versatile diffuse neutron scattering spectrometer with polarization analysis at FRM II: towards enhanced count rate and extended Q-range

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DNS is a versatile diffuse scattering instrument with polarization analysis operated by the JCNS at the research reactor FRM II. Compact design, a large double-focusing monochromator and a highly efficient supermirror-based polarizer provide an impressive polarized neutron flux in the range of 10^7 n/cm^{2}s. DNS is effectively used for the studies of highly frustrated spin systems [1], strongly correlated electrons [2], emergent functional materials [3] and soft condensed matter [4].

We present the current status of the instrument and recent scientific highlights at DNS as well as ongoing instrument developments. Within the upgrade project the coating of the neutron guide will be increased to m=2, which will extend the accessible Q-range towards higher values. In the combination with a large array of 1d position-sensitive detectors covering the solid angle of about 1.9sr and a high-frequency disc chopper system, both under development, DNS is expected to become a high count-rate cold time-of-flight spectrometer with medium resolution.

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Poster 2013-10

Field-induced spin reorientation in $EuFe_2(As_{0.85}P_{0.15})_2$ revealed by resonant magnetic x-ray scattering

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It was revealed from different experiments that there is a strong coupling between the Eu magnetism and the superconductivity in the P-doped $EuFe_2As_2$ compounds. However, it is still an open question with regard to the magnetic structure of Eu^{2+} moments in superconducting $EuFe_2(As_{1-x}P_x)_2$ [1-3]. Magnetic resonant x-ray scattering measurements on a superconducting $EuFe_2(As_{0.85}P_{0.15})_2$ single crystal were carried out to study the magnetism of Eu^{2+} sublattice in the unit cell. Evidences for ferromagnetic ordering of Eu^{2+} along *c*-axis in the ground state were found, which coexist with robust superconductivity. With the increase of applied in-plane magnetic field, the moment direction of ferromagnetic Eu^{2+} spins flops gradually from the *c* direction to the in-plane field direction. The phase diagram of the Eu magnetism in superconducting $EuFe_2(As_{0.85}P_{0.15})_2$ with the change of temperature and applied field was obtained and compared with that of the non-superconducting parent $EuFe_2As_2$ compound [4].

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Poster 2013-11

Single crystal diffraction studies on new magnetic and superconducting compounds with HEiDi

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The instrument HEiDi at the Heinz Maier-Leibnitz Zentrum (MLZ) uses hot neutrons for single crystal diffraction analysis of structural and magnetic properties of samples for which other methods are not applicable [1].

Various multiferroic compounds were studied on HEIDI due to required high precision like the pyroxene $NaFeGe_2O_6$ which shows a complex incommensurate magnetic structure below 12 K or various manganites of $REMnO_3$ type whose highly absorbing and heavy rare earth elements (RE=Gd, Dy) make it normally extremely difficult to get accurate structural and magnetic diffraction data [3]. In all of these cases the unique capabilities of this instrument offering high resolution, large penetration depth and large q range were very important.

Also new superconductors, like the recently discovered FeAs pnictides are an important topic of studies on HEIDI. These metal alloys show significant similarities to the ceramic high Tc cuprates having a layered structure which undergoes for certain compositions and dopings a structural, magnetic and/or superconducting phase transitions. An example is the $EuFe_2As_2$ compound with its complexity of the orthorhombic phase (reflection splitting due to appearance of domains and twinning) and high Eu absorption making precise data collections as well as their accurate interpretation very challenging but offer a deep insights to details of structural phase transitions and magnetic order at low temperatures of these compounds [4].

This contribution will give an overview of the instrument and examples of its contributions to various topics of magnetism and correlated electron systems.

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Poster 2013-12

Presence of chiral character in the spin resonance of the unconventional superconductor $CeCoIn_5$

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In various unconventional superconductors, cuprates, iron pnictides, and chalcogenides and heavy fermion systems, there exists characteristic magnetic response so-called 'spin resonance'. This mode is observed in inelastic neutron scattering below the superconducting transition temperature T_c at the wave vector for which the superconducting gap Δ changes sign and at an energy $\Omega res/2\Delta \approx 0.64$. While there is no consensus on the origin of such an excitation and its relevance to the pairing mechanism, it provides crucial information on the superconducting gap, and therefore has a particular importance to be studied.

In order to get microscopic insights into the spin resonance, the heavy-fermion superconductor $CeCoIn_5$ which has the highest T_c of 2.3 K among the Ce-based compound, was investigated via polarized inelastic neutron scattering under a magnetic field. We found that the spin resonance at 0.6 meV at zero field splits under magnetic fields. The magnetic excitation under the field is characterized as two Zeeman split peaks with a chiral nature, and an additional non-chiral contribution that appears at the same energy as the lower mode of the Zeeman split peaks. This observation evidences that the spin resonance in $CeCoIn_5$ is a degenerated mode, which has three fluctuation channels under magnetic field.

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Poster 2013-13

Magnetic excitation in intermediate-valence $EuCu_2Si_2$

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The magnetic spectral response in the intermetallic compound $EuCu_2Si_2$ has been studied by inelastic neutron scattering. The measurement were performed on the time-of-flight spectrometer SEQUOIA (SNS neutron source, ORNL) at incident neutron energies 225 and 125 meV, temperature T=5K and within the neutron scattering angle range 4° to 50°. ^{153}Eu-based sample (99.7% enrichment ^{153}Eu) was used to avoid neutron absorption by the sample.

$EuCu_2Si_2$ is an intermediate valence systems with the europium ions fluctuating between the Eu^{2+} and Eu^{3+} states. This compound is a member of the Eu-1-2 2 series demonstrating a variety of ground states ranging from the nonmagnetic Kondo singlet to the magnetically ordered states. The primary goal of the study was to collect detailed experimental information on the momentum transfer dependence of the magnetic spectral response in $EuCu_2Si_2$. A procedure has been developed to discriminate between the phonon and the magnetic contribution to the spectra. Two well-defined magnetic peaks have been observed in the neutron spectrum of $EuCu_2Si_2$, one of them is related to modified spin-orbit transition, another is inherent to the specific ground state in $EuCu_2Si_2$ The neutron momentum transfer dependence of the magnetic peaks is discussed.

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Poster 2013-14

Effects of magnetic order and lattice dynamics in $CuCrS_2$

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The transition metal dichalcogenide $CuCrS_2$ shows a strong crystalline anisotropy with a quasi-two dimensional layered structure and layers of S-Cr-S separated by a large van der Waals gap. The triangular arrangement of Cr^{3+} ions is prone to geometrical frustration, as the main magnetic exchange is antiferromagnetic.
Below T_N=37K a complex magnetic structure with an incommensurable magnetic propagation vector develops. The magnetic order is coupled to a structural transition from R3m (at RT) to Cm (at low T) giving evidence for magneto-elastic coupling in the system. [1] At higher temperatures ionic conductivity of the weakly bound Cu ions emerges.
Inelastic neutron scattering experiments on the thermal time-of-flight spectrometers IN4 and IN6 show the emergence of a strong non-dispersive magnetic signal with an intensity modulation typical for dimerisation of magnetic moments. Additionally an enhanced intensity has been observed at crossings of phonon and magnon modes at about 8meV.
Temperature dependent measurements of phonon density of states show a strong change of low lying phonon branches. The strongest change appears at about 150K with a strong change in intensity at about 8meV. Ab-initio calculations assign this energy to in plane motions of the Cu atoms.

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Poster 2013-15

Detailed investigation of magnetic structure in peculiar multiferroic $Ba_2CoGe_2O_7$

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Recently, $Ba_2CoGe_2O_7$ has attracted significant scientific interest due to its peculiar magnetoelectric behavior [1] and its giant directional dichroism in resonance with both electrically and magnetically active spin excitations located in the terahertz region [2]. Nevertheless that different theoretical models have been developed the detailed magnetic structure in the ground state has not been determined yet.

The detailed structural refinement of the spin order in $Ba_2CoGe_2O_7$ has been performed using single crystal neutron diffraction. The antiferromagntic order below 6.7 K where the spins of the Co2+ ions form a square-lattice Néel order within the (a,b) plane, while their alignment is ferromagnetic along the c axis has been determined. The magnitude of the ordered moment, fully lying within the (a,b) plane, is found to be 2.9(1) $\mu B/Co^{2+}$ and the easy axis of the sublattice magnetizations corresponds to the [110] direction. [3]

A non-collinear spin structure due to small canting is allowed by the magnetic symmetry and non-polarized diffraction data. In order to address the question about the noncollinearity of the magnetic structure the polarized neutron diffraction both using flipping ratio method and spherical polarimetry have been performed. The results show that value of the spin canting at the ground state is below 0.2°. The formation of the antiferromagnetic 180° domains was investigated using spherical polarimetry. Small external field of 0.1 T applied by cooling over the T_N lead to the formation of the one or two domain structure depending on the field direction.

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Poster 2013-16

Fabrication of transition metal oxide thin films by molecular beam epitaxy: New offer for users of the Heinz Maier-Leibnitz Zentrum at the FRM II

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Transition metal oxide thin films and heterostructures are of general interest due to their possible application in technological devices [1]. A characteristic property is the reconstruction of the charge, spin and orbital states at interfaces on the nanometre scale. Examples are interface superconductivity, magneto-electric coupling, and the quantum Hall effect in oxide heterostructures [2].

We utilize Molecular Beam Epitaxy (MBE) technique to fabricate these systems with a state-of-the-art MBE system at the MLZ. The system is equipped with six effusion cells, two electron guns for electron-beam evaporation with four crucibles each and an oxygen plasma source. Standard in-situ surface analysis tools like reflection high and low energy electron diffraction, Auger electron spectroscopy are also available.

The Jülich Centre of Neutron Science offers the preparation of tailored samples to users for investigation with the JCNS neutron reflectometer MARIA (magnetic reflectometer with high incident angle) or other neutron instruments. We give information about the modalities for sample preparation and neutron experiments and present examples from our work.

In collaboration with the Walther-Meißner-Institute for Low Temperature Research, Garching we report on the optimization of Pt growth on Yttrium Iron Garnet (YIG). This heterostructure is very interesting for spintronics as YIG is a ferrimagnetic insulator while Pt is a paramagnetic conductor which enables the usage of it for spin currents and spin transfer torque and inverse spin hall effect [3].

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Poster 2013-17

Interface induced magnetism in $[LaMnO_3/SrMnO_3]_N$ heterostructures

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Multifunctional oxides open a wide field of physical properties due to the correlated electron system. Small variations of the electron system can lead to a wide range of physical properties. Especially the interface of two oxide thin films can exhibit different properties as found in the bulk.

Here we combine $LaMnO_3$ and $SrMnO_3$, which are antiferromagnetic bulk insulators, while the interfaces in a multilayer stack behave as a ferromagnetic material. The ferromagnetism of the $LaMnO_3$ layer at the $LaMnO_3/SrMnO_3$ interface is induced due to the vicinity of a subjacent $SrMnO_3$ layer, and was not yet observed in the opposite boundary. May et al. reported recently that the different interfaces $LaMnO_3/SrMnO_3$ and $SrMnO_3/LaMnO_3$ exhibit different roughness. These structural asymmetries could be the origin of magnetic asymmetries in the thin film system [1].

$SrMnO_3$ and $LaMnO_3$ have been grown with a state of the art oxide molecular beam epitaxy system on $SrTiO_3$ with interface roughness of the order of a unit cell. The grown samples do not exhibit the structural asymmetries mentioned above and thus we don't expect magnetic asymmetries. We present the preparation method of this complex oxide multilayer and the results of our in-house characterization methods, x-ray reflectometry and SQUID magnetometry. The magnetic depth profile was investigated by polarized neutron reflectometry measurements performed at D17 (ILL, Grenoble). To evaluate the data we assumed a model to refine our data with an extensible reflectivity refinement program utilizing differential evolution (GenX) [2].

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Poster 2013-18

Electrically induced magnetic transition at the LSMO/BTO interface

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The magnetoelectric coupling is one of the most fascinating and active research areas today. The control of the magnetism due to an applied electric field may lead to new device concepts. First principles calculations of $La_{(1-x)}Sr_xMnO_3/BaTiO_3(001)$ interfaces show magnetic reconstructions due to the change of the polarization of BTO by applying an external electric field [1]. The different electron densities influence the equilibrium between super- and double-exchange favoring a ferromagnetic or an antiferromagnetic order at the interface for the two different orientations of the polarization.

Here we report on LSMO/BTO, grown with an Oxide Molecular Beam Epitaxy system. The epitaxial layer-by-layer growth was confirmed by in-situ RHEED analysis and the crystalline quality of the surface was investigated by LEED and Atomic Force Microscopy. The structural characterization was carried out by X-ray reflectometry and X-ray diffraction. The macroscopic magnetic properties were determined by MOKE and SQUID magnetometry. The magnetic formation at the interface was investigated by polarized neutron reflectometry measurements performed at MARIA (FRM II).

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