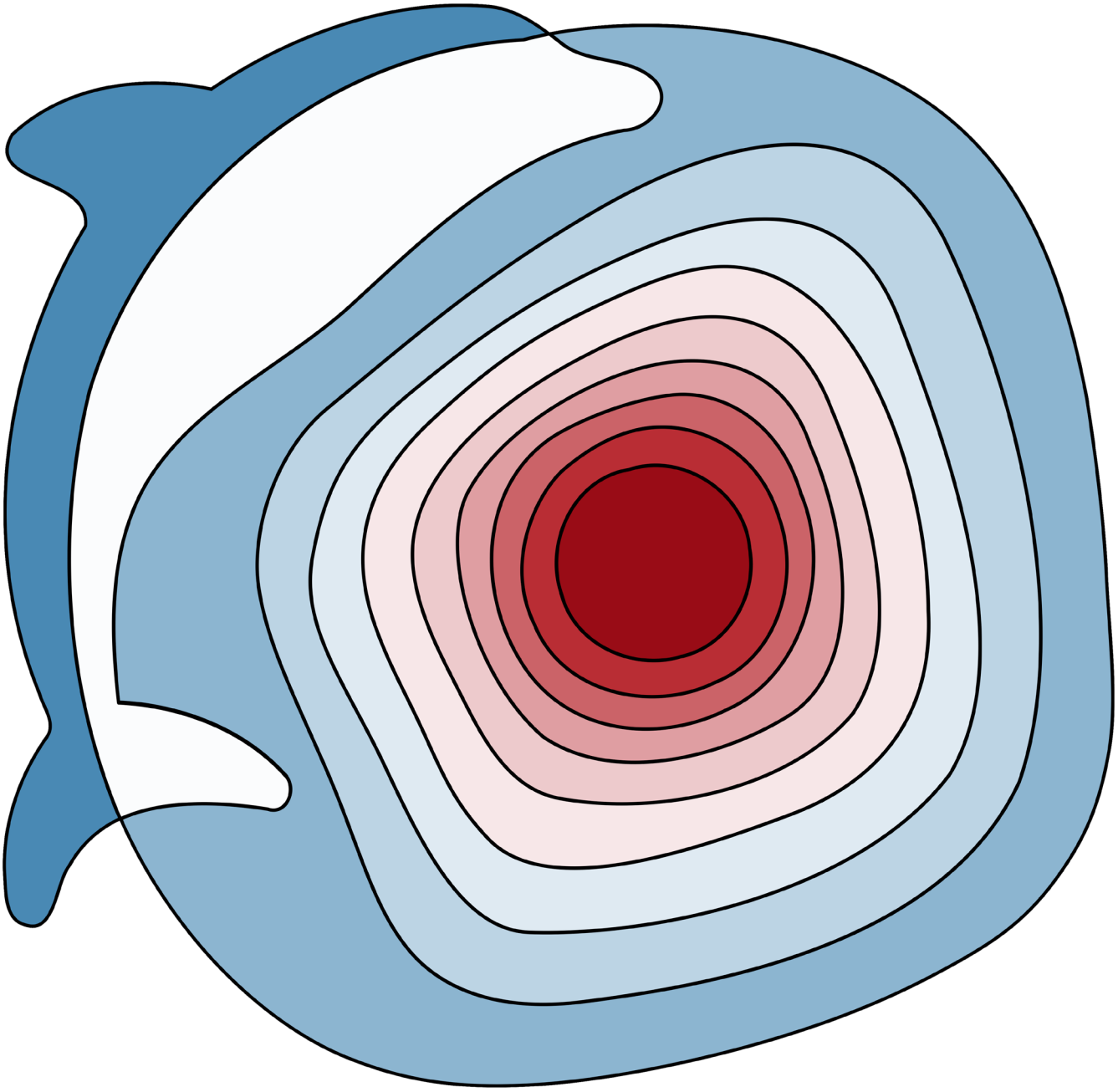


Member of the Helmholtz Association

Joint JCNS-Workshop and Flipper

Modern Trends in Neutron Scattering from Magnetic Systems and Single-crystal Diffraction with Polarized Neutrons

Program and Abstracts

3 – 7 Oct. 2016, Tutzing **www.fz-juelich.de/jcns/JCNS-Workshop2016**

Jülich Centre for Neutron Science
JÜLICH FORSCHUNGSZENTRUM
MLZ Heinz Maier-Leibnitz Zentrum

Dear colleagues,

In 2016 the JCNS-Workshop is dedicated to neutron scattering from magnetic systems. It will also host the workshop FLIPPER, Single-crystal Diffraction with Polarized Neutrons. This will bring related communities together and stimulate discussion and scientific exchange between them.

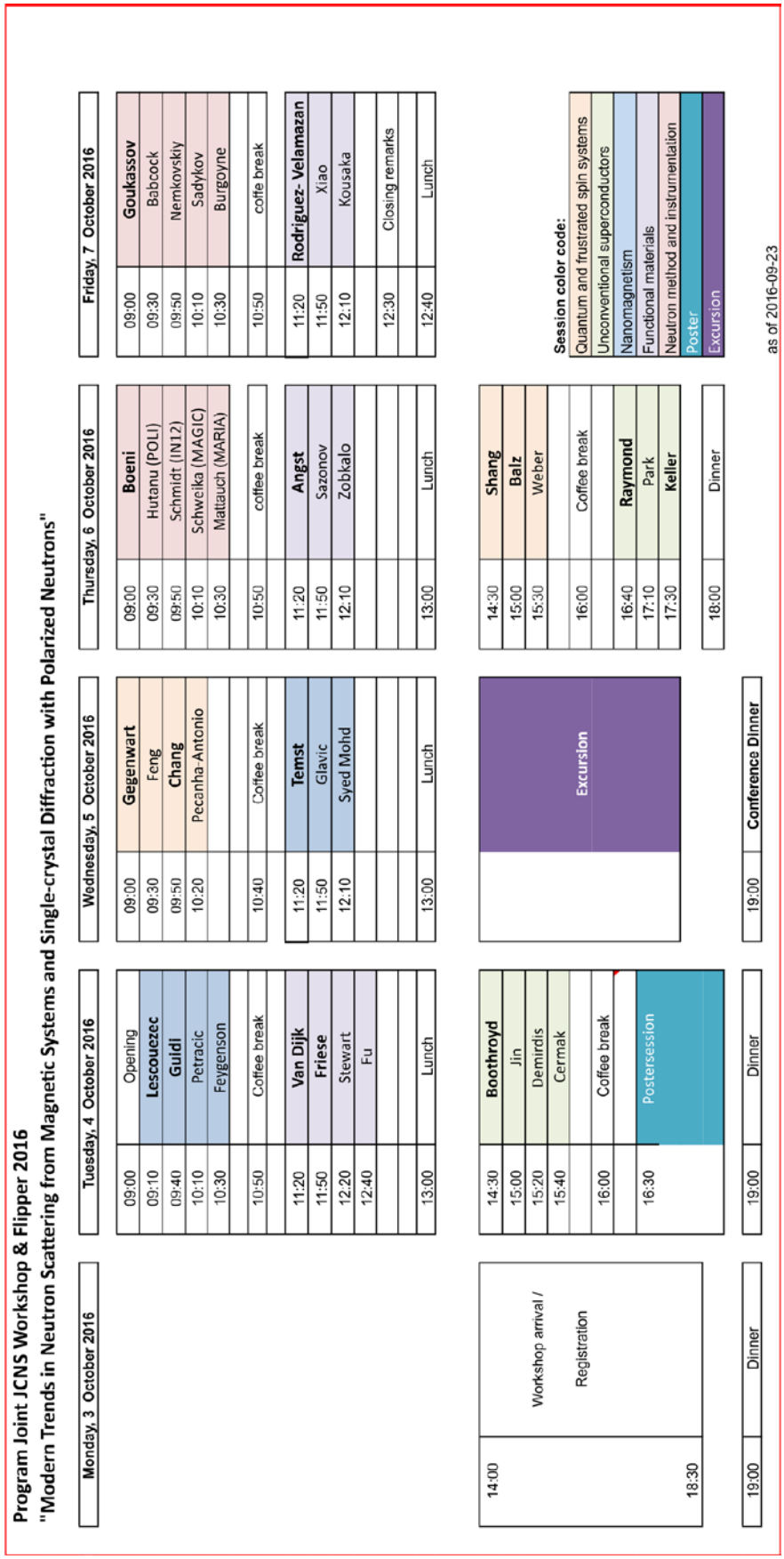
The topics addressed are:

- **Unconventional superconductors**
- **Quantum and frustrated spin systems**
- **Functional materials**
- **Neutron methods and instrumentation**
- **Nanomagnetism**

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.

Yixi Su Vladimir Hutanu

Presentation Schedule



Program Joint JCNS Workshop & Flipper 2016
"Modern Trends in Neutron Scattering from Magnetic Systems and Single-crystal Diffraction with Polarized Neutrons"

Monday, 3 October 2016		Tuesday, 4 October 2016		Wednesday, 5 October 2016		Thursday, 6 October 2016		Friday, 7 October 2016	
		09:00	Opening	09:00	**Gegenwart**	09:00	**Boeni**	09:00	**Goukassov**
		09:10	**Lescouezec**	09:30	Feng	09:30	Hutanu (POLI)	09:30	Babcock
		09:40	**Guidi**	09:50	**Chang**	09:50	Schmidt (IN12)	09:50	Nemkovskiy
		10:10	Petracic	10:20	Pecanha-Antonio	10:10	Schweika (MAGIC)	10:10	Sadykov
		10:30	Feygenson			10:30	Mattauch (MARIA)	10:30	Burgoyne
		10:50	Coffee break	10:40	Coffee break	10:50	coffee break	10:50	coffe break
		11:20	**Van Dijk**	11:20	**Temst**	11:20	**Angst**	11:20	**Rodriguez- Velamazan**
		11:50	**Friese**	11:50	Glavic	11:50	Sazonov	11:50	Xiao
		12:20	Stewart	12:10	Syed Mohd	12:10	Zobkalo	12:10	Kousaka
		12:40	Fu						
								12:30	Closing remarks
		13:00	Lunch	13:00	Lunch	13:00	Lunch	12:40	Lunch
14:00	Workshop arrival / Registration	14:30	**Boothroyd**		Excursion	14:30	**Shang**		
		15:00	Jin			15:00	**Balz**		
		15:20	Demirdis			15:30	Weber		
		15:40	Cermak						
		16:00	Coffee break			16:00	Coffee break		
		16:30	Postersession			16:40	**Raymond**		
18:30						17:10	Park		
						17:30	**Keller**		
19:00	Dinner	19:00	Dinner	19:00	**Conference Dinner**	18:00	Dinner		

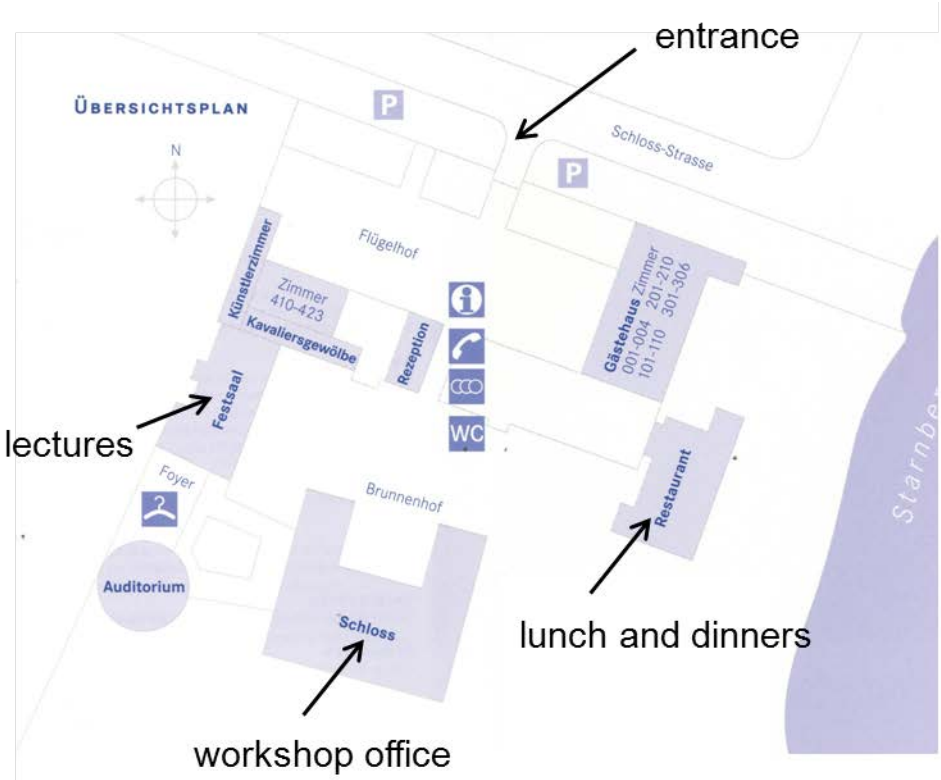
Session color code:

Quantum and frustrated spin systems
Unconventional superconductors
Nanomagnetism
Functional materials
Neutron method and instrumentation
Poster
Excursion

as of 2016-09-23

Evangelische Akademie Tutzing

Site Map



Joint JCNS-Workshop and Flipper 2016

"Modern Trends in Neutron Scattering from Magnetic Systems and Single-crystal Diffraction with Polarized Neutrons"

October 3 - 7, 2016, Tutzing

Program

Tuesday, October 4, 2016

09:00 Opening of the workshop and welcome

Nanomagnetism I (Molecular Magnets & Nanoparticles)

1 09:10 Rodrigue Lescouëzec, UPMC, France (invited)
Molecular Magnetic Materials:
Probing Magnetism at the local scale

2 09:40 Tatiana Guidi, ISIS, United Kingdom (invited)
Antiferromagnetic molecular rings: spin density and dynamics

3 10:10 Oleg Petracic, JCNS, Forschungszentrum Jülich, Germany
Magnetic and structural order in self-assembled 2d and 3d nanoparticle supercrystals

4 10:30 Mikhail Feygenson, JCNS, Forschungszentrum Jülich, Germany
Exchange bias effect in Au-Fe_3O_4 dumbbell nanoparticles induced by the charge transfer from gold

10:50 Coffee Break

Functional Materials I

5 11:20 Nils van Dijk, Delft University, The Netherlands (invited)
Neutron scattering studies on Fe_2P-based magnetocaloric materials

6 11:50 Karen Friese, JCNS, Forschungszentrum Jülich, Germany (invited)
Multiparametric studies on magnetocaloric compounds in the system $Mn_{5-x}Fe_xSi_3$

7 12:20 Ross Stewart, ISIS, United Kingdom
Static correlated spin fluctuations in single crystal $Fe_{65}Ni_{35}$ INVAR alloy, studied using small-angle neutron scattering with polarization analysis

7a 12:40 Zhendong Fu, JCNS at MLZ, Forschungszentrum Jülich, Germany
Magnetic structures and magnetoelastic coupling of Fe-doped hexagonal manganites $LuMn_{1-x}Fe_xO_3$ ($0 \leq x \leq 0.3$

13:00 Lunch

Tuesday, October 4, 2016 (continued)

Unconventional Superconductors I

8	14:30	Andrew Boothroyd, Oxford University, United Kingdom (invited) **Evidence for charge stripe correlations in the layered cobaltate $La_{5/3}Sr_{1/3}CoO_4$**
9	15:00	Wentao Jin, JCNS at MLZ, Forschungszentrum Jülich, Germany **Magnetism in $Eu(Fe_{1-x}Ir_x)_2As_2$ Iron Pnictides Studied by Complementary Scattering Methods**
10	15:20	Sultan Demirdis, JCNS at MLZ, Forschungszentrum Jülich, Germany **SANS Study of Vortex Lattice Structure in Iron-Based Superconductors**
11	15:40	Petr Cermak, JCNS at MLZ, Forschungszentrum Jülich, Germany **Magnetoelastic hybrid excitations in non-centrosymmetric heavy fermion compound $CeAuAl_3$**

16:00 Coffee Break

16:30 Postersession

19:00 Dinner

Wednesday, October 5, 2016

Quantum/Frustrated spin systems I

12 9:00 Philipp Gegenwart, Augsburg University, Germany (invited)
Frustrated quantum magnets with large spin-orbit coupling

13 9:30 Erxi Feng, JCNS at MLZ, Forschungszentrum Jülich, Germany
Neutron scattering investigation of rare earth pyrochlore iridates

14 09:50 Lieh-Jeng Chang, National Cheng Kung University, Taiwan (invited)
Low temperature magnetic properties of $Yb_2Ti_2O_7$

15 10:20 Viviane Pecanha-Antonio, JCNS at MLZ, Forschungszentrum Jülich, Germany
Neutron Scattering Studies on $Yb_2Ti_2O_7$ powder

10:40 Coffee Break

Nanomagnetism II (Films)

16 11:20 Kristiaan Temst, University of Leuven, Belgium (invited)
Exchange bias in thin Co-CoO films: inner secrets revealed by unpolarized neutron reflectivity

17 11:50 Artur Glavic, Paul Scherrer Institut, Switzerland
Complex Magnetism in Manganite Heterostructures Probed with Polarized Neutrons

18 12:10 Amir Syed Mohd, JCNS at MLZ, Forschungszentrum Jülich, Germany
Connecting MARIA with an MBE setup: first (quasi) in-situ neutron reflectivity measurements on thin films

13:00 Lunch

Excursion and Conference Dinner

Thursday, October 6, 2016

Neutron Methods and Instrumentation I

19 9:00 Peter Böni, Technische Universität München, Germany (invited)
Instrumentation with Polarized Neutrons

20 9:30 Vladimir Hutanu, RWTH Aachen Iniversity and JCNS at MLZ, Forschungszentrum Jülich, Germany
tbd

21 9:50 Wolfgang Schmidt, JCNS at ILL, Forschungszentrum Jülich, Germany
Polarization analysis on the new IN12

22 10:10 Werner Schweika, JCNS, Forschungszentrum Jülich, Germany, and ESS, Sweden
MAGiC – the polarized single crystal diffractometer at the ESS

23 10:30 Stefan Mattauch, JCNS at MLZ, Forschungszentrum Jülich, Germany
MARIA - The high-intensity polarized neutron reflectometer of JCNS

10:50 Coffee Break

Functional Materials II (Multiferroics)

24 11:20 Manuel Angst, JCNS-2 and PGI-4 , Forschungszentrum Jülich, Germany (invited)
tbd

25 11:50 Andrew Sazonov, RWTH Aachen University and JCNS at MLZ, For--schungszentrum Jülich, Germany
Magnetic structure and magnetic domain population in multiferroic $Ba_2CoGe_2O_7$ by polarized neutron diffraction

26 12:10 Igor Zobkalo, Petersburg Nuclear Physics Institute, Russia
On the antisymmetric exchange in $TbMn_2O_5$ by polarized neutron diffraction

13:00 Lunch

Quantum/Frustrated Spin Systems II

27 14:30 Shang Gao, Paul Scherrer Institute, Switzerland (invited)
Spiral spin liquid in $MnSc_2S_4$

28 15:00 Christian Balz, Helmholtz-Zentrum Berlin, Germany (invited)
Physical realization of a new quantum spin liquid based on a novel frustration mechanism

29 15:30 Tobias Weber, MLZ, Technische Univerität München, Germany
Field-dependence of the helimagnon dispersion in the chiral magnet MnSi

16:00 Coffee Break

Thursday, October 6, 2016 (continued)

Unconventional Superconductors II

30 16:40 Stephane Raymond, CEA-Grenoble, (invited)
Ising incommensurate Spin Resonance of $CeCoIn_5$: A dynamical precursor of the Q-phase

31 17:10 Jitae Park, MLZ, Technische Universität München, Germany
Transition from sign-reversed to sign-preserved Cooper-pairing symmetry in sulfur-doped iron selenide superconductors

31a 17:30 Thomas Keller, MPI für Festkörperforschung, Germany (invited)
Magnetostriction and magnetostructural domains in antiferromagnetic $YBa_2Cu_3O_6$

18:00 Dinner

Friday, October 7, 2016

Neutron Methods and Intrumentation II

32 9:00 Arsen Goukassov, LLB, CEA-CNRS, France (invited)
Area Detectors for Single-Crystal Neutron Diffraction

33 9:30 Earl Babcock, JCNS at MLZ, Forschungszentrum Jülich, Germany
Latest results of practical testing of PASTIS with a TOF beamline

34 9:50 Kirill Nemkovskiy, JCNS at MLZ, Forschungszentrum Jülich, Germany
Simulation and optimization of a new focusing polarizing bender for the diffuse neutron scattering spectrometer DNS@MLZ

35 10:10 Ravil Sadykov, Institute for Nuclear Research, Russia
Nonmagnetic high pressure clamp cells for neutron scattering at low temperature and high magnetic fields

36 10:30 John Burgoyne, Oxford Instruments, United Kingdom
Cryogen-free high magnetic field and low temperature sample environments for neutron scattering - latest developments

10:50 Coffee Break

Functional Materials III (Multiferroics)

37 11:20 J. Alberto Rodriguez Velamazan, Institute Laue-Langevin, France (invited)
Magnetic interactions and magneto-electric coupling mechanisms in iron penta-halide hybrid compounds

38 11:30 Yinguo Xiao, JCNS at MLZ, Forschungszentrum Jülich, Germany
Spin-wave and electromagnon dispersions in multiferroic $MnWO_4$ as observed by neutron spectroscopy

39 12:10 Yusuke Kosaka, Hiroshima University, Japan
Homo-chiral crystal growth and chiral helimagnetism in $CsCuCl_3$

12:30 **Closing remarks, end of the workshop**

12:40 Lunch

Poster Presentations

2016-1
Kirill Nemkovskiy, JCNS at MLZ, Forschungszentrum Jülich, Germany
Recent developments at DNS, diffuse neutron scattering spectrometer with polarization analysis at MLZ

2016-2
Artem Feoktystov, JCNS at MLZ, Forschungszentrum Jülich, Germany
Upgrade of the KWS-1 Small-Angle Neutron Scattering Instrument

2016-3
Henrik Thoma, RWTH Aachen University and JCNS at MLZ, Germany
New setup for polarized neutron diffraction at instrument POLI at MLZ

2016-4
Martin Meven, RWTH Aachen University and JCNS at MLZ, Forschungszentrum Jülich, Germany
Studies on new magnetic and superconducting compounds with Hot Single Crystal Diffraction on HEiDi

2016-5
Jörg Voigt, JCNS-2 and PGI-4 , Forschungszentrum Jülich, Germany
T-REX: a bispectral direct geometry chopper spectrometer at the ESS

2016-6
Liming Wang, JCNS-2 and PGI-4, Forschungszentrum Jülich, Germany
Strain and electric field control of magnetism in supercrystalline iron oxide nanoparticle - $BaTiO_3$ composites

2016-7
Michael Smik, JCNS-2 and PGI-4, Forschungszentrum Jülich, Germany
Structural and magnetic properties of self-assembled 3D nanoparticle macrocrystals

2016-8
Artur Glavic, Paul Scherrer Institut, Switzerland
The Polarized Small Sample Reflectometer Estia at ESS

Joint JCNS Workshop & Flipper 2016

Modern Trends in Neutron Scattering from Magnetic Systems and Single-crystal Diffraction with Polarized Neutrons

Abstracts

Status: 23 September 2016

October 4, 2016, 9:10h Nanomagnetism I (Molecular Magnets & Nanoparticles)

Molecular Magnetic Materials:
Probing Magnetism at the local scale

Siddhartha DE,[1] Delphine GARNIER,[1] Alexandrine FLAMBARD,[1] **Rodrigue LESCOUEZEC**,[1] Karl RIDIER,[2] Grégory CHABOUSSANT,[2] Béatrice GILLON,[2] Corentin BOILLEAU,[3] Olivier CADOR,[3] Boris LE GUENNIC,[3] Karine COSTUAS,[3] Frank H. Kohler.[4]

[1] UPMC Sorbonne Univ., Institut Parisien de Chimie Moléculaire, Paris, France

[2]CEA-CNRS UMR12, Laboratoire Léon Brillouin, Gif-sur-Yvette, France

[3]Univ. Rennes, Institut des Sciences Chimiques de Rennes, Laboratory, Rennes, France

[4] Technische Universität München, Munich, Germany

The understanding of the magnetic properties at the atomic scale is crucial to design molecule-based magnetic materials with original properties. There are only a few experimental techniques that enable to probe the magnetism at the local scale. EPR spectroscopy provides information about the *g* tensors and hyperfine constants. X-ray magnetic circular dichroism (XMCD) gives access to local magnetic moments. Nuclear Magnetic Resonance (NMR) spectroscopy allows to probe very small amount of spin density in paramagnetic species. Polarized Neutron Diffraction (PND) has proven to be one of the most efficient tools to enlighten the magnetic interaction mechanisms in molecule-based materials. In the present study, we intend to show the complementarities between the NMR spectroscopy and the PND to probe the local magnetic structure of cyanide-based molecular materials. We also show that both techniques exhibit other interesting specific assets for the study of molecular-based materials: on the one hand NMR can provide accurate local structural information and on the other hand PND can be used to access the local magnetic anisotropy in molecular compounds.

[1] A. Flambard, F.H. Köhler, R. Lescouëzec, B. Revel, *Chem. Eur. J.*, **17**, 11567 (2011).
[2] N. Baumgärtel, A.Flambard, F.H. Köhler, R. Lescouëzec, *Inorg. Chem.*, **52**, 12634 (2013).
[3] K. Ridier, A. Mondal, C. Boilleau, O. Cador, B. Gillon, G. Chaboussant, B. Le Guennic, K. Costuas, R. Lescouëzec, *Angew. Chem.*, **128**, 4031 (2016).

E-mail of the corresponding author: Rodrigue.lescouezec@upmc.fr

October 4, 2016, 9:40h Nanomagnetism I (Molecular Magnets & Nanoparticles)

Antiferromagnetic molecular rings: spin density and dynamics

Tatiana GUIDI[1], Beatrice GILLON[2], Stefano CARRETTA[4], Sax MASON[3], Anne STUNAULT[3], Elena GARLATTI[4], Paolo SANTINI[4], Grigore TIMCO[5], Richard WINPENNY[5]

[1]ISIS facility, Rutherford Appleton Laboratory, United Kingdom

[2]Laboratoire Léon Brillouin CEA-CNRS, Saclay, France

[3]Institut Laue-Langevin, 71 avenue des Martyrs, 38042 Grenoble Cedex 9, France

[4]Dipartimento di Fisica, Università di Parma, I-43100 Parma, Italy

[5]School of Chemistry and Photon Science Institute,University of Manchester,Manchester, UK

Finite spin chains made of a few magnetic ions are the ultimate-size structures that can be engineered to perform spin manipulations for quantum information devices. Their spin structure is expected to show finite size effects and its knowledge is of great importance both for fundamental physics and applications. The experimental realization of finite spin chains is offered by the chemistry of antiferromagnetic molecular rings.

We have investigated the spin dynamics and local moment distribution of two prototypical members of this family of molecules, the homonuclear Cr_8 "closed" ring and the heteronuclear Cr_8Cd "open" ring. Homonuclear AF rings, like Cr_8, are characterized by a singlet ground state and periodic boundary conditions. The replacement of one Cr ion with a non-magnetic atom (Cd) breaks the cyclic symmetry with an open-boundary condition resulting in an effective model system for an "open" finite chain. We used polarized neutron diffraction for determining the experimental spin distribution in Cr_8Cd in non-zero spin ground states induced by applying a magnetic field at low temperature [1]. From the data refinement it is found that most of the spin density is located at the Cr position. Moreover, there is an accumulation of spin density at the edges of the open ring and negligible spin density at the Cr positions further away from the Cd. The distribution of local magnetization is consistent with a non collinear spin arrangement as predicted by theory for an even AF finite open chain. This is in contrast with the uniform spin distribution observed in the parent closed chain and the collinear arrangement in odd open chains.

[1] T. Guidi, B. Gillon, S. A. Mason, E. Garlatti, S. Carretta, P. Santini, A. Stunault, R. Caciuffo, J. van Slageren, B. Klemke, A. Cousson, G. A. Timco and R. E. P. Winpenny, Nature Communications **6**, 7061 (2015).

E-mail of the corresponding author: tatiana.guidi@stfc.ac.uk

October 4, 2016, 10:30h Nanomagnetism I (Molecular Magnets & Nanoparticles)

Exchange bias effect in Au-Fe_3O_4 dumbbell nanoparticles induced by the charge transfer from gold

Mikhail FEYGENSON[1]

[1] Jülich Centre for Neutron Science, Forschungszentrum Jülich, 52428 Jülich, Germany

We have studied the origin of the exchange bias effect in the Au-Fe_3O_4 dumbbell nanoparticles in two samples with different sizes of the Au seed nanoparticles (4.1 and 2.7 nm) and same size of Fe_3O_4 nanoparticles (9.8 nm). The magnetization, small-angle neutron-scattering, synchrotron x-ray diffraction, and scanning transmission electron microscope measurements determined the antiferromagnetic FeO wüstite phase within Fe_3O_4 nanoparticles, originating at the interface with the Au nanoparticles. The interface between antiferromagnetic FeO and ferrimagnetic Fe_3O_4 is giving rise to the exchange bias effect. The strength of the exchange bias fields depends on the interfacial area and lattice mismatch between both phases. We propose that the charge transfer from the Au nanoparticles is responsible for a partial reduction of the Fe_3O_4 into the FeO phase at the interface with Au nanoparticles. The Au-O bonds are formed, presumably across the interface to accommodate an excess of oxygen released during the reduction of magnetite.

[1] M. Feygenson et al, Phys. Rev. B, **92**, 054416 (2015).

E-mail of the corresponding author: m.feygenson@fz-juelich.de

Neutron scattering studies on Fe_2P-based magnetocaloric materials

Niels VAN DIJK[1], Ekkes BRÜCK[1]

[1]Delft University of Technology, Radiation Science & Technology,
Mekelweg 15, 2629 JB Delft, The Netherlands.

In the last two decades growing research efforts have focused on the development of magnetocaloric materials. Materials that show a magnetocaloric effect near room temperature are excellently suited for magnetic cooling and for energy conversion of waste heat into electricity. For systems that show a ferromagnetic transition that is accompanied by latent heat a giant magnetocaloric effect is found. Since our discovery of a giant magnetocaloric effect in $(Fe,Mn)_2(P,X)$ compounds (X = As, Ge, Si) [1] we have focused our attention on optimizing the materials properties for magnetic cooling applications and on the fundamental understanding of the origin of the unusual magnetoelastic transition [2]. Compositional tuning of the Fe_2P-based alloys allows for a detailed control of the operating temperatures and performance characteristics. Neutron scattering [3-7] has been applied to unravel the nature of the magnetic order, the competition with other types of magnetic order, the Fe/Mn and P/X site occupation at the different crystallographic sites in the Fe_2P structure and the short-range magnetic order.

[1] O. Tegus, E. Brück, K. H. J. Buschow, F. R. de Boer, Nature **415**, 150 (2002).
[2] N. H. Dung *et al.*, Adv. Energy Mater. **1**, 1215 (2011).
[3] N. H. Dung *et al.*, Phys. Rev. B **86**, 045134 (2012).
[4] Z. Q. Ou *et al.*, J. Magn. Magn. Mater. **340**, 80 (2013).
[5] X. F. Miao *et al.*, Phys. Rev. B **89**, 174429 (2014).
[6] X. F. Miao *et al.*, Appl. Phys. Lett. **107**, 0242403 (2015).
[7] X. F. Miao *et al.*, Phys. Rev. B, in press.

E-mail of the corresponding author: n.h.vandijk@tudelft.nl

October 4, 201, 11:50h Functional Materials I

Multiparametric studies on magnetocaloric compounds in the system $Mn_{5-x}Fe_xSi_3$

Karen FRIESE[1], Paul HERING[1], Mamuka CHIKOVANI[1], A. GRZECHNIK[2], Martin MEVEN[2], Anatoliy SENYSHYN[3], Jörg PERSSON[1], Thomas BRÜCKEl[1], Jörg VOIGT[1]

[1]Jülich Centre for Neutron Science JCNS-2 and Peter Grünberg Institut PGI-4, Forschungszentrum Jülich GmbH, Jülich, Germany

[2] Institute for Crystallography, RWTH Aachen University, Jägerstr. 17-19, Aachen, Germany

[3] Heinz Maier-Leibnitz Zentrum, Technische Universität München, Garching, Germany

Magnetic cooling based on the magnetocaloric effect could replace conventional vapor compression cooling, as it has a potentially lower energy consumption and does not rely on environmental hazardous gases. The compounds within the system $Mn_{5-x}Fe_xSi_3$ undergo a variety of magnetic phase transitions at different temperatures depending on their iron content. The iron is distributed on at least one mixed Mn/Fe site and one pure iron site [1,2]. Magnetic and structural properties of the compounds in the system were investigated macroscopically and on an atomic scale. Compounds with low iron content order antiferromagnetically, while compounds with higher iron content show ferromagnetic order. Of special interest is $MnFe_4Si_3$ as it has a phase transition to a ferromagnetically ordered phase at approximately 300 K. It displays a strong anisotropy of the magnetization and the magnetocaloric effect with the easy axis of magnetization in the *a,b*-plane. Refinements of combined neutron and X-ray single crystal diffraction data introduce a new structural model for the compound with x=4 in space group *P-6* characterized by partial ordering of Mn and Fe into layers perpendicular to *c* on one of the transition metal sites. The magnetic structure was refined in the magnetic spacegroup *Pm`*. It shows that the spins on the sites with mixed occupancy of Mn and Fe are aligned in the *a,b*-plane. A significant magnetic moment for the site exclusively occupied by iron could not be unambiguously refined [3]. The thermal evolution of the lattice parameters of the compounds in the system exhibits an anisotropic behavior and clearly reflects the onset of magnetic ordering.

We performed multiparametric studies as a function of temperature, chemical composition and hydrostatic pressure in the system at laboratory, synchrotron and neutron sources. The aim for these studies was twofold: we wanted to elucidate, - on one hand - whether the influence of hydrostatic and "chemical pressure" (i.e. through the variation of composition) is equivalent, and - on the other hand – we wanted to learn about the magnetic and associated structural transitions varying these thermodynamic parameters to gain deeper insight into the coupling of lattice and spin degrees of freedom. Conspicuous similarities of the observed behavior when compared to other magnetocaloric systems will be pointed out.

[1] Binczyska, at al., Phys. Stat. Sol., Sect. A, 19, 13-17 (1973).
[2] Songlin, et al., J. Alloys Comp. 334, 249-252 (2002).
[3] Hering et. al., Chem. Materials 27, 7128-7136 (2015).

E-mail of the corresponding author: k.friese@fz-juelich.de

Static correlated spin fluctuations in single crystal $Fe_{65}Ni_{35}$ INVAR alloy, studied using small-angle neutron scattering with polarization analysis

Ross STEWART[1], Sean GIBLIN[2], Jon TAYLOR[3]

[1]ISIS Neutron and Muon Facility, Didcot, UK

[2]Departement of Physics, University of Cardiff, UK

[3]European Spallation Source, Lund, Sweden

The origin of the INVAR effect, whereby certain ferromagnetic alloys exhibit near zero thermal expansion around room temperature, is still not understood. Various models have been put forward, including two-state models, canted moments and longitudinal spin-fluctuations, but experimental evidence is lacking, if not opposed to the theories.

Some time ago, the group of Menshikov and co-workers [1] used polarized neutrons (D5, ILL) to measure powder samples of INVAR ($Fe_{65}Ni_{35}$) and off-INVAR ($Fe_{50}Ni_{50}$) and found considerable small-angle magnetic neutron scattering for the INVAR alloy – and none for the off-INVAR alloy – indicating the presence of transverse magnetization components which were inferred to come from low-spin Fe clusters.

We have now used the D33 polarized SANS diffractometer with 3He spin-analysers to measure single-crystal FeNi alloys with the same concentrations as the study of Menshikov. We confirm the presence of static spin-fluctuations in INVAR – both longitudinal and transverse – in a single magnetic domain. These fluctuations also are present in the off-INVAR concentration, but are significantly suppressed. While the transverse magnetization in INVAR does indeed appear to be associated with finite clusters, we find that the range of these is much larger than Menshikov found – extending to ~100 Å. Interestingly, the longitudinal fluctuations appear only weakly correlated with a flat dependence on momentum transfer.

Clearly this is more evidence that the presence of static fluctuations is likely to be associated to the INVAR effect.

[1] Menshikov, A. Z. & Schwinger, J. The transverse magnetization components in the ground state of invar γ-$Ni_{1-c}Fe_c$ alloys. Solid State Communications, **100**, 251–255 (1996).

Email of corresponding author: ross.stewart@stfc.ac.uk

Magnetic structures and magnetoelastic coupling of Fe-doped hexagonal manganites $LuMn_{1-x}Fe_xO_3$ ($0 \leq x \leq 0.3$)

Zhendong FU[1], Harikrishnan S. NAIR[2], Yinguo XIAO[3], Anatoliy SENYSHYN[4,5], Vladimir Y. POMJAKUSHIN[6], Erxi FENG[1], Yixi SU[1], W. T. JIN[1], and Thomas BRÜCKEL[3]

[1]Jülich Centre for Neutron Science JCNS at Heinz Maier-Leibnitz Zentrum MLZ, Forschungszentrum Jülich GmbH, Garching, Germany

[2]Highly Correlated Matter Research Group, Physics Department, University of Johannesburg, South Africa

[3]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany

[4]Institute for Material Science, Darmstadt University of Technology, Darmstadt, Germany

[5]Forschungsneutronenquelle Heinz-Maier Leibnitz FRM-II, Technische Universität München, Garching, Germany

[6]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, Villigen, Switzerland

We have studied the crystal and magnetic structures of Fe-doped hexagonal manganites $LuMn_{1-x}Fe_xO_3$ (x = 0, 0.1, 0.2, and 0.3) by using bulk magnetization and neutron powder diffraction methods. The samples crystalize consistently in a hexagonal structure and maintain the space group $P6_3cm$ from 2 to 300 K. The Néel temperature T_N increases continuously with increasing Fe-doping. In contrast to a single Γ_4 representation in $LuMnO_3$, the magnetic ground state of the Fe-doped samples can only be described with a combination of Γ_3 ($P6_3'cm'$) and Γ_4 ($P6_3'c'm$) irreducible representations, whose contributions have been quantitatively estimated. The drastic effect of Fe-doping is highlighted by composition-dependent spin reorientations. A phase diagram of the entire composition series is proposed based on the present result and those reported in literature. Our result demonstrates the importance of tailoring compositions in increasing magnetic transition temperatures of multiferroic systems [1].

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E-mail of the corresponding author: z.fu@fz-juelich.de

Evidence for charge stripe correlations in the layered cobaltate $La_{5/3}Sr_{1/3}CoO_4$

P. Babkevich[1], P. G. Freeman[2], M. Enderle[3], D. Prabhakaran[4], **A. T. Boothroyd[4]**

[1]Institute of Condensed Matter Physics (ICMP), EPFL, Lausanne, Switzerland

[2]Jermiah Horrocks Insititute, University of Central Lancashire, Preston, U.K.

[3]Institut Laue–Langevin, Grenoble, France

[3]University of Oxford, Department of Physics, Oxford, U.K.

Stripe phases are a form of complex matter involving coupled spin and charge order. They are observed in certain copper oxide superconductors, as well as in layered nickelates and manganites. Some theoreticians believe that stripe fluctuations are important to the mechanism of cuprate high temperature superconductivity. A key piece of evidence for this idea is the universal form of the magnetic spectrum of hole-doped copper oxide superconductors as measured by neutron scattering, which is in the shape of an hourglass. This type of spectrum emerges naturally from a stripe-ordered ground state.

In 2011, an insulating, layered cobalt oxide $La_{5/3}Sr_{1/3}CoO_4$ was also found to have an hourglass magnetic spectrum [1]. At the time, there was indirect evidence for stripe order in this material, but direct evidence was missing. The failure to observe stripes in layered cobaltates in experiments with several different techniques motivated an alternative stripe-free model to explain the hourglass spectrum [2].

Here we present evidence for charge stripes in $La_{5/3}Sr_{1/3}CoO_4$ from polarized neutron diffraction measurements [3]. The results show that the magnetic ground state can be described interpreted in terms of a nanoscopic coexistence of (i) spin- and charge-stripe order, and (ii) checkerboard charge order of Co^{2+} and Co^{3+} However, the measurements reinforce the hypothesis of charge stripe correlations as the underlying mechanism for the hourglass magnetic spectrum in the cobaltates and, by extension, in the cuprate superconductors.

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E-mail of the corresponding author: a.boothroyd@physics.ox.ac.uk

Magnetism in $Eu(Fe_{1-x}Ir_x)_2As_2$ Iron Pnictides Studied by Complementary Scattering Methods

Wentao JIN[1], Yinguo XIAO[2], Yixi SU[1], Shibabrata NANDI[3], Wenhe JIAO[4], Martin MEVEN[1, 5], Andrew SAZONOV[1, 5], Gareth NISBET[6], Sultan DEMIRDIS[1], Erxi FENG[1], Guanghan CAO[7], Thomas BRÜCKEL[1, 2]

[1] Jülich Center for Neutron Science JCNS at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, 85748 Garching, Germany

[2] Jülich Center for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

[3] Department of Physics, Indian Institute of Technology, Kanpur 208016, India

[4] Zhejiang University of Science and Technology, Hangzhou 310023, China

[5] RWTH Aachen University, Institut für Kristallographie, 52056 Aachen, Germany

[6] Diamond Light Source Ltd., Oxfordshire OX11 0DE, United Kingdom

[7] Department of Physics, Zhejiang University, Hangzhou 310027, China

Doped $EuFe_2As_2$ is a unique representative of the 122 type family of iron based superconductors due to the two magnetic sublattices and the strong coupling between spin-, lattice- and charge degrees of freedom. In present work, the magnetic ground states of the localized Eu^{2+} spins in underdoped, nonsuperconducting $Eu(Fe_{0.94}Ir_{0.06})_2As_2$ and optimally doped, superconducting $Eu(Fe_{0.88}Ir_{0.12})_2As_2$ (T_{SC} = 22 K) were investigated by polarized and unpolarized single-crystal neutron diffraction measurements, respectively [1, 2]. The Eu^{2+} spins in the underdoped (x = 0.06) crystal were found to order within the *ab* plane in the A-type antiferromagnetic (AFM) structure. However, the Eu^{2+} spins in the optimally doped (x = 0.12) crystal were found to be ferromagnetically aligned along the *c* direction with an ordered moment of 7.0(1) μ_B at 2.5 K, coexisting with the bulk superconductivity. In addition, compared with the parent compound $EuFe_2As_2$, which shows the AFM order of the Fe^{2+} moments below $T_{N,Fe}$ = 190 K, $T_{N,Fe}$ was significantly suppressed to 85(2) K and completely suppressed, by 6% and 12% Ir doping, respectively. Most strikingly, the x-ray resonant magnetic scattering measurements on the underdoped (x = 0.06) crystal revealed the magnetic polarization of the 5*d* Ir dopant atoms and suggested a possible interplay between the localized Eu^{2+} moments and the conduction *d* electrons on the FeAs layers.

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E-mail of the corresponding author: w.jin@fz-juelich.de

SANS Study of Vortex Lattice Structure in Iron-Based Superconductors

S. DEMIRDIS[1], Cornelis J. VAN DER BEEK[2], S. MÜHLBAUER[3], Y. SU[1], Th. WOLF[4]

[1]Jülich Center for Neutron Science (JCNS), Forschungszentrum Jülich GmbH, JCNS at MLZ, Lichtenberstr, D-85747 Garching, Germany
[2]Laboratoire des Solides Irradiés, CNRS UMR 7642
& CEA/DSM/IRAMIS, Ecole Polytechnique, 91128 Palaiseau cedex, France
[3]Technische Universität München, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II) D-85748 Garching, Germany
[4]Karlsruher Institut für Technologie, Institut für Festkörperphysik, D-7602 Karlsruhe, Germany

We have used small-angle neutron scattering to study the vortex lattice (VL) in high quality optimally doped $(Ba_{1-x}K_x)Fe_2As_2$ single crystals. Where previous SANS studies, as well as real-space imaging methods applied to the study of the vortex ensemble in single crystalline $(Ba_{1-x}K_x)Fe_2As_2$, Co-, and P-substituted $BaFe_2As_2$, have consistently reported highly disordered vortex structures [1]-[7], the present SANS study reveals sharp vortex lattice Bragg peaks. This is the first iron-based superconductor, apart from the ``clean'' end-compound KFe_2As_2 [8] in which an triangular VL is observed.
In this contribution we present SANS data taken in a magnetic field ranging between 0.25 and 2 Tesla, performed on optimally doped $(Ba_{1-x}K_x)Fe_2As_2$. The data show clear resolution-limited sharp Bragg spots, indicating the existence of a long-range ordered Bragg glass in this compound. The magnetic field dependence of the vortex structure factor, obtained by correction of the intensity by the field-dependent vortex form factor, shows a sharp drop well below the second critical field. This vortex structural transition shows clear correlations with features observed around the so-called ''second magnetization peak'' observed in isothermal hysteresis loop measurements, and the behavior of magnetic hysteresis between zero-field cooling and field-cooling.

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E-mail of the corresponding author: s.demirdis@fz-juelich.de

Magnetoelastic hybrid excitations in non-centrosymmetric heavy fermion compound $CeAuAl_3$

Petr Čermák[1], Astrid Schneidewind[1], Christian Franz[2,3], Rudolf Schönmann[2], Oleg Sobolev[2,4], and Christian Pfleiderer[2]

[1]Jülich Centre for Neutron Science, MLZ, Garching, Germany

[2]Physik-Department, Technische Universität München, Garching, Germany

[3]FRM II, Technische Universität München, Garching, Germany

[4]Institute for Physical Chemistry, Georg-August-University, Göttingen, Germany

Hybridized excitations that comprise of well-understood collective modes have received increasing interest as the possible origin of unconventional materials properties and novel functionalities. In strongly correlated electron systems the effects of electron-phonon interactions are typically neglected, being deemed not important for an overall understanding. However, recently neutron time-of-flight spectroscopy on polycrystalline $CeCuAl_3$ have provided putative evidence for a vibron, i.e., a combined crystal field – optical phonon excitation [1], whereas no such excitation could be detected in the isostructural sister compound $CeAuAl_3$ [2]. This raises the question to what extent such hybrid modes represent a generic property of the series of Ce*T*Al_3 compounds (*T*: transition metal element) or even f-electron systems in general. To pursue this question, we have revisited the properties of $CeAuAl_3$ using triple axis neutron spectroscopy on a float-zoned high-quality single-crystal. In contrast with early conjectures, we find two pieces of strong evidence suggesting strong crystal field – phonon interactions and the formation of a novel hybrid mode. First, at the zone center there is clearly a hybridized excitation between the crystal-field and phonons, which appears to be in general agreement with vibronic bound state reported for $CeCuAl_3$ [1]. Second, we observe a distinct anticrossing of the longitudinal acoustic phonon with the $\Gamma_7^{(1)}$ crystal field level. To the best of our knowledge such an anti-crossing has not been reported before. Both phenomena are in agreement with observed dominant phonon scattering processes by the localized 4f electrons [3]. Taken together, our results suggest that strongly hybridized crystal field – phonon excitations may, in fact, be rather common in f-electron compounds.

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E-mail of the corresponding author: p.cermak@fz-juelich.de

Frustrated quantum magnets with large spin-orbit coupling

Philipp GEGENWART

Experimentalphysik VI, Center for Electronic Correlations and Magnetism, Augsburg University, Germany

Heavy transition metal oxides with large spin orbit coupling and threefold coordinated effective ½ spins are discussed as promising materials to realize a particular bonding dependent anisotropic exchange called Kitaev interaction, which supports topological quantum spin liquid behavior. I will present experiments on two-and three-dimensional honeycomb iridates and rhodates.

I will also discuss recent results on the quantum spin liquid candidate $YbMgGaO_4$ with effective ½ spins on a perfect triangular lattice.

Work in collaboration with Yuesheng Li, A. Tsirlin, F. Freund, A. Jesche, R. Manna, S. Manni, I. Pietsch, S. Bachus, Y. Tokiwa, Yogesh Singh, S. Choi, S. Williams, R. Coldea, P. Khuntia, M. Baenitz.

E-mail of the corresponding author: philipp.gegenwart@physik.uni-augsburg.de

Neutron scattering investigation of rare earth pyrochlore iridates

Erxi FENG[1*], Yixi SU[1], Thomas WOLF[2], Thomas BRÜCKEL[3,1]

[1]Jülich Centre for Neutron Science JCNS at MLZ, Forschungszentrum Jülich, D-85747 Garching, Germany

[2]Institut für Festkörperphysik, Karlsruhe Institute of Technology KIT, D-76021 Karlsruhe, Germany

[3]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA- FIT, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

The pyrochlore iridate compounds $A_2Ir_2O_7$, where the A sites are occupied by rare-earth (RE) local moments and the B site by 5d transition metal Ir^{4+} ions with strongly spin-orbit coupled (SOC) electrons, have attracted strong interests because they sit in the intersection of the two emerging research fields in condensed matter physics: quantum spin ice [1] and correlated topological phases [2]. An intriguing "all-in-all-out" magnetic order at the Ir^{4+} sites has been found in recent resonant magnetic X-ray scattering experiments on $Eu_2Ir_2O_7$ [3] and $Sm_2Ir_2O_7$ [4] respectively. The magnetic order of Ir^{4+} is suggested being responsible for the metal-to-insulator transition observed in earlier transport and magnetization studies [5]. However, the interplay between the Ir^{4+} magnetic order and the localized magnetism of RE ions at very low temperatures has not been systematically studied, except the cases in the Tb^{3+} and Er^{3+} based compounds [6]. We have recently synthesized a series of high quality polycrystalline samples covering a full range of RE ions by solid-state synthesis methods. X-ray and high-resolution neutron powder diffraction were employed to determine sample quality. Heat capacity and magnetization were measured to investigate their low temperature physical properties. Comprehensive polarized neutron diffraction and inelastic neutron scattering experiments were performed to investigate their magnetic ground states in the mK regime. An updated phase diagram based mainly on new neutron scattering studies will be presented. Our results point out the important role of both RE single-ion anisotropy and the Ir-RE coupling. In metallic $Pr_2Ir_2O_7$, evidence for an exotic ground state has been obtained [7].

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Low temperature magnetic properties of $Yb_2Ti_2O_7$

Lieh-Jeng CHANG

Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan.

$Yb_2Ti_2O_7$ with pyrochlore structure shows ferromagnetic phase transition at T_c = ~0.2 K. Above T_c, the compound is realized to be a quantum spin ice state which exhibits two-in-two-out classical spin ice spin configuration together with the quantum fluctuation of the magnetic components perpendicular to the <111> Ising axis. Below T_c, Yb^{3+} possesses moment of ~1.3 μB and points to [100] orientation. However, this ferromagnetic ground state is sample-dependent and can only be observed in high quality single crystals or polycrystalline samples [1]. This fact leads the difficulty of the study of $Yb_2Ti_2O_7$ in the past one and a half decades, and causes the constructions of theoretical frames incompletely.

In this talk, I will be on behalf of our collaborative group to present our studies on our $Yb_2Ti_2O_7$ crystal which is still the unique crystal showing ferromagnetic ground state in the world until now. Besides our earlier studies by using polarized neutron scattering, μSR [2], low temperature magnetization [3] and heat capacity, synchrotron x-rays, we have also carried out inelastic neutron scattering experiments to further investigate low energy excitations in the same $Yb_2Ti_2O_7$ crystal. Below T_c, a broad mode at ~0.2 meV with little dispersion is observed along the <111> direction on LET, ISIS. This mode corresponds to the localized quantum spin ice monopole excitations. While at the pinch point (111), the collective monopole excitations with energy gap ~0.04 meV is seen in the backscattering spectra from DNA, J-PARC. On the other hand, at ~0.35 K, i.e. above T_c, only gapless continuum excitations are revealed in the experiments. TEM had also been adapted to clarify the sample-dependent issue [4].

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E-mail of the corresponding author: ljchang@mail.ncku.edu.tw

Neutron Scattering Studies on $Yb_2Ti_2O_7$ powder

Viviane PECANHA-ANTONIO[1], Erxi FENG[1], Yixi SU[1] , Thomas BRÜCKEL[1,2]

[1]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Lichtenbergstr. 1, 85748 Garching, Germany

[2]Jülich Centre for Neutron Science (JCNS) and Peter Grünberg Institut (PGI), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

In this talk, we present our studies of a powder sample of $Yb_2Ti_2O_7$. A well-characterised stoichiometric sample is particularly important when studying this compound due to the strong sample-dependence of its behaviour [1,2]. We have proven the stoichiometry of our sample to the greatest extent possible with the powder neutron diffraction technique and shown that it presents the low temperature specific heat anomaly characteristic of pristine samples of $Yb_2Ti_2O_7$. We report neutron diffraction data that clearly display a phase transition to a long-range, ferromagnetic state at T_C=0.28 K, in disagreement with the recent allegations that the phase transition seen in neutron scattering is unrelated to that seen in heat capacity measurements [3,4]. The observed absence of the (200) magnetic Bragg peak in our work indicates that the canting angle of the spins out of the cubic axis is much smaller than previously reported [3], making the structure a *quasi-collinear* ferromagnet with an ordered moment of 0.87(2) μ_B. Our results therefore raise questions about the existence of gapless magnetic excitations as a universal feature of S_{eff}=1/2 Yb-based pyrochlores [5]. Additionally, we show that our sample does not adopt any other symmetry-allowed l*ong-range* magnetic order below T_C and that in fact we observe no evidence of multiple phase transitions or a multi-step ordering process [6].

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E-mail of the corresponding author: v.pecanha.antonio@fz-juelich.de

October 5, 2016, 11:20h Nanomagnetism II (Films)

Exchange bias in thin Co-CoO films: inner secrets revealed by polarized neutron reflectivity

Kristiaan TEMST[1], Enric MENENDEZ[1], Joost DEMETER[1], Roland STEITZ[2], Andrew R. WILDES[3], Amir S. MOHD[4], Alexandros KOUTSIOUMPAS[4], Earl BABCOCK[4], Stefan MATTAUCH[4], André VANTOMME[1]

[1]Instituut voor Kern- en Stralingsfysica, KU Leuven, Belgium

[2]Helmholtz-Zentrum Berlin fur Materialien und Technologie, Berlin, Germany

[3]Institut Laue-Langevin, Grenoble, France

[4]Jülich Centre for Neutron Science at MLZ, Garching, Germany

Exchange bias (EB) is the interfacial coupling between a ferromagnet (FM) and an antiferromagnet (AFM). It induces a unidirectional magnetic anisotropy in the FM upon cooling in a magnetic field. Since its discovery, this phenomenon has been widely studied in bilayers, core-shell clusters, and patterned films. Polarized neutron reflectivity has played an important role in the study of exchange bias, in particular for the identification of the unusual asymmetry in the magnetization reversal mechanism that is present in e.g. Co/CoO and Fe/FeF_2. Recently we explored a new approach, namely EB systems produced by oxygen ion implantation into Co thin films [1]. The oxygen implantation leads to the local formation of antiferromagnetic CoO buried within the ferromagnetic Co layer, thus creating multiple internal FM/AFM interfaces. Polarized neutron reflectivity allows reconstructing the magnetization depth profile in such an implanted system.

Ferromagnetic Co layers with a thickness of 100 nm were prepared by molecular beam epitaxy. These layers were implanted with oxygen ions using an implantation energy of 60 keV. A strong exchange bias shift is observed once a minimum oxygen fluence has been implanted. We have investigated the correlation between the implantation depth profile and the magnetic depth profile using specular polarized neutron reflectometry (PNR) and found that the local Co magnetization varies in depth as a result of the Gaussian-like implantation profile. PNR experiments also indicated that the implanted exchange bias system does not have the asymmetric magnetization reversal modes typically observed in Co/CoO bilayers.

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E-mail of the corresponding author: Kristiaan.Temst@kuleuven.be

Complex Magnetism in Manganite Heterostructures Probed With Polarized Neutrons

Artur Glavic[1], Hemant Dixit[2], Valentino R. Cooper[3], Kirill Nemkovskiy[4], Adam A. Aczel[5]

[1]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

[2]GLOBALFOUNDRIES Engineering Private Limited, 9th Floor, N1 Building, Manyata Embassy Business Park, Bangalore, 560045 INDIA

[3]Materials Science and Technology Division, Oak Ridge National Laboratory, PO Box 2008, MS6114, 37831 Oak Ridge, TN, USA

[4]Jülich Center for Neutron Science (JCNS) at Hienz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Lichtenbergstraße 1, 85748 Garching, Germany

[5]Quantum Condensed Matter Division, Oak Ridge National Laboratory, PO Box 2008, MS6475, 37831 Oak Ridge, TN, USA

An intrinsic property of antiferromagnetic (AFM) systems is the overall compensation of the atomic magnetic moments that prohibits the direct interaction of the spin-lattice with an external magnetic field. To overcome this limitation we have created artificial spin structures by heteroepitaxy between two bulk AFM $SrMnO_3$ (SMO) and $NdMnO_3$ (NMO). Thin superlattices with 1:2 ratio of SMO:RMnO$_3$ (R=Lanthanide) are known to exhibit ferromagnetism (FM) due to electronic reconstruction[1,2]. We demonstrate that charge transfer at the interface can be used to create thin FM layers adjacent to *A*-type AFM using thicker NMO layers as a magnetic *"handle"* to couple to the adjacent AFM spins [3].

Neutron scattering is the ideal probe for this complex magnetic state when combined with atomic layer controlled thin film growth. We will present polarized neutron reflectometry data (MR@SNS) that shows the existence of FM around the thin SMO layers. Presence and interlayer coupling of the AFM state was measured with unpolarized neutron diffraction (HB1A@HFIR), which proofs the presence of the anticipated magnetic ordering [3]. Recent xyz-polarization analysis data (DNS@MLZ) was taken to analyze spin direction in the AFM state and measure the influence of a small cooling field on the AFM ordering.

The results show that it's possible to analyze novel complex magnetic order in thin heterostructures with neutron scattering, not accessible with other techniques, using specifically designed layer structures.

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E-mail of the corresponding author: *artur.glavic@psi.ch*

Connecting MARIA with an MBE setup: first (quasi) in-situ neutron reflectivity measurements on thin films

Amir SYED MOHD[1] , Sabine PÜTTER[1], Stefan MATTAUCH[1], Alexander WEBER[1], Alexandros KOUTSIOUBAS[1], Harald SCHNEIDER[1], and Thomas BRÜCKEL[1,2]

[1] Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Lichtenbergstr. 1, 85747 Garching, Germany

[2]Jülich Centre for Neutron Science (JCNS) and Peter Grünberg Institut, JCNS-2, PGI-4: Scattering Methods, Forschungszentrum Jülich GmbH, Jülich, Germany

MARIA is a dedicated instrument for neutron reflectometry of thin films. However, due to limited space a UHV system for thin film growth and in-situ measurements cannot be placed on-site. Hence, up to now ultra thin films which are sensitive to ambient air have been fabricated in the MBE system located in the thin film laboratory nearby and were covered by protecting cap layers in-situ. However these layers may change the physical properties of the sample, which is undesirable and prevents from further manipulation of the sample, e.g. growth of additional layers.

Recently, we have solved this problem by developing a handy mini UHV-chamber which is capable for both, sample transfer and quasi in-situ measurements at the neutron reflectivity instrument, respectively. Quasi in-situ polarized neutron reflectivity (PNR) measurements can be performed at room temperature in magnetic fields of up to 600 mT at MARIA.

Our solution consists of a DN CF-40 cube with two opposing sapphire windows for the neutron beam, a combined non evaporable getter and ion pump for keeping the vacuum, a wobble stick, which is needed for in-situ sample transfer and also serves as sample holder for samples of up to 1 cm^2 and a valve for sample exchange by mounting the chamber on the MBE system. The pressure in the transfer chamber is kept in the 10^{-10} mbar range during transport and PNR measurement.

We present first polarized neutron reflectivity measurements on Co thin films at room temperature at different magnetic fields in the Q-range up to 0.2 $Å^{-1}$.

Booking of the access to the MBE system as well as the transport chamber is possible via the MLZ user office system in combination with an application for a beam time at neutron instruments like MARIA.

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E-mail of the corresponding author: a.syed.mohd@fz-juelich.de

October 6, 2016, 9:00h Neutron Methods and Instrumentation I

Instrumentation with Polarized Neutrons

Peter BÖNI[1]

[1]Physik-Department E21, Technische Universität München, D-85748 Garching, Germany

Neutron scattering with polarization analysis is an indispensable tool for the investigation of novel materials exhibiting electronic, magnetic, and orbital degrees of freedom. In addition, polarized neutrons are necessary for neutron spin precession techniques that path the way to obtain extremely high resolution in space and time. Last but not least, polarized neutrons are being used for fundamental studies as well as for neutron imaging.

Typically, neutron beam lines are simply adapted for polarized beam applications by adding polarization equipment leading usually to unacceptable losses in neutron intensity. Recently, more and more beam lines are designed such that an optimum use of polarized neutrons is facilitated. In addition, marked progress has been obtained in the technology of ^{3}He polarizers and in improving the reflectivity and polarization of the polarizing supermirrors with large critical angles. Therefore, if properly designed, only factors of approximately 2-3 in neutron intensity are lost when compared with the use of unpolarized neutrons.

In my presentation, I will give a short overview about the various polarization techniques available. Then I shall discuss various routes of how to equip an existing beam line with a polarized beam option. Finally, possibilities of how to improve the polarization of neutron beams and how to implement polarization in the design of new beam lines shall be discussed.

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E-mail of the corresponding author: pboeni@frm2.tum.de

October 6, 2016, 9:50h Neutron Methods and Instrumentation I

Polarization analysis on the new IN12

Wolfgang SCHMIDT[1], Karin SCHMALZL[1], Stephane RAYMOND[2], Thomas BRÜCKEL[3]

[1]Forschungszentrum Jülich, JCNS at ILL, Grenoble, France

[2]CEA-Grenoble, INAC SPSMS MDN, Grenoble, France

[3]Forschungszentrum Jülich, JCNS, Jülich, Germany

IN12, a three-axis spectrometer for cold neutrons, is operated as a CRG-instrument from the Jülich Centre for Neutron Science (JCNS) at the Institute Laue Langevin in Grenoble. In the framework of the Millenium Program of the ILL IN12 has been relocated to a new position at the end of a new guide. Along with this relocation the whole primary spectrometer has been upgraded with new state-of-the-art components [1].

For the use of polarized neutrons a new transmission polarizer (cavity) has been installed in the neutron guide, mounted on a guide changer together with a standard guide element. This guarantees high intensities and an easy change from non-polarized to polarized mode.

Together with a new spin flipper and a focusing Heusler analyser IN12 presents state-of-the-art techniques for advanced polarized neutron experiments. Polarization analysis with high magnetic fields on the sample as well as a Cryopad set-up can be offered for measurements.

We will present details of the relevant neutron optical components and also show results from polarized experiments on the refurbished IN12 spectrometer.

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E-mail of the corresponding author: w.schmidt@fz-juelich.de

October 6, 2016, 10:10h Neutron Methods and Instrumentation I

MAGiC - the polarized single crystal diffractometer at the ESS

Xavier FABRÈGES[1], Sergey KLIMKO[1], Arsen GOUKASOV[1], Uwe FILGES[2], Michel KENZELMANN[2], **Werner SCHWEIKA[3,4]**

[1] Laboratoire Léon Brillouin, CEA-CNRS, Gif-sur Yvette, France

[2] Paul Scherrer Institut, LDM, Villigen PSI, Switzerland

[3] Forschungszentrum Jülich, JCNS, Germany

[4] European Spallation Source ESS ERIC, Lund, Sweden

MAGiC is a dedicated polarized single crystal diffractometer for the broad research field in magnetism proposed for the European Spallation Source [1]. MAGIC will be build in a collaboration with JCNS, PSI and the leading partner LLB.

The combination of the intense long pulse of the ESS with the time-of-flight Laue technique will provide a new performance to explore diffuse magnetic scattering and to determine magnetic structures even from very small crystals and weak magnetic moments. It will allow for studies of "x-ray sized" crystals and epitaxial films on a daily basis.

MAGiC will make versatile use of the optimized peak fluxes of the thermal and cold ESS moderators. The peak cold neutron flux can be favorably applied for high Q-resolution studies of complex magnetic structures or diffuse scattering, while thermal neutrons will enable to correlate atomic positions with magnetic properties. The polarizing neutron optic elements yield a highly polarized beam (<P>=98%) from 0.6 to 6Å with a flux as high as $3x10^9$ n/s/cm^2 at the sample position combined with polarization analysis for cold neutrons. The flexible wavelength spectrum and a (2 sr) position sensitive detector give a large access to reciprocal space with tunable 3 dimensional resolution.

In this talk, we present the science case supporting the MAGIC instrument, the technical design and potential future upgrades. Virtual (McStas) experiments on MAGiC will illustrate various challenging cases for micro-crystals, tiny magnetic contributions in superconductors, spin correlations in spin-ice systems, and spin-densities in molecular magnets.

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E-mail of the corresponding author: Werner.Schweika@esss.se

MARIA – The high-intensity polarized neutron reflectometer of JCNS

Stefan MATTAUCH[1] , Alexandros KOUTSIOUBAS[1], Sabine PÜTTER[1], Amir Syed MOHD[1], Earl BABCOCK[1], Zahir SALHI[1], Alexander IOFFE[1] and Thomas BRÜCKEL[2]

[1]Jülich Centre for Neutron Science JCNS at MLZ, Forschungszentrum Jülich, Garching, Germany

[2]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institute PGI, JARA-FIT, Forschungszentrum Jülich, Jülich, Germany

The high-intensity reflectometer MARIA of JCNS is installed in the neutron guide hall of the FRM II reactor in Garching and is using a velocity selector, Fermi-Chopper combination for the monochromatization of the neutron beam (1%,3%,5% or 10%). The full cross section of the beam is polarized by a double-reflecting super mirror and in the vertical direction the elliptically focussing neutron guide increases the flux at the sample position and consequently reduces the required sample size or measuring time. A flexible Hexapod, as sample table, can be equipped with an electromagnet (up to 1.1T) or a cryomagnet (up to 5T), low temperature sample environment, a UHV-chamber (10^{-10} mbar range) for the measurement of Oxide MBE samples (transfer forth and back) and last but not least with various soft matter cells. Together with the 400 x 400 mm² position sensitive detector and a time-stable ^{3}He polarization analyser based on Spin-Exchange Optical Pumping (SEOP), the instrument is well equipped to investigate specular reflectivity and off-specular scattering from magnetic layered structures down to the monolayer regime. Furthermore the GISANS option can be used to investigate lateral correlations in the nm range. All the options, like GISANS, polarization and ^{3}He polarization analyser can be moved in and out of the beam in seconds by remote controlled push button operation and do not require any realignment.
MARIA is a state of the art reflectometer at a constant flux reactor. It gives you the opportunity to investigate easily reflectivity curves in a dynamic range of up to 7-8 orders of magnitude including off-specular scattering and GISANS measurement. Furthermore the high intensity allows for kinetic measurements down to a few seconds over a dynamic range of 3-4 orders.

E-mail of the corresponding author: s.mattauch@fz-juelich.de

October 6, 2015, 11:50h Functional Materials II (Multiferroics)

Magnetic structure and magnetic domain population in multiferroic $Ba_2CoGe_2O_7$ by polarized neutron diffraction

Andrew SAZONOV[1,2], Vladimir HUTANU[1,2], Georg ROTH[2]

[1]Institute of Crystallography, RWTH Aachen University, Aachen, Germany

[2]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany

Emergence of ferroelectricity in several members of the melilite family, including $Ba_2CoGe_2O_7$, below their magnetic ordering temperature has been recently discovered [1,2]. The remarkable and complex response of these materials to magnetic and electric fields can be predicted by considering their magnetic symmetries [3,4]. In order to study experimentally the magnetic properties of $Ba_2CoGe_2O_7$ in the multiferroic state, we performed polarized neutron diffraction experiments.

Depends on the orientation of the antiferromagnetic component, the following types of magnetic space groups (MSGs) are possible in $Ba_2CoGe_2O_7$: $P2'_12_12'$ with moment along [100], $Cm'm2'$ along [110] or $P112'_1$ for a more general direction in the *ab* plane [3-6]. Moreover, small canting leading to the existence of the tiny spontaneous magnetization in the *ab* plane below $T_N \approx 6.7$ K is allowed according to the magnetic symmetry. In zero magnetic field, it is impossible to distinguish between those MSGs with conventional unpolarized neutron diffraction due to the presence of the symmetry-related energetically equivalent magnetic domains in each case.

In order to differentiate between the possible magnetic structures in $Ba_2CoGe_2O_7$, zero-field spherical neutron polarimetry (SNP) experiments were performed with a CRYOPAD on the polarized single-crystal diffractometers POLI (MLZ) and D3 (ILL). To study the influence of external field on the magnetic domain distribution the sample was cooled in the external field over the Néel temperature, the field was switched off and additional zero-field SNP measurements were done. The full polarization matrices were measured for dozens of Bragg reflections and treated within different magnetic models. It was found that even weak magnetic fields (20 mT) lead to a noticeable change of the ratio between the magnetic domain volumes. In contrast, applied electric fields (6 kV/mm) do not lead to the domain redistribution. The weak canting angle was also found in agreement with unpolarized neutron diffraction and bulk magnetization data. Thus, SNP sheds a new light on the complex properties of this multiferroic material.

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[4] P. Toledano, D. D. Khalyavin and L. C. Chapon, Phys. Rev. B **84**, 094421 (2011).
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E-mail of the corresponding author: mail@sazonov.org

On the antisymmetric exchange in $TbMn_2O_5$ by polarized neutron diffraction

Igor ZOBKALO[1,2], Sergey GAVRILOV[1], Andrey SAZONOV[3], Vladimir HUTANU[3]

[1]B.P. Konstantinov Petersburg Nuclear Physics Institute, Kurchatov Institute, Laboratory of Physics of Crystals, Gatchina, Russia
[2]Saint-Petersburg State University, Saint-Petersburg, Russia
[3]Institute of Crystallography, RWTH Aachen University and Jülich Centre for Neutron Science at Heinz Maier- Leibnitz Zentrum, Garching, Germany

Magnetic multiferroic family RMn_2O_5 (R – rare-earth element) demonstrate, probably, the most interesting and close interrelations between magnetism and ferroelectricity. Being now one of the most intriguing challenges in the physics of strongly correlated systems, magnetic multiferroicity is hopeful for potential application in functional devices. Notwithstanding on the great amount of the experimental and theoretical works devoted to RMn_2O_5, the mechanisms of ferroelectricity in this family still are not obvious.

In order to make a new approach to the elucidation of the microscopic mechanisms of multiferroicity in family RMn_2O_5 we carried out experiments on $TbMn_2O_5$ single crystal using polarized neutron techniques diffraction in different modifications. We employed technique of polarized neutron diffraction without analysis after scattering, XYZ-polarization analysis, and technique of spherical neutron polarimetry (SNP). Measurements with SNP were undertaken with external electric field also.

We observed the difference in the population of domains with “right” and “left” spirals in all magnetically ordered phases which are characteristic for $TbMn_2O_5$ [1] i.e. in high-temperature incommensurate, commensurate magnetic, and low-temperature incommensurate ones. This difference can be controlled by the external electric field in field-cooled mode, which correspond to rather rigid domain structure.

For the analysis of our results we employed model of the antisymmetric superexchange through anion [2, 3]. The analysis of results bears evidence that antisymmetric Dzyaloshinsky-Moria exchange is effective in all magnetic phases in $TbMn_2O_5$.

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E-mail of the corresponding author: zobkalo@pnpi.spb.ru

Hidden ordered magnetic states on hyperkagome lattices.

P. P. DEEN[1,2] J. A. M. PADDISON[3,4] H. JACOBSEN[2,1] O. A. PETRENKO[5], M.T. FERNANDEZ-DIAZ[6] , A. L. GOODWIN[3]

[1]European Spallation Source, Lund, Sweden.

[2]Niels Bohr Institute, University of Copenhagen, Denmark.

[3]University of Oxford, Inorganic Chemistry Laboratory, U.K.

[4]ISIS Facility, Rutherford Appleton Laboratory, Didcot, U.K.

[5]Department of Physics, University of Warwick, U.K.

[6]Institut Max von Laue–Paul Langevin, Grenoble , France

The search for new states of matter is a fundamental theme of condensed matter science. Frustrated magnetic materials are promising candidates for new states because lattice geometry suppresses conventional magnetic dipole order. Frustration thus drives novel emergent states. $Gd_3Ga_5O_{12}$ is the canonical frustrated magnet as the compound that does not order via the pervasive "order by disorder" mechanism down to the lowest temperatures probed, 25 mK [1 and ref. therein]. Short-range correlations, determined via neutron diffraction, have long been assumed to originate from near neighbour short-range interactions.
A non-dipole ("hidden") order has been uncovered via recent developments in Reverse Monte Carlo techniques [2] in conjunction with optimised neutron scattering instrumentation that enabled S(Q) of non-isotope enriched $Gd_3Ga_5O_{12}$ to be probed. The hidden-order state of $Gd_3Ga_5O_{12}$, the only known example of a magnetic multipole crystal in a spin liquid, does not break the crystal symmetry and is built from individually fluctuating groups of spins.

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E-mail of the corresponding author: pascale.deen@esss.se

Physical realization of a new quantum spin liquid based on a novel frustration mechanism.

Christian BALZ[1,2], Bella LAKE[1,2], Johannes REUTHER[1,3], Hubertus LUETKENS[4], Rico SCHÖNEMANN[5], Thomas HERRMANNSDÖRFER[5] Yogesh SINGH[6], A. T. M. Nazmul ISLAM[1], Elisa M. WHEELER[7], Jose A. RODRIGUEZ-RIVERA[8], Tatiana GUIDI[9], Giovanna G. SIMEONI[10], Chris BAINES[4], Hanjo RYLL[1]

[1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany.

[2]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany.

[3]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Germany.

[4]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, Villigen, Switzerland.

[5]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf, Germany.

[6]Indian Institute of Science Education and Research Mohali, Mohali, India.

[7]Institut Laue-Langevin, 38042 Grenoble, France.

[8]Center for Neutron Research, NIST, Gaithersburg, USA.

[9]ISIS Facility, STFC Rutherford Appleton Laboratory, Oxfordshire OX11 0QX, UK.

[10]Heinz Maier-Leibnitz Zentrum, Technische Universitat München, 85748 Garching

Unlike conventional magnets where the magnetic moments are partially or completely static in the ground state, in a quantum spin liquid they remain in collective motion down to the lowest temperatures. The importance of this state is that it is coherent and highly entangled without breaking local symmetries. Such phenomena is usually sought in simple lattices where antiferromagnetic interactions and/or anisotropies favoring specific alignments of the magnetic moments, are frustrated by lattice geometries incompatible with such order. Despite an extensive search among such compounds, experimental realizations remain very few. Here we investigate the new spin-1/2 magnet, $Ca_{10}Cr_7O_{28}$, which has a novel unexplored lattice with several isotropic interactions consisting of strong ferromagnetic and weaker antiferromagnetic couplings. Despite its unconventional structure and Hamiltonian, we show experimentally that it displays all the features expected of a quantum spin liquid. Bulk properties measurements, neutron scattering and muon spin relaxation reveal coherent spin dynamics in the ground state, the complete absence of static magnetism and diffuse spinon excitations. Pseudo-Fermion renormalization group calculations verify that the Hamiltonian of $Ca_{10}Cr_7O_{28}$ supports a dynamical ground state which furthermore is robust to significant variations of the exchange constants.

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E-mail of the corresponding author: christian.balz@helmholtz-berlin.de

October 6, 2015, 15:30h Quantum/Frustrated Spin Systems II

Field-dependence of the helimagnon dispersion in the chiral magnet MnSi

Tobias WEBER[1,2], Johannes WAIZNER[3], Robert GEORGII[2], Gregory TUCKER[4], Max KUGLER[1,2], Andreas BAUER[1], Markus GARST[3], Peter BÖNI[1]

[1]Physik-Department E21, Technische Universität München (TUM), James-Franck-Str. 1, 85748 Garching, Germany

[2]Heinz-Maier-Leibnitz-Zentrum (MLZ), TUM, Lichtenbergstr. 1, 85747 Garching, Germany

[3]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77a, 50937 Köln, Germany

[4]Laboratory for Neutron Scattering and Imaging (LNS), Paul-Scherrer-Institut (PSI), 5232 Villigen PSI, Switzerland

MnSi is a chiral magnetic compound hosting an abundance of different magnetic phases [1], among them a helimagnetic, a conical, and a ferromagnetic phase, with the most prominent of them being the A-phase featuring a hexagonal Skyrmion lattice [2]. The different magnetic phases originate from a competition of three distinct interactions: the ferromagnetic exchange *J*, the Dzyaloshinsky-Moriya interaction *D* and the weak crystal electric field *C* [3].

The helimagnetic dispersion relation forms a band structure, which was identified and mapped out by Janoschek et al. [3] and Kugler et al. [4], respectively, using zero magnetic field in the former and a low field inducing a single-domain state in the latter case.

In the present study, we mapped out the magnon dispersion relations in MnSi near the second-order transition between the conical and the field-polarised ferromagnetic phase. For increasing magnetic fields the dispersion branches converge towards a single excitation in the ferromagnetic phase at the upper critical field B_{c2}. In contrast to a normal ferromagnet, the field-polarised magnons above B_{c2} show a strong damping compared to the helimagnetic phase. A deconvolution of the spectra shows an increased interaction of the magnon modes that is marked by anomalous deviations of the measured to the predicted energies.

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E-mail of the corresponding author: tweber@frm2.tum.de

Ising incommensurate Spin Resonance of $CeCoIn_5$: A dynamical precursor of the Q-phase

Stéphane RAYMOND

CEA-Grenoble and Univ. Grenoble Alpes, INAC-MEM-MDN, 38054 Grenoble, France

The concept of soft mode is central to condensed matter physics; it emphasizes the relationship between the excitation spectrum and the ground state of different phases of matter in a variety of situation ranging from lattice dynamical instability in ferroelectrics to Bose-Einstein condensation of magnons in magnetic insulators. Unconventional superconductivity often occurs on the verge of magnetic ordering or charge density-wave formation asking the question whether these states of matter are competitive or collaborative phases. Unconventional superconductivity modifies the magnetic excitation spectrum of a metal by a feedback effect corresponding to the apparition of a new collective mode, the spin resonance. It was recently shown by detailed inelastic neutron scattering experiments performed on the model *d*-wave unconventional superconductor $CeCoIn_5$ that the spin resonance mode has the same symmetry [1] as the adjacent field induced magnetic ordered phase, the Q-phase [2]. This fact, together with the known softening of the dynamical mode under applied magnetic field [3,4], strongly supports a scenario where the static magnetic order is realized by a condensation of the superconducting spin resonance.

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E-mail of the corresponding author: raymond@ill.fr

Transition from sign-reversed to sign-preserved Cooper-pairing symmetry in sulfur-doped iron selenide superconductors

Qisi WANG[2], **Jitae PARK**[1], Y. FENG[2], Y. SHEN[2], Y. HAO[2], B. PAN[2], J. W. LYNN[3], A. IVANOV[4], S. CHI[5], M. MATSUDA[5], R. J. BIRGENAEAU[6], D. V. EFREMOV[7], Jun ZHAO[2]

[1] Heinz Maier-Leibnitz Zentrum (MLZ), TUM, 85748 Garching, Germany
[2] Department of Physics, Fudan University, Shanghai 200433, China
[3] NIST Center for Neutron Research, Maryland 20899, USA
[4] Institut Laue-Langevin, 38042 Grenoble, France
[5] Quantum Condensed Matter Division, ORNL, Tennessee 37831-6393, USA
[6] Department of Physics, University of California, California 94720, USA
[7] IFW Dresden, 01069 Dresden, Germany

An essential step toward elucidating the mechanism of superconductivity is to determine the sign/phase of superconducting order parameter, as it is closely related to the pairing interaction. In conventional superconductors, the electron-phonon interaction induces attraction between electrons near the Fermi energy and results in a sign-preserved s-wave pairing. For high-temperature superconductors, including cuprates and iron-based superconductors, prevalent weak coupling theories suggest that the electron pairing is mediated by spin fluctuations which lead to repulsive interactions, and therefore that a sign-reversed pairing with an s± or d-wave symmetry is favored. Here, by using magnetic neutron scattering, a phase sensitive probe of superconducting gap, we report the observation of a transition from the sign-reversed to sign-preserved Cooper-pairing symmetry with insignificant changes in Tc in the S-doped iron selenide superconductors $K_xFe_{2-y}(Se_{1-z}S_z)_2$. We show that a rather sharp magnetic resonant mode well below the superconducting gap (2Δ) in the undoped sample ($z = 0$) is replaced by a broad hump structure above 2Δ under 50% S doping. These results cannot be readily explained by simple spin fluctuation-exchange pairing theories and, therefore, multiple pairing channels are required to describe superconductivity in this system. Our findings may also yield a simple explanation for the sometimes contradictory data on the sign of the superconducting order parameter in iron-based materials [1].

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E-mail of the corresponding author: jitae.park@frm2.tum.de

Magnetostriction and Magnetostructural Domains in Antiferromagnetic $YBa_2Cu_3O_6$

B. NÁFRÁDI, **Thomas KELLER**, F. HARDY, C. MEINGAST, A. ERB, B. KEIMER

MPI für Festkörperforschung, Outstation at FRM II, Garching, Germany

We use high-resolution neutron Larmor diffraction and capacitative dilatometry to investigatespontaneous and forced magnetostriction in undoped, antiferromagnetic $YBa_2Cu_3O_{6.0}$, the parent compound of a prominent family of high-temperature superconductors. Upon cooling below the Néel temperature TN=420 K, Larmor diffraction reveals the formation of magnetostructural domains of characteristic size ~240 nm. In the antiferromagnetic state, dilatometry reveals a minute (4×10^{-6}) orthorhombic distortion of the crystal lattice in external magnetic fields. We attribute these observations to exchange striction and spin-orbit coupling induced magnetostriction, respectively, and show that they have an important influence on the thermal and charge transport properties of undoped and lightly doped cuprates.

[1] Nafradi et al., PRL 116, 047001 (2016).

E-mail of the corresponding author: t.keller@fkf.mpg.de

Area Detectors for Single-Crystal Neutron Diffraction

Arsen GUKASOV

Leon Brillouin Laboratory CEA-CNRS, CE de Saclay, 91191, Gif sur Yvette, France

Neutron single-crystal diffraction is the tool of choice to determine the accurate positions of hydrogen atoms in solids and the arrangements of magnetic moments. Since neutron fluxes are low compared to those available at synchrotron X-ray facilities much emphasis has been placed in particular on the provision of large area detector systems. They provide unique possibility for real-time exploration of reciprocal space and rapid data collection through phase transitions.

Diffractometer at the LLB (5C1 and 6T2) which combines a large area detector and a polarized neutron beam demonstrate very high efficiency both in conventional diffraction experiments and in the measurement of spin densities. In this talk some recent results illustrating the efficiency of the "area detector" diffractometers will be given, as well as the trends of their development.

E-mail of the corresponding author: arsen.goukassov@cea.fr

October 7, 2016, 9:30h Neutron Methods and Instrumentation II

Latest results of practical testing of PASTIS with a TOF beamline

Earl BABCOCK[1], Zahir SALHI[1], Ramil GAINOV[2], Robin WORACEK[4], Helmut SOLTNER[3], Patrick PISTEL[3], Fabian BEULE[5], Klaus BUSSMANN[6], Achim HEYNEM[3], Hans KAMMERLING[3], Frank SUXDORF[5], Margarita RUSSINA[2], Jörg VOIGT[6], Alexander IOFFE[1]

[1]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH . 85747 Garching, Germany

[2]Helmholtz-Zentrum Berlin fuer Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

[3]Engineering und Technologie (ZEA-1), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

[4]European Spallation Source ERIC, S-221 00 Lund, Sweeden

[5]Jülich Centre for Neutron Science JCNS and Institute for Complex Systems ICS Forschungszentrum Jülich GmbH 52425 Jülich, Germany

[6] Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

A complete XYZ polarization analysis solution is under development for the new thermal time of flight spectrometer TOPAS [1], to be operated in the new East neutron guide hall at the FRM II. Polarization Analysis Studies on a Thermal Inelastic Spectrometer, commonly called PASTIS [2], is based on polarized ^{3}He neutron spin filters and an XYZ field configuration for the sample environment and a polarization preserving neutron guide field. The complete system was calculated to provide adiabatic transport of the neutron polarization to the sample position while maintaining the homogeneity of the XYZ field. This system has now been tested on the polarized time of flight ESS test beamline V20 at Helmholtz Zentrum Berlin[3]. To the minimum wavelength of the instrument of 1.6 Å the magnetic configuration worked ideally neutron spin transport while giving full experimental freedom to change between the X, Y or Z field configuration. Additionally a graphite powder hydrated with H_20 was measured to verify performance under practical measuring conditions. The ^{3}He cell used was polarized at the ^{3}He lab in Garching and transported to HZ-Berlin via car in a permanent magnet transporter box. We present results of this test and the next steps forward.

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E-mail of the corresponding author: e.babcock@fz-juelich.de

Simulation and optimization of a new focusing polarizing bender for the diffuse neutron scattering spectrometer DNS@MLZ

Kirill NEMKOVSKI[1], Alexander IOFFE[1], Yixi SU[1], Earl BABCOCK[1], Werner SCHWEIKA[2,3] and Thomas BRÜCKEL[2]

[1] Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Garching, Germany

[2] Jülich Centre for Neutron Science (JCNS) und Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany

[3] European Spallation Source ESS AB, Lund, Sweden

DNS is a versatile diffuse neutron scattering instrument with polarization analysis operated by JCNS at the Heinz Maier-Leibnitz Zentrum (MLZ) [1]. It is used for studies of highly frustrated spin systems, strongly correlated electrons, emergent functional materials and soft condensed matter. During the last years the instrument has been considerably upgraded; here the concept and the results of simulations for a new polarizer are presented.

The concept of the polarizer is based on the idea of a bender [2] made from the stack of the silicon wafers with a double-side supermirror polarizing coating and absorbing spacers in between [3]. Owing to its compact design, such a system provides more free space for the arrangement of other instrument components. Additionally, to reduce the activation of the polarizer we plan to use the Fe/Si coating instead of currently used FeCoV/Ti:N one.

As the polarizer at DNS is positioned after the double-focusing crystal monochromator, it is required to accept a high divergence of the incoming neutron beam. Using the VITESS package [4] we have performed simulations for horizontally focusing polarizing benders in combination with the double-focusing monochromator. Neutron transmission and polarization efficiency as well as the effects of the focusing for convergent conventional C-benders and S-benders have been analyzed both for wedge-like and plane-parallel convergent geometries of the channels. The results of these simulations and the advantages/disadvantages of the various configurations are discussed.

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E-mail of the corresponding author: k.nemkovskiy@fz-juelich.de

Nonmagnetic high pressure clamp cells for neutron scattering at low temperature and high magnetic fields.

Ravil Sadykov [1,2]

[1]Institute For Nuclear Research, Moscow, Troitsk, Russia,

[2]Institute for High Pressure Physics, Moscow, Troitsk, Russia

The increased interest in quantum phase transitions and the study of new magnetic state-skyrmions under pressure demands the creation of new non-magnetic high-pressure cells. High pressure clamp cells made of hard nonmagnetic alloys: TiZr (zero), Al, 40HNU (NiCrAl) and CuBe for use by TOF-method on pulse and reactor neutron sources are presented in this report. The cells fit for powder and single crystal studies, both for diffraction and inelastic neutron scattering. They can be placed in typical cryostats (as well as in dilution fridge insert) and high magnetic field cryostat up to 6-10T. Single crystal or powder NaCl (a pressure calibrant) and Fluorinert (a pressure medium) were used in experiments on the neutron sources SINQ (Swiss), ISIS (UK), HMI (Germany), ILL (France) and SNS (USA). We tested a number of types of Fluorinert and found that the limits of solidification differ for various Fluorinerts with the maximum for mixture of FC84/87=23kbar [1]. Some of these cells were used for investigations of magnetic spirals in $ZnCr_2S_4$, $CsCuCl_3$ and MnSi [2] under pressure. A new nonmagnetic two layer piston/cylinder type cell made of TiZr+40HNU was used for determination of form-factor dependence of localized magnetic moments in $CePd_2Si_2$ under pressures up to 40kbar and H=10T with polarized neutrons on D3 (ILL) [3].

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E-mail of the corresponding author: rsadykov@inr.ru

Cryogen-free high magnetic field and low temperature sample environments for neutron scattering – latest developments

John BURGOYNE[1], Christoph KARL[2]

[1]Oxford Instruments NanoScience, Tubney Woods, Abingdon, OX13 5QX, UK

[2]Oxford Instruments GmbH, Borsigstrasse 15a, 65205 Wiesbaden, Germany

Continuous progress has been made over many years now in the provision of low- and ultra-low temperature sample environments, together with new high-field superconducting magnets and increased convenience for both the user and the neutron research facility via new cooling technologies. Within Oxford Instruments' experience, this has been achieved in many cases through close collaboration with neutron scientists, and with the neutron facilities' sample environment leaders in particular.

Superconducting magnet designs ranging from compact Small Angle (SANS) systems up to custom-engineered wide-angle scattering systems have been continuously developed. Recondensing, or "zero boil-off" (ZBO), systems are well established for situations in which a high field magnet is not conducive to totally cryogen-free cooling solutions, and offer a reliable route with the best trade-offs of maximum system capability versus running costs and user convenience. Fully cryogen-free solutions for cryostats, dilution refrigerators, and medium-field magnets are readily available.

Here we will present the latest technology developments in these options, describing the state-of-the art, the relative advantages of each, and the opportunities they offer to the neutron science community.

E-mail of the corresponding author: john.burgoyne@oxinst.com

Magnetic interactions and magneto-electric coupling mechanisms in iron penta-halide hybrid compounds

J. Alberto RODRIGUEZ VELAMAZAN[1], Oscar FABELO[1], Laurent CHAPON[1], Juan RODRIGUEZ-CARVAJAL[1], Javier CAMPO[2]

[1]Institut Laue-Langevin, Grenoble, France

[2]Instituto de Ciencia de Materiales de Aragón (CSIC-Univ. Zaragoza), Zaragoza, Spain

In magnetoelectric multiferroic materials, a subtle competition between different magnetic interactions is at the origin of multiferroicity, as this competition is the responsible of the formation of a magnetic structure able to induce ferroelectric polarization. The difficulty in controlling this interplay of interactions explains the scarce number of these materials reported. Recently, $A_2[FeCl_5(H_2O)]$ (A = Cs, K, Rb) have been identified as new linear magnetoelectric materials, while $(NH_4)_2[FeCl_5(H_2O)]$ was established as a type II multiferroic, with strong magnetoelectric coupling and with a rich phase diagram upon application of magnetic field.[1,2] The crystal and magnetic structures of $(ND_4)_2[FeCl_5(D_2O)]$ [3] and $Cs_2[FeCl_5(D_2O)]$ in different regions of their phase diagrams have been studied by neutron diffraction, trying to understand the mechanisms of magneto-electric coupling in these compounds. Spherical neutron polarimetry has been used to elucidate the occurrence of a collinear magnetic structure in a particular region of the phase diagram of $(ND_4)_2[FeCl_5(D_2O)]$ and to determine the nature and population of the coexisting magnetic domains at 2K. 1D polarimetry (flipping ratio method) has been employed to obtain spin-density maps that could shed light on the magnetic interactions at the origin of the magnetic structures and, ultimately, of the magneto-electric coupling.

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Corresponding author: velamazan@ill.eu

October 7, 2016, 11:50h Functional Materials III (Multiferroics)

Spin-wave and electromagnon dispersions in multiferroic $MnWO_4$ as observed by neutron spectroscopy

Y. XIAO[1], C. M. N. KUMAR[2], S. NANDI[1,3], Y. SU[3], W. T. JIN[1,3], Z. FU[3], E. FAULHABER[4], A. SCNEIDEWIND[3,4], and Th. BRÜCKEL[1,3]

[1] Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

[2] Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at SNS, POB 2008, 1 Bethel Valley Rd. Oak Ridge, TN 37831-6473, USA

[3] Jülich Centre for Neutron Science JCNS at Heinz Maier-Leibnitz Zentrum, Forschungszentrum Jülich GmbH, Lichtenbergstraße 1, 85747 Garching, Germany

[4] Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM-II), TU München, 85747 Garching, Germany

So-called spin-driven ferroelectrics, for which the inversion symmetry is broken in the ferroelectric phase due to the appearance of a particular magnetically ordered state, provide a path to the required coupling. As a prototypical multiferroic material with spiral magnetic order, $MnWO_4$ has been widely studied concerning its magnetic and ferroelectric properties. However, a deeper insight into the coupling between the electric and magnetic degrees of freedom can be gained by studying not only the respective order but also the excitation spectra. In present work, high resolution inelastic neutron scattering reveals that the elementary magnetic excitations in multiferroic $MnWO_4$ consist of low energy dispersive electromagnons in addition to the well-known spin-wave excitations. The latter can well be modeled by a Heisenberg Hamiltonian with magnetic exchange coupling extending to the 12^{th} nearest neighbor. They exhibit a spin wave gap of 0.61(1) meV. Two electromagnon branches appear at lower energies of 0.07(1) meV and 0.45(1) meV at the zone center. They reflect the dynamic magnetoelectric coupling and persist in both, the collinear magnetic and paraelectric AF1 phase, and the spin spiral ferroelectric AF2 phase. These excitations are associated with the Dzyaloshinskii-Moriya exchange interaction, which is significant due to the rather large spin-orbit coupling.

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E-mail of the corresponding author: y.xiao@fz-juelich.de

Homo-chiral crystal growth and chiral helimagnetism in $CsCuCl_3$

Y. Kousaka[1,2], T. Koyama[1], K. Ohishi[3], K. Kakurai[3], V. Hutanu[4], T. Brueckel[5] J. Campo[6], J. Suzuki[3], Y. Miyamoto[1], A. Sera[1], K. Inoue[1,2], and J. Akimitsu[1,2]

[1]Graduate School of Science, Hiroshima University, Higashi-hiroshima, Japan

[2]Center for Chiral Science, Hiroshima University, Higashi-hiroshima, Japan

[3]Research Center for Neutron Science and Technology, CROSS, Tokai, Japan

[4]RWTH Aachen University, Aachen, Germany

[5]Jülich Centre for Neutron Science, Garching, Germany

[6]Aragón Materials Science Institute (CSIC-Universidad de Zaragoza), Zaragoza, Spain

Chiral helimagnetic ordering, forming only right- or left-handed spiral magnetic structure, has attract much attention due to unique magnetic textures such as skyrmion and chiral magnetic soliton lattice [1, 2]. Therefore, it is very important to investigate interplay between crystallographic and helimagnetic chirality because sense of the helical spin structure depends on the right- or left-handed chiral crystal structure that allows an asymmetric Dzyaloshinskii-Moriya interaction. However, there have been few experimental results due to the difficulty to synthesize homo-chiral single crystals, having only right- or left-handed crystalline domains. $CsCuCl_3$ has a chiral crystal structure with chiral space groups of right-handed $P6_122$ and left-handed $P6_522$. Cooling temperature below T_N = 10.5 K, unpolarized neutron diffraction studies show helimagnetic ordering [3]. Some experimental groups have performed polarized neutron diffraction experiments to determine the domain ratio between right- and left-handed helimagnetic ordering in the right-handed crystalline $CsCuCl_3$. However, their results are different due to problems in growing and evaluating the homo-chiral crystals [4, 5].

We will present a unique crystallization technique to make homo-chiral crystals for $CsCuCl_3$ By adapting our crystallization technique, we succeeded in growing the cm-ordered enantiopure single crystals. Polarized neutron diffraction studies were performed at BL15 (TAIKAN) in J-PARC, and at POLI in FRM-II. We prepared 2 crystalline samples for the measurements, having only right- and left-handed crystalline domains. We observed magnetic satellite intensity, depending on neutron polarization. The polarization dependence indicates that the right-handed crystalline $CsCuCl_3$ forms right-handed helimagnetic structure, and the left-handed crystal forms left-handed helimagnetic structure.

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E-mail of the corresponding author: koyu@hiroshima-u.ac.jp

Posters

Poster 2016-01

Recent developments at DNS, diffuse neutron scattering spectrometer with polarization analysis at MLZ

Yixi SU[1], **Kirill NEMKOVSKI[1]**, Sultan DEMIRDIŞ[1], Werner SCHWEIKA[2,3], Alexander IOFFE[1] and Thomas BRÜCKEL[2]

[1] Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Garching, Germany

[2] Jülich Centre for Neutron Science (JCNS) und Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany

[3] European Spallation Source ESS AB, Lund, Sweden

DNS is a versatile diffuse scattering instrument with polarization analysis operated by JCNS at the Heinz Maier-Leibnitz Zentrum (MLZ). A compact design, a large double-focusing PG monochromator and a highly efficient supermirror-based polarizer provide a polarized neutron flux of about 10^7 n/cm^{2}s. DNS is used for the studies of highly frustrated spin systems, strongly correlated electrons, emergent functional materials and soft condensed matter.

Here we present the recent developments and scientific highlights at DNS as well as the ongoing instrument upgrades. In the frame of this project, the neutron guide with m=1.2 has been replaced by the new one with m=2. Respectively, the flux for the short-wavelength range has been considerably enhanced. The available short wavelength range has been extended from 2.4 Å to 1.5 Å, with an accessible Q-range up to 7.8 Å^{-1} instead of 4.8 Å^{-1}. In order to deal with the increased neutron flux, the monochromator shielding has been replaced and improved. In addition, a neutron velocity selector has been installed and successfully commissioned. It allows us to suppress the high-order contamination of the monochromatized beam. Alternatively, the velocity selector can be used for selecting a shorter wavelength by the PG004 reflection with better resolution and without moving the secondary spectrometer. An important step toward a user-friendly instrument has been achieved by switching to the new generation instrument control software TANGO and NICOS. The new option for the data reduction and visualization in diffraction mode has been developed and implemented based on the Mantid project.

E-mail of the corresponding author: k.nemkovskiy@fz-juelich.de

Poster 2016-02

Upgrade of the KWS-1 Small-Angle Neutron Scattering Instrument

Artem FEOKTYSTOV[1], Henrich FRIELINGHAUS[1], Marie-Sousai APPAVOU[1], Vitaliy PIPICH[1], Earl BABCOCK[1], Zahir SALHI[1], Romuald HANSLIK[2], Ralf ENGELS[3], Günter KEMMERLING[4], Georg BRANDL[1], Harald KLEINES[4], Alexander IOFFE[1], Dieter RICHTER[5],Thomas BRÜCKEL[4]

[1]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Garching, Germany

[2]Central Institute for Engineering, Electronics and Analytics ZEA-1, Forschungszentrum Jülich GmbH, Jülich, Germany

[3]Central Institute for Engineering, Electronics and Analytics ZEA-2, Forschungszentrum Jülich GmbH, Jülich, Germany

[4]Jülich Centre for Neutron Science JCNS-2 and Peter Grünberg Institute PGI-4, JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany

[5]Jülich Centre for Neutron Science JCNS-1 and Institute of Complex Systems ICS-1, Forschungszentrum Jülich GmbH, Jülich, Germany

The KWS-1 small-angle neutron scattering (SANS) instrument operated by JCNS at the research reactor FRM II of the MLZ in Garching has been recently upgraded [1]. The instrument obtained new components, including: transmission supermirror polarizer, adiabatic radio-frequency spin flipper, chopper and neutron lenses. The double-disc chopper is used to reduce the wavelength spread from the standard 10% to about 1%. The lenses allow the enhancement of the neutron flux at the sample by using larger sample aperture. The polarizer, with an average polarization > 93%, is positioned in a custom designed changer of revolver type. The flipper provides high flipping efficiency of more than 99.9%. A custom designed hexapod allows heavy loads and precise sample positioning in beam for SANS and GISANS experiments under applied magnetic field. A new flexible instrument control system (NICOS) is installed and its utilization opens new possibilities at the instrument.

The performance of the new components was checked by means of the standard samples as well as ^{3}He neutron spin filter for polarizer and spin flipper characterization. Test measurements on a ferrofluid in a magnetic field with polarized and nonpolarized neutrons are presented. Recent developments in the field of polarization analysis at the instrument are presented along with the results of the first test.

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E-mail of the corresponding author: a.feoktystov@fz-juelich.de

Poster 2016-03

New setup for polarized neutron diffraction at instrument POLI at MLZ

Henrik THOMA[1,2], Vladimir HUTANU[1,2]

[1] Institut für Kristallographie RWTH Aachen, Jägerstr. 17–19, 52056 Aachen, Germany

[2] Jülich Centre for Neutron Science JCNS at MLZ, Lichtenbergstr. 1, 85747 Garching

Polarized neutron diffraction (PND) is a powerful method to investigate magnetic structures. It allows very precise magnetization measurements even for weak magnetic contributions. In this technique, spin flip measurements are carried out on a sample, located in a magnetic field. Optionally, the scattered beam can be analyzed to perform a polarization analysis along the given field direction at the sample.

A new PND setup has been developed for the hot neutron single crystal diffractometer POLI [1] at MLZ, which is commonly used for 3D polarization analysis or non-polarized structure refinements. This setup consists of a new high Tc superconducting magnet producing fields up to 2.2 T and a ^{3}He spin filter cell [2] for polarization. Because the magnet was originally not designed for the use with polarized neutrons but has weak stray fields, a guide field system was designed and the polarization feed-through simulated. Furthermore, a Mezei flipper optimized for hot neutrons was constructed.

By using either a Heusler crystal at the sample position or a second spin filter cell as analyzer, the polarization losses in the setup were confirmed to be below 2% over the total field range of the magnet. With the ^{3}He cell as polarizer, a beam polarization over 90% at a wavelength of 0.7 A is reachable. The magnetic stray fields did not affect the ^{3}He polarization, which had a relaxation time above 100 h. First experiments with antiferromagnetic and paramagnetic sample using the new setup have been successfully performed.

New developed guide field system and flipper are also suitable to be used with the new 8 T asymmetric field, actively shielded magnet which is under production and planned to be implemented on POLI in 2017.

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E-mail of the corresponding author: henrik.thoma@frm2.tum.de

Poster 2016-04

Studies on new magnetic and superconducting compounds with hot single crystal diffraction at HEiDi

Martin Meven[1,2], Vladimir Hutanu[1,2], Andrew Sazonov[1,2], Georg Roth[1]

[1]RWTH Aachen University, Institute of Crystallography, 52056 Aachen, Germany

[2]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science, Outstation at Heinz Maier-Leibnitz Zentrum (MLZ), 85747 Garching, Germany

At the Heinz Maier-Leibnitz Zentrum (MLZ) the single crystal diffractometer HEiDi uses hot neutrons for detailed studies of structural and magnetic properties of crystalline samples [1].

Concerning magnetic systems various multiferroic compounds have been thoroughly studied in the past like different melilites [2, 3], ferromagnetic compounds [4] and various frustrated antiferromagnetic systems [5, 6]. In all of these cases the unique capabilities of this instrument offering high resolution, large penetration depth and large q range were very important.

New superconductors like the recently discovered FeAs pnictides are also an important topic of studies on HEIDI. Examples are the highly absorbing $EuFe_2As_2$ compound and its doped members [7] or LiFeAs [8]. Their complex structural properties and their magnetic order in the undoped states require precise data collections and very accurate interpretation but yield deep insights into the details of their phase diagrams referring to structure, magnetism and superconductivity.

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

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E-mail of the corresponding author: martin.meven@frm2.tum.de

Poster 2016-05

T-REX: a bispectral direct geometry chopper spectrometer at the ESS

Nicolò Violini[1], Jörg Voigt[1], Andrea Orecchini[2,3], Thomas Brückel[1], Earl Babcock[1], Alessandro Paciaroni[2], Francesco Sacchetti[2], Zahir Salhi[1], Marco Zanatta[2]

[1] Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH, Wilhelm-Johnen Strasse, 52425 Jülich, Germany

[2] Department of Physics and Geology, Università di Perugia, 06123 Perugia, Italy

[3] CNR-IOM c/o Department of Physics and Geology, Università di Perugia, 06123 Perugia, Italy

We present the concept of T-REX, a bispectral direct geometry chopper spectrometer for the ESS neutron source. The instrument is designed to explore a wide dynamic range that extends from 20 μeV to 160 meV in energy transfer and from 0.01 $Å^{-1}$ to 17 $Å^{-1}$ in wave vector transfer. The science to be covered extends from high-energy coherent excitations, e.g. magnetic excitations in strongly correlated electron systems or phonon spectra in novel materials, to diffusion and relaxational processes in soft matter, energy materials or life science. In all fields, the application of polarization analysis combined with high energy resolution will provide completely new opportunities to identify the microscopic origin of the observed dynamic features.

T-REX features a removable cold neutron extraction system to provide an undisturbed performance when using thermal neutrons. The polychromatic operation of a chopper spectrometer provides features that resemble the performance of a three axis spectrometer: As the lower energy loss part of the excitation spectrum is always re-probed by the subsequent pulse, the chopper system can be used to optimize for a narrow dynamic range, namely the high energy loss, while still covering a wide dynamic range from all the individual pulses. The long secondary time-of-flight of the down-scattered neutrons allow a longer illumination of the sample, but require a narrower wavelength/velocity definition. Basically such an operation focuses a narrow dynamic range by a single pulse similar to a TAS instrument, but with the wide overall coverage of excitation energies by all pulses and the large solid angle coverage of a direct geometry chopper spectrometer. Hence it is appropriate to state that T-REX will serve the science case of thermal and polarized TAS at the ESS.

Polarization analysis over the full spectral range is envisaged by combination of polarizing supermirror assemblies at the position of the cold neutron extraction and continuously pumped SEOP ^{3}He spin filter cells the thermal neutrons. Wide angle polarization analysis will be realized based on the experience gained in the development of the magic PASTIS device for the TOPAS instrument.

E-mail of the corresponding author: j.voigt@fz-juelich.de

Poster 2016-06

Strain and electric field control of magnetism in supercrystalline iron oxide nanoparticle - $BaTiO_3$ composites

L.-M. Wang,[1] O. Petracic,[1] E. Kentzinger,[1] U. Rücker,[1] A. Koutsioumpas[2], S. Mattauch[2] and Th. Brückel[1,2]

[1)] Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich, Jülich, Germany
[2)]Jülich Centre for Neutron Science JCNS at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich, Lichtenbergsrtr. 1, Garching, Germany

Magnetoelectric (ME) materials have a large potential for use in spintronic and multifunctional devices [1-2]. In particular artificial composites composed of a ferroelectric and ferro- or ferrimagnetic component attracted intense research interest, since the ME coupling effect is much stronger and can be easier realized compared to intrinsic magnetoelectric materials.

In our case the composite is a self-assembled monolayer of iron oxide nanoparticles on top of a Ti film buffered $BaTiO_3$ (BTO) substrate. Grazing incident small angle x-ray scattering (GISAXS) and scanning electron microscopy (SEM) confirm a hexagonal close-packed well-ordered NP monolayer.
Strain-induced ME coupling (MEC) effect was observed in this composite as shown in Figure 2. MEC is demonstrated by measurements of both the magnetization and magneto-electric ac susceptibility (MEACS). The magnetization, coercivity, remanent magnetization and MEACS signal shows abrupt jumps at the BTO phase transition temperatures.

We find that for efficient strain coupling an additional Au layer embedding the NPs is crucial. The strain is very likely mediated through the Au layer. Our works open up viable possibilities for energy-efficient electronic devices fabricated by simple self-assembly techniques. [3]

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E-mail of the corresponding author: li.wang@fz-juelich.de

Poster 2016-07

Structural and magnetic properties of self-assembled 3D nanoparticle macrocrystals

Michael SMIK[1], Genevieve WILBS[1], Elisa VOLKMANN[1,] Alexandros KOUTSIOUMPAS[2], Stefan MATTAUCH[2], Emmanuel KENTZINGER[1], Jörg PERSSON[1], Ulrich RÜCKER[1], Oleg PETRACIC[1], Thomas BRÜCKEL[1]

[1] Jülich Centre for Neutron Science (JCNS) and Peter Grünberg Institut (PGI), JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

[2] Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Lichtenbergstr. 1, 85748 Garching, Germany

We have used centrifuge assisted sedimentation to fabricate 3D nanoparticle 'macrocrystals' from commercially available spherical iron oxide nanoparticles. The fabrication process was optimized to reliably produce macrocrystals up to 300µm in size. The samples were analyzed using scanning electron microscopy, which allowed for the identification of single crystals, which could then be isolated for further study. Using small angle x-ray scattering (SAXS) on the new in-house instrument 'GALAXI' (Gallium Anode Low-Angle X-ray Instrument) the supercrystalline structure could be identified to be face-centered cubic. The magnetic structure was investigated by a variety of magnetometric methods, including zero field cooled and field cooled curves, thermo remanent and isothermal remanent magnetization. The appearance of an "inverse" memory effect was observed, which cannot be explained yet. All methods point to a spin-glass-like structure; however, deviations from the expected results for a spin-glass indicate a novel kind of magnetic ordering. Semi-polarized small angle neutron scattering was also performed using MARIA, the high intensity reflectometer at the Heinz Maier-Leibnitz Zentrum (MLZ). As the samples were still very small, the neutron experiment proved to be challenging, but a signal could be observed.

E-mail of the corresponding author: m.smik@fz-juelich.de

2016-08

The Polarized Small Sample Reflectometer Estia at ESS

Artur Glavic[1], Jochen Stahn[1], Sven Schütz[2]

[1]Laboratory for Neutron Scattering and Imaging,
Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

[2]Laboratory for Scientific Developments and Novel Materials,
Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

The European Spallation Source (ESS) being build in Lund, Sweden, is the future flagship facility for neutron scattering. One of the instruments that will be operational when the facility starts the user program in 2023 is the polarized reflectometer Estia[1]. Based on the focusing Selene neutron guide concept[2,3], the beamline will make full use of the high ESS brilliance and a large divergence to allow specular reflectivity from tiny samples down to 1 mm² surface area as well as fast, time resolved studies with sub second resolution.

The instrument operates with horizontal scattering geometry with optional polarization and analysis. An elliptical neutron feeder extracts the beam from the cold moderator followed by a single frame definition chopper that is sufficient for the desired wavelength band (4-11Å) when using the natural resolution of the long-pulse source. A set of absorbers (virtual source) within the neutron bunker already reduces the beam to the sample size, so only the actually used neutrons are transported down to the experimental cave. Further down stream, two elliptical mirrors form the Selen guide that projects the virtual source onto the sample position. The experimental cave houses the sample environment and detector with -10 to 145 degree angular coverage. Polarization and analysis is performed with large, curved transmission mirrors, allowing polarization >99% with up to 88% polarized transmission.

We will present the overall instrument design and details of key instrument components distinguishing Estia from typical neutron instruments. Most notable focus of the design effort is the high precision Selene guide, which allows independent control of the beam size and divergence far away from the sample position. Although this property can be used to perform novel kinds of experiments and substantially reduce background for small samples it requires an unprecedented accuracy for the guide alignment, two orders of magnitude higher than for conventional guide systems.

[1] https://www.psi.ch/lns/estia .

[2] J. Stahn, U. Filges, and T. Panzner. Focusing specular neutron reflectometry for small samples. *Eur. Phys. J. Appl. Phys.*, **58**(1):11001, (2012).

[3] J. Stahn and A. Glavic. Focusing neutron reflectometry: Implementation and experience on the ToF-Reflectometer Amor. *Nuc. Instr. Meth. A*, **821**:44–54, (2016).

E-mail of the corresponding author: *artur.glavic@psi.ch*