Magnetic Small Angle Neutron Scattering – from Nanoscale Magnetism to Long-Range Magnetic Structures

725. WE-Heraeus-Seminar

31 May - 03 June 2021
ONLINE

WILHELM UND ELSE HERAEUS-STIFTUNG

Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the 725. WE-Heraeus-Seminar:

This WE-Heraeus-Seminar focuses on the technique of magnetic small angle neutron scattering, which is one of the most important methods for magnetic microstructure determination in condensed-matter physics and materials science. Magnetic SANS provides access to bulk properties and yields, quite uniquely, information on the mesoscopic length scale (roughly 1-1000 nm). This is an important size regime where many macroscopic materials properties are realized. Currently, the magnetic SANS community can be roughly subdivided into two larger groups: the research of one group is anchored in the domain of condensed-matter physics with a focus on fundamental questions such as skyrmion crystals and topological spin structures, complex long-range-ordered spin structures, and vortex lattices in superconductors, while the second group of scientists employs the magnetic SANS method for scrutinizing nanoscale magnetism in terms of a micromagnetic continuum description; materials classes which are studied are e.g. permanent magnets, magnetic steels, nanoparticles and ferrofluids, or complex alloys. It is one of the central aims of this Heraeus seminar to bring both groups of researchers closer together by providing a stage for intra- and interdisciplinary scientific exchange. Besides, in view of the upcoming European Spallation Source, a further focus will be on future challenges related to neutron instrumentation, sample environment, and neutron data analysis.

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Program

Program

Monday, 31 May 2021		Time CET
09:00 – 09:15	Scientific organizers	**Welcome** **Organizational Details**
09:15 – 09:30	Stefan Jorda	**About the Wilhelm and Else Heraeus Foundation**
09:30 – 10:00	**Mingling** (MeetAnyway – join the Mingling Area in the Networking floor)	
10:00 – 10:30	Christian Pfleiderer	**Experimental Perspectives of Skyrmions in Chiral Magnets**
10:30 – 11:00	**Discussion and questions to the talks**	
11:00 – 11:30	**Discussion at the virtual tables**	
11:30 – 13:00	*LUNCH BREAK*	
13:00 – 15:00	**Poster Session I** **30 min. Flash talks +** **90 min. Poster**	
15:00 – 15:30	*COFFEE BREAK*	
15:30 – 16:00	Chris Leighton	**Quantitative Understanding of Superparamagnetism in Soft Ferromagnetic Metallic Nanoparticles via Polarized Small-Angle Neutron Scattering**
16:00 – 16:30	Artem Feoktystov	**Small-angle neutron scattering for magnetic nanoparticles**
16:30 – 17:00	Philipp Bender	**Investigating magnetic nanostructures by small-angle neutron scattering**
17:00 – 17:30	**Discussion and questions to the talks**	
17:30 – 18:00	**Discussion at the virtual tables**	

Program

Tuesday, 1 June 2021	Time CET	
09:00 – 09:30	Dmitry Berkov	**Analyzing neutron scattering data by micromagnetic modeling: state of the art and perspectives**
09:30 – 10:00	Karin Everschor-Sitte	**Magnetic skyrmions for unconventional computing and revealing latent information**
10:00 – 10:30	**Discussion and questions to the talks**	
10:30 – 11:00	**Discussion at the virtual tables**	
11:00 – 13:00	*LUNCH BREAK*	
13:00 – 13:30	Nicolas Martin	**Field-induced vortex-like spin textures in reentrant spin glasses**
13:30 – 14:00	Kathryn Krycka	**Interplay Between Internal Magnetic Morphology and the Response of Solvated Nanoparticles**
14:00 – 14:30	**Discussion and questions to the talks**	
14:30 – 15:00	**Discussion at the virtual tables**	
15:00 – 15:30	*COFFEE BREAK*	
15:30 – 16:00	Morten Eskildsen	**Vortex lattice studies in UPt_3**
16:00 – 16:30	Johanna Jochum	**MIEZE-SANS: a spin-echo technique for magnetic phenomena**
16:30 – 17:00	**Discussion and questions to the talks**	
17:00 – 17:30	**Discussion at the virtual tables**	

Program

Wednesday, 2 June 2021	Time CET	
09:00 – 09:30	Dominika Zákutná	**Unravelling the magnetic and chemical morphologies of nanoparticles by SANS**
09:30 – 10:00	Sergey Grigoriev	**Measurements of spin wave stiffness in helimagnets by small-angle polarized neutron scattering**
10:00 – 10:30	**Discussion and questions to the talks**	
10:30 – 11:00	**Discussion at the virtual tables**	
11:00 – 13:00	*LUNCH BREAK*	
13:00 – 15:00	**Poster Session II** **30 min. Flash talks +** **90 min. Poster**	
15:00 – 15:30	*COFFEE BREAK*	
15:30 – 16:00	Elizabeth Blackburn	**Pauli paramagnetism and superconducting flux line lattices**
16:00 – 16:30	Marc Janoschek	**High-Precision Studies of Ferromagnetic Quantum Matter**
16:30 – 17:00	**Discussion and questions to the talks**	
17:00 – 17:30	**Discussion at the virtual tables**	
19:00 – 21:00	**Virtual Conference Party** (MeetAnyway – join a table in the Networking floor)	

Program

Thursday, 3 June 2021 **Time CET**

09:00 – 09:30	Verónica Salgueiriño	**Synthesis and Characterization of Nanocrystals of Transition Metal Oxides**
09:30 – 10:00	Andrew Wildes	**Neutron diffuse scattering from magnetically disordered compounds**
10:00 – 10:30	**Discussion and questions to the talks**	
10:30 – 11:00	**Discussion at the virtual tables**	
11:00 – 13:00	*LUNCH BREAK*	
13:00 – 13:30	Dirk Honecker	**Data analysis for magnetic small-angle scattering with SasView**
13:30 – 14:00	Markus Bleuel	**Recent Small Angle Neutron Scattering (SANS) Measurements using dynamic B-fields**
14:00 – 14:30	Sara Majetich	**Spin Canting in Magnetic Spinel Nanoparticles**
14:30 – 15:00	**Discussion and questions to the talks**	
15:00 – 15:30	**Discussion at the virtual tables**	
15:30 – 15:45	Scientific organizers	**Poster awards and Closing remarks**

End of seminar

Posters

Poster Session I

Monday, 31 May 2021 / Posters 1 – 13

1	Alexander Backs	**Vortex Matter of Intertype Superconductors studied by Neutron Methods and Molecular Dynamics Simulations**
2	Aicha Bouhlala	**Ab-initio study of the structural, magnetic and electronic properties of Ce0.75W0.25O2: spintronic application**
3	Xaver Simon Brems	**Current-induced self-organisation of mixed superconducting states**
4	Grace Causer	**Grazing Incidence SANS from Helimagnet MnSi Thin Films**
5	Adil Chakir	**Structure and dielectric study**
6	Cynthia Paola Contreras Medrano	**Low dimensional substructures in hulsite oxyborates**
7	Jonathan Gaudet	**Weyl mediated helical magnetism in NdAlSi**
8	Elliot Gilbert	**QUOKKA, the Pinhole Monochromatic Small Angle Neutron Scattering (SANS) instrument for Magnetic Studies**
9	Cecilia Granados-Miralles	**Rare-Earth-Free Permanent Magnets based on Exchange-Coupled and Decoupled Composites**
10	Maksym Karpets	**Investigation of structural and magnetic changes in transformer oil-based ferrofluids induced by electric field**
11	Naëmi Leo	**Small-angle neutron scattering for magnetic nanoparticles of nanomagnetic gyroid structures**

Poster Session I

12	Artem Malyeyev	**Magnetic Guinier Law**
13	Elizabeth Martín Jefremovas	**Coexistence of disorder and antiferromagnetism in $NdCu_2$ nanoparticles**

Poster Session II

Wednesday, 2 June 2021 / Posters 14 – 25

14	Flore Mees	**Dipolar correlations in square arrays of magnetic nanoparticles**
15	Denis Mettus	**Kinetic small-angle neutron scattering of skyrmion lattice order in chiral magnets**
16	Nileena Nandakumaran	**Investigating self-assembly of Au-Fe3O4 dumbbell nanoparticles using advanced scattering techniques**
17	Frédéric Ott	**Investigations of the magnetization reversal in Co nanowires bundles by Polarized SANS**
18	Yousra Ounza	**Spin-glass transition and magnetic properties in manganite perovskite $LaBiCaMn_2O_7$**
19	Leonhard Rochels	**Effects of pyrolysis on the magnetic structure and dipolar interactions in iron oxide mesocrystals**
20	Evelyn Pratami Sinaga	**Magnetic neutron scattering of nanoparticles: failure of the superspin model**
21	Paula Steinberg	**Aggregation study of sodium ibuprofenate and 1-butyl-3-methilimidazolium ibuprofenate in aqueous solutions by SANS**
22	Annika Stellhorn	**Interplay of proximity effects in Superconductor/Ferromagnet heterostructures**
23	Mohamed Tadout	**Engineered Gd-Co based multilayer stack to enhanced magneto-caloric effect and relative cooling power**

Poster Session II

24	R. Paxton Thedford	**Engineering Mesoscale Architecture in Superconductors via Block Copolymer Self-Assembly**
25	Ulrike Zweck	**Antiferromagnetically coupled anti-phase domains under external magnetic fields**

Abstracts of Lectures

(in alphabetical order)

Investigating magnetic nanostructures by small-angle neutron scattering

P. Bender[1]

[1]*Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, D-85747 Garching, Germany*

Small-angle neutron scattering (SANS) is a powerful technique to resolve structural and magnetic correlations on the mesoscale (~ 1-500 nm) and is therefore perfectly suited to investigate magnetic nanostructures such as magnetic nanoparticle (MNP) samples. In recent years, we used magnetic SANS to study a large variety of different MNP samples including exotic systems such as magnetotactic bacteria [1] and nanoflowers [2]. Furthermore, we applied magnetic SANS to investigate dipolar-coupled moment correlations in dense MNP assemblies [3] and developed new approaches to analyze the scattering data [4]. In this talk I will give an overview about the potential application of magnetic SANS for the characterization of magnetic nanostructured samples with a focus on novel numerical approaches for the analysis of 2D scattering patterns. A recent example is shown in **Figure 1**.

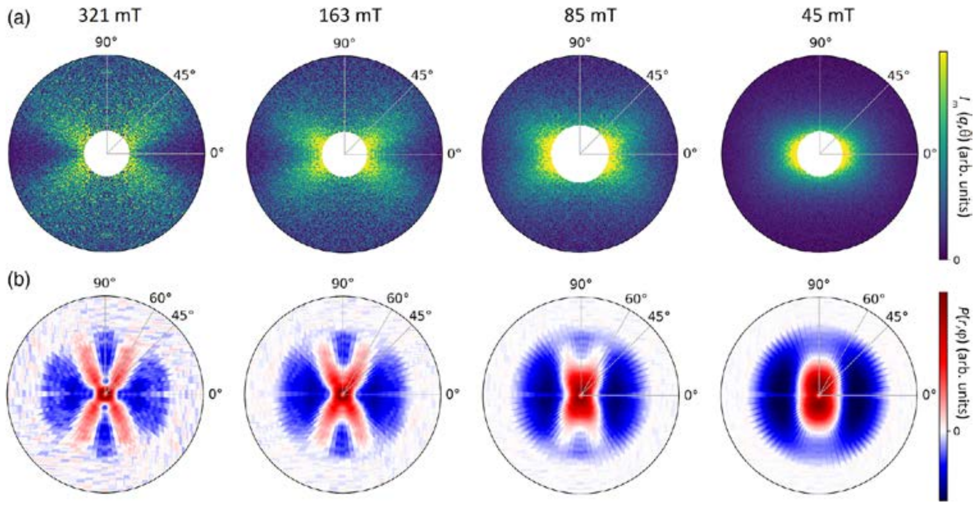

Figure 1: (a) Experimental 2D magnetic SANS patterns of Nanoperm measured at four different magnetic field strengths (field applied in horizontal direction).
(b) Corresponding 2D correlation functions extracted from the above scattering patterns using a fast iterative algorithm (from Bender et al., Small Sci. (2021)).

References

[1] Orue et al., Nanoscale **10**, 7407 (2018) & Bender et al., Nanoscale Adv. **2**, 1115 (2020).
[2] Bender et al., J. Phys. Chem. C **122**, 3068 (2018) & Bender et al., APL **115**, 132406 (2019).
[3] Bender et al., PRB **98**, 224420 (2018) & Honecker et al., PRB **101**, 134401 (2020).
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Analyzing neutron scattering data by micromagnetic modeling: state of the art and perspectives

S. Erokhin and D. Berkov

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We have developed a new micromagnetic methodology for modeling magnetization reversal in bulk magnetic materials including polycrystalline systems and nanocomposites [1]. This methodology is based on the polyhedral finite element mesh, what allows to overcome the main difficulty of the finite-element micromagnetics – efficient treatment of the long-ranged magnetodipolar interaction. It is achieved by utilizing the mapping of a disordered particle system onto a regular grid and the subsequent usage of the lattice Ewald algorithm employing the Fast Fourier transformation.

In this talk we present several physical examples, demonstrating the accuracy of our method by simulations of magnetization distributions in a wide range of systems: from particles in a non-magnetic matrix and magnetically soft nanocomposites to permanent magnet materials. In particular, we demonstrate how micromagnetic framework allows to optimize the magnetic performance of a material before its actual manufacturing.

Special attention is paid to the quantitative analysis of the experimentally obtained SANS data, including the decryption of the total magnetic SANS patterns (Fig. 1). Further, we discuss the anisotropic nature of the real-space magnetic correlations [2] in magnetic nanocomposites and their impact on the neutron scattering picture.

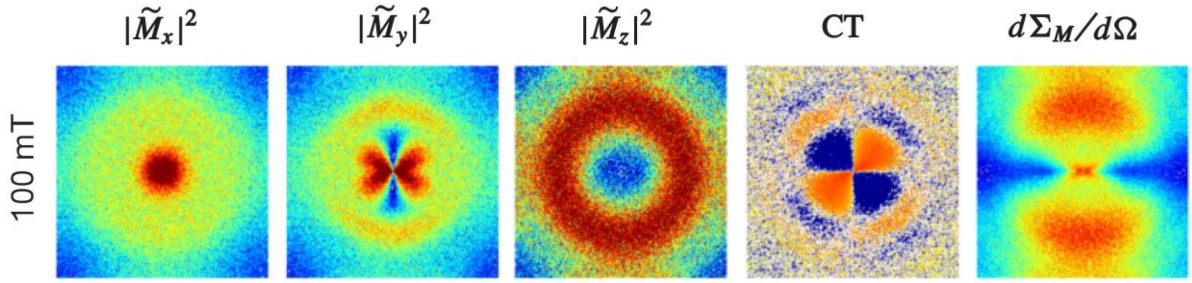

Fig. 1. Results of micromagnetic modeling for the Fourier components of magnetization and the total magnetic neutron scattering.

References

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Pauli paramagnetism and superconducting flux line lattices

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When flux lines enter superconductors, they give rise to large length-scale fluctuations in magnetic field that can be probed to investigate the superconducting parameters, such as the coherence length and penetration depth. The flux line cores can be thought of as regions of normal state inside the superconducting state, and if that normal state is affected by the magnetic field in an unusual way, this can also be seen. The most common reason for this is enhanced Pauli paramagnetic effects, which act to split Cooper pairs by favouring alignment of the electron spins. A clear signature of this has been observed in $CeCoIn_5$ [1] and $CeCu_2Si_2$ [2], and is also thought to be responsible for weaker anomalies seen in $TmNi_2B_2C$ [3] and possibly $YBa_2Cu_3O_7$ [4,5] To bring these results together, we will present a physically-motivated algebraic expression for the vortex lattice factor in Pauli-limited superconductors, drawing on results obtained from first-principles calculations [6].

References

[1] Bianchi, A. D. *et al. Science* 319, 177–180 (2008).
[2] Campillo, E. *et al.*, submitted to *Nature Communications* (2021).
[3] DeBeer-Schmitt, L. *et al. Phys. Rev. Lett*. 99, 167001 (2007).
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[5] Campillo, E. *et al.*, in preparation (2021).
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Recent Small Angle Neutron Scattering (SANS) Measurements using dynamic B-fields

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This presentation will discuss selected recent experiments using magnetic sample environments at NCNR-SANS beamlines. Key design parameters and choices of the setups as well as the data analysis will be discussed with a focus on experiments with dynamic B-fields. The potential use of advanced techniques to prepare the neutron beams like time focusing [1] and phase locking [2] of chopper signals will be part of the outlook for magnetic SANS as this talk aims to give an optimistic perspective for future steps and possibilities based on these experiments.

References

[1] R. Gähler et al., ILL SC, 99 (1999), p. 73
[2] M. Bleuel NIM A 921 (2019), p. 184

Vortex lattice studies in UPt_3

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Subjecting a type-II superconductor to a magnetic field will cause the formations of quantized vortices. The vortices introduce singularities in the order parameter and may be used as probes of the superconducting state in the host material. Moreover, the structural and dynamical properties of vortex matter is of both fundamental interest as well as practical importance. Here I will discuss our small-angle neutron scattering studies of the vortex lattice in UPt_3 from both of the above-mentioned perspectives.

Identification of broken time-reversal symmetry (BTRS), a key component of chiral symmetry, of the superconducting order parameter has presented a challenge in bulk superconductors. The two leading candidates for bulk chiral superconductors are UPt_3 and Sr_2RuO_4, although evidence for comes largely from surface-sensitive measurements and have recently been called into question for the latter. In our SANS studies of UPt_3 we discovered a previously unknown non-monotonic VL rotation in the so-called B-phase with increasing field. Furthermore, the VL rotation depends on the field history, demonstrating that the vortices possess an internal degree of freedom and providing direct evidence for bulk BTRS in this material.

The UPt_3 VL undergoes a gradual disordering on a time scale of tens of minutes as it is subjected to a beam of cold neutrons. The disordering is due to local heating events caused by neutron induced fission of ^{235}U, which leaves an increasing fraction of the sample in a quenched vortex glass state. The disordering rate is proportional to the vortex density, suggesting a direct relation to collective VL properties such as the elastic moduli. While the system does not spontaneously re-order once the local heating has been dissipated, it is possible to re-anneal the VL by the application of a small-amplitude field oscillation. This shows that no permanent radiation damage of the UPt_3 crystal occur within experimental time scales. Our results demonstrate a novel avenue for vortex matter studies, allowing an introduction of localized and reversible quenched disorder.

References

[1] K. E. Avers *et al*., Nat. Phys. **16**, 531-535 (2020).
[2] K. E. Avers *et al*., arXiv:2103.09843.

Magnetic skyrmions for unconventional computing and revealing latent information

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Novel computational paradigms in combination with proper hardware solutions are required to overcome the limitations of our state-of-the-art computer technology. [1-3] In this talk, I will focus on the potential of topologically stabilized magnetic whirls – so-called skyrmions for reservoir computing. Reservoir computing is a computational scheme that allows to drastically simplify spatial-temporal recognition tasks. We have shown that random skyrmion fabrics provide a suitable physical implementation of the reservoir [4,5] and allow to classify patterns via their complex resistance responses either by tracing the signal over time or by a single spatially resolved measurement. [6]

In a second part of the talk I will introduce two new data analysis tools. While often a significant effort is made in enhancing the resolution of an experimental technique to obtain further insight into the sample and its physical properties, an advantageous data analysis has the potential to provide deep insights into given data set. [7, 8]

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Small-angle neutron scattering for magnetic nanoparticles

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Small-angle neutron scattering is a widely used technique in studies of magnetic materials. The unique properties of neutrons like the sensitivity for light elements and interaction with unpaired electrons of atoms make them a powerful probing tool. The magnetic nanoparticles are usually coated with a organic shell for stabilization in a solvent and the application of small-angle neutron scattering allows to determine magnetic as well as structural properties of the nanoparticles simultaneously. In this talk the application of small-angle neutron scattering for determination of magnetic properties of the nanoparticles is presented. Some theoretical considerations are presented on the possibility of magnetic size determination from contrast variation experiments only [1]. An utilization of polarized neutron beam in small-angle scattering together with polarization analysis is presented for detailed magnetic structure determination. Limitations, peculiarities of experimental data as well as advantages of the technique are shown together on few examples [2, 3].

References

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[2] D. Zákutná, D. Nižňanský, L.C. Barnsley, et al., Phys. Rev. X **10**, 031019 (2020)
[3] T. Köhler, A. Feoktystov, O. Petracic, et al., submitted to Nanoscale (2021)

Measurements of spin wave stiffness in helimagnets by small-angle polarized neutron scattering

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We have developed a method for measuring the spin wave stiffness in helimagnets with Dzyaloshinsky-Moriya interaction in a completely polarized state using small-angle scattering of polarized neutrons [1]. It has been experimentally proved that the dispersion of magnons in this state has an anisotropic appearance, since the neutron scattering intensity pattern is registered as two circles for neutrons with the gain and loss of magnon energy, respectively. The centers of the circles are shifted by the momentum transfer value equal to the helix wave vector ± $\mathbf{k}_S$, which is oriented along the applied magnetic field H. The radius of the circles is directly related to the spin wave stiffness of the magnetic system, but depends on the magnitude of the magnetic field. This scattering depends on the polarization of neutrons, showing the chiral nature of the spin waves in the Dzyaloshinsky-Moriya helimagnet in the polarized state.

We have measured the temperature dependence of the spin wave stiffness of the following compounds: MnSi [1], $Mn_{1-x}Fe_xSi$ with x = 0.03, 0.06, 0.09, 0.10 [2], $Fe_{1-x}Co_xSi$ with x = 0.25, 0.30, 0.50 [3], FeGe [4], $Mn_{1-x}Fe_xGe$ with x = 0.80 [5], as well as Cu_2OSeO_3 [6].

References

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Data analysis for magnetic small-angle scattering with SasView

D. Honecker

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SasView[1] is an open-source data analysis package for small-angle scattering, developed by an international collaboration of facilities and universities. Primarily, SASview provides an easy-to-use interface for model fitting to 1D and 2D scattering patterns, supporting oriented anisotropic particle systems, including resolution smearing, and—as one of the latest developments—considering a 3D magnetic field geometry and longitudinal neutron polarimetry. A variety of alternative approaches to obtain structural parameters from the data are also implemented in the software, including model-free analysis by integral parameters like the radius of gyration, Porod behavior, and scattering invariants, as well as an inversion to the real-space pair-distance distribution and correlation function.

SasView provides a large library of form and structure factors and allows for easy construction of user-defined compound models. New models not already available in the model repository can be easily shared with the community via the online model marketplace. SasView also supports calculations on Graphical Processing Units (GPUs), which allows for faster evaluation of complex model functions. Additionally, SasView enables processing multiple data sets simultaneously with a shared set of (constrained) parameters as needed to coherently analyse a set of magnetic field-dependent measurements or polarised neutron data. More complex magnetic structures beyond uniformly magnetised particles commonly demand micromagnetic simulation using software packages like OOMMF and Mumax^3. A scattering calculator tool allows generating from a micromagnetic simulation the corresponding SANS scattering cross-section.

One of the challenges is developing a user-oriented state-of-the-art analysis for magnetic SANS to improve data inspection and to effectively retrieve the information entailed in the data. In this talk, I will present the latest developments in SASview to analyse magnetic scattering data and discuss how to contribute to its further enhancement.

References

[1] http://www.sasview.org

High-Precision Studies of Ferromagnetic Quantum Matter

M. Janoschek[1,2]

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[2] *Department of Physics, University of Zurich*

In the vicinity of ferromagnetic quantum phase transitions a host of interesting quantum matter states including the formation of spin density waves [1], topological non-Fermi liquid behavior [2] and chiral p-wave superconductivity [3] have been reported. Here the latter is considered a possible route to implement decoherence free quantum computing [4]. Although, Belitz-Kirkpatrick-Vojta (BKV) theory shows excellent agreement with experiments both on clean [5] and disordered materials [6], currently little information is available on the underlying low-energy spin fluctuations that are widely believed to be crucial for the formation of ferromagnetic quantum matter. Notably, the outstanding challenge is that the underlying characteristic energy scales that drive these quantum matter states are tiny compared to typical electronic energy scales in solids, and are, in turn, notoriously difficult to measure. Here we discuss some of our recent results to showcase current advances in the resolution of neutron spectroscopy. Using the novel Modulated IntEnsity by Zero Effort (MIEZE) technique implemented at the neutron spectrometer RESEDA in Munich in SANS geometry, we achieve ultra-high energy resolution of 1 μeV and reveal that the spin fluctuations in the prototypical ferromagnet UGe_2 exhibit a dual nature arising from the interplay of localized and itinerant electronic degrees of freedom consistent with spin-triplet superconductivity proposed for this material [7].

References

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MIEZE-SANS: a spin-echo technique for magnetic phenomena

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Small angle neutron scattering (SANS) represents an exceptionally important probe for a wide range of scientific problems. In recent years, the interplay of processes on the nanoscale with macroscopic quantum phenomena with long range order has attracted great interest in many different areas of condensed matter physics. Despite this strong case for SANS, there is essentially no dedicated instrumentation for studies of the dynamical properties in the SANS parameter range.

The MIEZE (Modulation of Intensity with Zero Effort) technique, is in essence a high-resolution, spin-echo, time-of-flight technique. In contrast to classical neutron spin-echo, all beam preparation and therefore all spin manipulation is done BEFORE the sample, opening up the possibility of introducing depolarizing conditions at the sample position. Therefore, magnetic or strongly incoherently scattering samples can easily be measured without loss of signal. Furthermore, it is possible to apply large magnetic fields at the sample position, making MIEZE an excellent tool for studying the dynamic behavior of magnetic phenomena [1-3].

The combination of MIEZE and SANS allows for the study of dynamical properties in the SANS regime, which offers the possibility to explore for example fluctuations at quantum phase transitions, magnon dynamics, or the melting of superconducting vortex or skyrmion lattices.

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Interplay Between Internal Magnetic Morphology and the Response of Solvated Nanoparticles

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The ability to construct and functionalize magnetic nanostructures for biological applications and medicine has increased dramatically during the past two decades, and this has expanded potential biomedical uses including therapeutic heating (hyperthermia), magnetic particle tagging of tissues, and magnetic particle imaging. When exposed to alternating magnetic fields, magnetic nanoparticles can generate heat through loss power mechanisms that continue to challenge a complete physical description. Here we shall discuss the dramatic differences observed among measured specific loss power generated by three magnetic iron oxide nanoparticle constructs having comparable size and chemical composition [1]. Small angle neutron scattering with polarization analysis of the neutron spin reveals unexpected and complex coupling among magnetic domains within the nanoparticle cores that influence their interactions with external magnetic fields. These results underscore the important contribution of internal magnetic domains for hysteresis heating, in addition to the recognized contributions of particle size, shape, and magneto-crystalline anisotropy. The idea of internal magnetic domains can be further exploited to alter the tendency of the nanoparticles to chain when exposed to external magnetic fields. This in turn impacts techniques such as magnetic relaxometry (which can differentiate nanoparticles that are "free" from "bound", *e.g.* to a tissue of interest) and magnetic particle imaging (which uses the non-linear response of the magnetization to an applied magnetic field to create an image). To this end, we demonstrate how ferrite nanoparticles composed of similar magnetic domain sizes, but of dissimilar total radii, exhibit markedly different responses to the presence of a static magnetic fields from remanence up to 0.5 T.

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Quantitative Understanding of Superparamagnetism in Soft Ferromagnetic Metallic Nanoparticles *via* Polarized Small-Angle Neutron Scattering

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Thanks to advances in synthesis that enable control over size, structure, properties, and functionalization, magnetic nanoparticles (NPs) present unique opportunities in data storage, cancer treatment, biomedical imaging, *etc.* While superparamagnetism (SP) dominates the properties of magnetic NPs, *quantitative* understanding of SP blocking in NP assemblies remains a challenge. We address this here *via* comprehensive magnetic characterization and analysis of model soft ferromagnetic NP ensembles based on elemental Ni. NPs were synthesized by hot injection of a Ni-oleylamine (OAm) complex into trioctylphosphine (TOP), with tight size control achieved *via* the TOP:OAm ratio, reaction time, and differential centrifugation.[1] X-ray diffraction, transmission electron microscopy, and various spectroscopies reveal polycrystalline/twinned FCC Ni NPs with mean diameter ($<D>$) from 4 to 22 nm, dispersity down to 10%, and TOP/OAm ligands.[1] SP blocking temperatures (T_B) are carefully determined, quantitatively accounting for the substantial yet frequently ignored effects of dispersity, yielding mean T_B ($<T_B>$) from 5 to >300 K.[1] Remarkably, *quantitative* reproduction of the size-dependent $<T_B>$ is achieved, *with no adjustable parameters*, by accounting for the size distribution, effective ferromagnetic volume (V_{mag}), temperature-dependent bulk magnetocrystalline anisotropy, and random shape anisotropy due to statistical deviations from spherical.[1] Critically, unpolarized and polarized SANS provides detailed quantitative insight into the internal chemical and magnetic structure of the NPs, including a sub-nanometric non-ferromagnetic shell that limits V_{mag}, arising from phosphide formation due to reactivity with TOP ligands.[2] Accounting for this, the size-, temperature-, and field-dependent SANS is then *quantitatively* reproduced using the bulk magnetic properties of Ni.[2] Small discrepancies related to potential surface and defect effects[1] will be discussed. 3M and the DOE Center for Quantum Materials are thanked for support of this work.

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Spin Canting in Magnetic Spinel Nanoparticles

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The saturation magnetization of spinel phase magnetic nanoparticles is often reduced for small particle sizes, and this talk will examine the origin of this phenomenon, highlighting how magnetic small angle neutron scattering (SANS) has been critical to understanding the effect of spin canting. Early work postulated the existence of an empirical magnetic "dead" layer, without providing a physical mechanism. Kodama and Berkowitz postulated the existence of a surface spin glass, which was consistent with experimental data for ball-milled particles that contained a lot of structural disorder, but could not explain the behavior of highly crystalline nanoparticles. Scanning transmission electron microscopy has shown that particles containing subtle antiphase boundaries can have reduced magnetization due to changes in the proportion of ferromagnetic and antiferromagnetic superexchange interactions. SANS with polarized neutrons provides an alternative technique to determine magnetic correlations, and it has been particularly useful in understanding complex phenomena in spinel ferrite nanoparticles. We focus on cases where the particles are monodisperse, single crystal, and have self-assembled into close-packed lattices, which leads to additional Bragg contrast at the superlattice peak. The simplest case if $CoFe_2O_4$, where the large magnetocrystalline anisotropy leads to uniform magnetization within the particles and slight canting of different particle moments within the assembly. Fe_3O_4, which has moderate anisotropy, shows unusual behavior parallel and perpendicular to the applied field. Perpendicular magnetization is reversibly induced in large fields and at higher temperatures. This is consistent with earlier Mössbauer spectroscopy measurements at high fields, where spin canting was a suggested mechanism by no direct evidence of magnetic correlations lengths was available. Finally results for Fe_3O_4/$MnFe_2O_4$ core shell and $MnFe_2O_4$ nanoparticles are discussed. Both have low anisotropy Mn ferrite components, but stronger interparticle coupling effects are seen in the core-shell case.

Field-induced vortex-like spin textures in reentrant spin glasses

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Spin glasses (SG) are archetypal disordered magnetic systems that have mobilized continuous efforts for decades. In a mean-field approach, a "canonical" SG forms when the average magnetic interaction term is smaller than the width of the interaction distribution. Otherwise, ferromagnetic and SG order coexist in so-called "reentrant" spin glasses (RSG) [1].

In the end of the 80^{ies}, it was discovered that nanoscopic magnetic textures could be stabilized under an applied magnetic field in several RSGs [2-4]. These textures correspond to the cancellation of the transverse magnetization over a finite length scale, thereby resembling spin vortices. Not predicted by current theories, they are therefore good candidates to help refining our understanding of the microscopic properties of the RSGs.

We have recently revisited the properties of these vortices using magnetic SANS on two kinds of RSGs, with the aim of *(i)* extending the explored field range [5] and *(ii)* crossing the RSG → SG transition line for the first time [6]. We will show that these defects obey generic scaling laws, independent of the sample nature (crystalline or amorphous), and vanish in the SG phase. We will also discuss how this apparent "universality" can be tested against Monte Carlo simulations, which in turn allow clarifying the nature and spatial distribution of the spin vortices.

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Experimental Perspectives of Skyrmions in Chiral Magnets

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The discovery of skyrmion lattices and isolated skyrmions in magnetic materials exhibiting bulk or interface inversion-asymmetry and associated Dzyaloshinskii-Moriya interactions has triggered massive research activities towards the development of devices and applications based on topological spin solitons in real space, alluding to skyrmions as most prominent examples.

Early studies of the fundamental properties of skyrmion systems have revealed strong effects of Berry phases that may be described by emerging electric and magnetic fields. Recent advances focus in addition on skyrmions in antiferromagnetic and geometrically frustrated materials, tailored creation and decay routes of skyrmions, the dynamical properties of skyrmions, and skyrmions in the quantum limit as well as avenues towards more sophisticated topological textures such as hopfions.

Experimental and theoretical evidence that thin films, nano-wires and nano-dots are particularly amenable to the formation of topological spin solitons, underscore their potential for major breakthroughs in applications. Moreover, advances in thin-film heterostructures demonstrate that skyrmions stabilized by interface-mediated Dzyaloshinskii-Moriya interactions as well as further stabilization mechanisms may be tailored for applications at room temperature.

In this talk I will review recent progress in research on Skyrmions in magnetic materials, with a particular focus on the potential of small-angle neutron scattering as a particularly powerful experimental probe.

Synthesis and Characterization of Nanocrystals of Transition Metal Oxides

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Nanocrystals of magnetic materials can show interesting behaviors stemming from the combination of chemistry and magnetic configuration, which also determines or directs their final purpose.
Different examples of magnetic nanocrystals of antiferro- and ferrimagnetic transition metal oxides, synthesized and manipulated by wet-chemistry methods, will be detailed describing the magnetic behavior.
Their magnetism originates from the increased complexity in spin textures, topology and/or frustration in three dimensions, and associated to different internal interfaces, grain boundaries or surface facets.

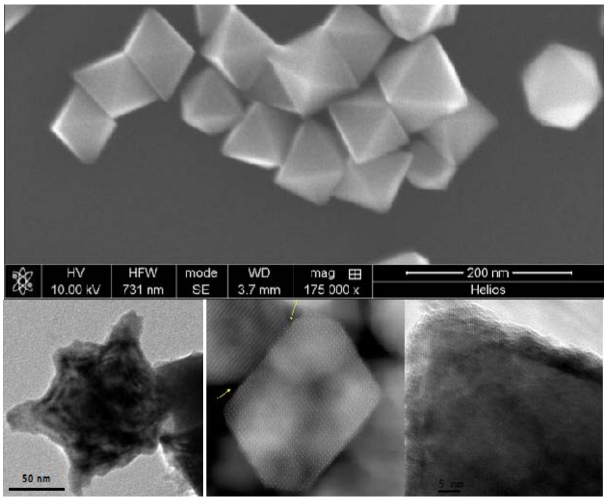

Figure 1. TEM images of: CoO-Co_3O_4 octahedron-shaped nanocrystals (top), FeO-Fe_3O_4 cubic nanostructures with elongated tips (bottom, left), $ZnFe_2O_4$ truncated octahedral (bottom, center) and an internal interface between spinel crystalline structures in a polyhedron shaped nanocrystal (bottom, right).

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Neutron diffuse scattering from magnetically disordered compounds

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Neutron scattering is a well-established method to determine magnetic structures and correlations in condensed matter. The methods extend to diffuse scattering, with the aim of determining pair-correlation functions in compounds with magnetic disorder. The magnetic disorder is usually due to frustration from competing interactions which may be associated with chemical or structural disorder, or may be geometric due to the local coordination of the magnetic moments. Polarization analysis techniques are particularly powerful, allowing the separation of the chemical and magnetic contributions to the scattering and providing directional information on the moment orientations in the magnetic structures. Initial scientific interest focused on intermetallics, and particularly spin glasses, resulting in the construction in the 1970s and 1980s of neutron diffractometers with polarization analysis dedicated to measure diffuse scattering. Interest in the techniques has waxed and waned, but it is currently in the midst of an unprecedented surge that began in the late-2000s. The current enthusiasm is primarily driven by three developments: the availability of significantly improved instrumentation, the creation of powerful data analysis software, and the discovery of exotic physics in geometrically frustrated magnetic compounds with spin ice being an archetypal example.

I will strive to summarize the developments and highlight some applications of neutron diffuse scattering with polarization analysis, with an emphasis on experimental examples that may also be of interest to the SANS community.

Unravelling the magnetic and chemical morphologies of nanoparticles by SANS

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Magnetic nanoparticles (MNPs) reveal unique magnetic properties, such as superparamagnetism, which make them relevant for data storage, electronic and mechanical engineering, and biomedical applications. Being intrinsic to nanomaterials, the performance of MNPs is crucially determined by their chemical composition and surface effects, such as surface spin disorder, which have a strong impact on the resulting magnetic properties of MNPs and their performance [1-2]. Despite lots of scientific attention of the MNPs, it is challenging to isolate surface-related effects from the effective anisotropy using integral magnetization measurements. Thus, a key challenge in MNPs research remains in quantitative interpretation of the spin configuration and the nanoscale distribution of the magnetization and spin disorder. Polarized small-angle neutron scattering (SANS) is a versatile technique, which allows investigating nanoparticle magnetization with the necessary spatial resolution [3]. In this contribution, we will present our recent results on the spin disorder in ferrite nanoparticles induced during the synthesis. The nanoparticles show an overall homogeneous distribution of Co:Fe, only the sensitivity of polarized SANS to the density variation reveals the exact chemical core-shell morphology of the as-prepared samples. By using polarized SANS, we disentangle the magnetic field response of the core and shell magnetization.

For fully oxidized single phase MNPs, we will show that the magnetization is still affected by a near-surface magnetic disorder. We have recently shown [4], that the magnetization configuration inside of MNPs may not be static – as often presumed – but rather susceptible to the magnetic fields with the occurrence of field-dependent magnetization processes. In consequence, we could observe a significant field-induced growth of the total magnetic moment by a magnetic ordering transition at the structurally disorder surface. Our study challenges the traditional macroscopic magnetic characterization with polarized SANS revealing the surface spin disorder apart from magnetic disorder in the MNP interior.

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Abstracts of Posters

(in alphabetical order)

Vortex Matter of Intertype Superconductors studied by Neutron Methods and Molecular Dynamics Simulations

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In the intermediate mixed state (IMS) in superconducting niobium, the mixed attractive and repulsive vortex interaction leads to the clustering of vortices into domains [1]. Featuring behavior outside the conventional categories of type-I and type-II, this regime is also denoted intertype superconductivity [2].

Using a combination of several neutron techniques, we have investigated the hierarchical properties of the IMS in bulk niobium on length scales of the vortex lattice (~100nm, SANS), the domain structure (~10mum, VSANS/USANS) and the sample size (~10mm, NGI) [3,4,5].
In addition we have performed molecular dynamics simulations to access the microscopic vortex arrangement and domain structure. In a novel approach, the simulations use results from an extended Ginzburg-Landau formalism to model the vortex interactions [2].

The combined results give detailed insight into the properties of the vortex domain and the underlying vortex lattice in a field cooled IMS transition. A special focus of the study was on the influence of vortex pinning and the external magnetic field, which highlights the well-defined properties of the IMS and its fundamental character.

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Ab-initio study of the structural, magnetic and electronic properties of $Ce_{0.75}W_{0.25}O_2$: spintronic application

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Comprehension of materials physics requires fundamental knowledge of its properties; simulation plays an important role in determining these properties. The latter minimizes the costs of expensive and dangerous requirements of an experiment or various models about specific phenomenon that is difficult to achieve experimentally. In this study, we discussed an ab initio analysis of the structural, electronic and magnetic properties of W doped CeO2 compound. Our assessments were performed by the augmented plane wave method FP LAPW founded on the DFT (density functional theory) and introduced in the Wien2k calculation code. This investigation of the electronic band, structural, and magnetic properties were performed using a WC-GGA for exchange-correlation potential. The host compound CeO2 had doped with transition metal atoms W in the doping concentration of 25% to replace the Ce atom. After substitution of atom, the compound of W0.25Ce0.75O2 was formed. The band structure of this doped compound was plotted for elucidate the semiconductor nature of material, with band gap at the Fermi level (EF), the band structure shows that CeO2 doped by Tungsten (W) has a direct gap (M–M) in the both spin channel. In our study, Volume optimization predicts that the compound is more stable in ferromagnetic state than in the paramagnetic state. The doped atom plays a vital role in increasing the magnetic moment of the super cell with magnetic moment of around 1.998 μB. Calculated results indicate that the electronic and magnetic properties provide a new route to the experimentalist for the potential applications in spintronics devices.
Keywords: CeO_2, FP-LAPW, Wien2k, WC-GGA, Properties.

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Current-induced self-organisation of mixed superconducting states

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Small-angle neutron scattering is used in combination with transport measurements to investigate the current-induced effects on the morphology of the intermediate mixed state domains in the intertype superconductor niobium. We report the robust self-organisation of the vortex lattice domains to elongated parallel stripes perpendicular to the applied current in a steady-state. The experimental results for the formation of the superstructure are supported by theoretical calculations, which highlight important details of the vortex matter evolution. The investigation demonstrates a mechanism of a spontaneous pattern formation that is closely related to the universal physics governing the intermediate mixed state in low-κ superconductors [1].

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Grazing Incidence SANS from Helimagnet MnSi Thin Films

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In 2009, small-angle neutron scattering (SANS) was used to study the complex phase diagram of bulk MnSi, revealing a topological skyrmion phase [1]. However, to date, a consistent determination of the magnetic order of thin film MnSi remains elusive. Data obtained and interpreted by different research groups employing different measurement techniques often paints two very clear, but different, pictures of the non-collinear magnetic order of thin film MnSi [2,3]. These discrepancies are fuelled by the lack of a single, direct, and microscopic probe of skyrmions in thin films. While SANS proved to be an absolute probe of skyrmions in bulk materials, the technique is not suitable for thin films due to the limited scattering volume of the sample [3]. However, a SANS measurement performed under grazing incidence opens the possibility to obtain distinct scattering patterns from thin-film samples by SANS. In this work we employ grazing-incidence SANS to characterise the phase diagram of thin film MnSi [4] alongside susceptibility, first-order reversal and planar Hall data in search of a topological skyrmion lattice. Grazing incidence SANS data identifies the formation of an out-of-plane helical spin texture with a field-dependent propagation length which vanishes below H_{c2} potentially indicating the presence of an additional phase close to the field-polarised phase boundary, as detected in our first-order reversal and planar Hall data. The work provides insight into the effects of shape anisotropy, surface anisotropy and dimensionality on the magnetic phase diagram of MnSi, and will help to obtain the necessary knowledge required for the design of skyrmion-based spintronic devices.

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Structure and dielectric study

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Dielectric materials with high energy density are currently in high demand. The dielectrics with a medium dielectric constant, high breakdown strength, and low polarization hysteresis are the most promising candidates for high-power energy storage applications (1). In this perspective we have studied the compounds with general formula Re (A 3+ B 4+) O5, These compounds constitute a class of oxides with remarkable magnetic and electrical properties that make them interesting for the fundamental and technological levels. They are promising in a wide range of applications such as multiferroic devices, spintronics and cathode materials with high energy densities. PrFeTiO5 compound was synthesized using solid-state reaction method. X-ray diffraction (XRD) measurements were performed at room temperature and the data were analyzed using Rietveld method. The analysis of XRD patterns shows a single phase indexed in orthorhombic system. This compound is isostructural with ReMn 2 O 5 the dielectric properties and the ac-conductivity were studied in the frequency range 10-106 Hz and the temperature range 305-625 °K. The experimental results indicate that the ac-conductivity σ ac (f), the dielectric constant ε', and the loss dielectric ε" depend on temperature and frequency.

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Low dimensional substructures in hulsite oxyborates

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Magnetic oxyborates of the 3d transition metals are good examples of strongly correlated systems. Low-dimensional substructures are characteristic of these insulating compounds, and they are present in the form of ladders in ludwigites, ribbons in warwickites, and planes in hulsites. These compounds have shown complex and intriguing physical properties that depend on their elementary composition and have been studied for decades. Among magnetic oxyborates, those with hulsite structures are less studied, it is composed of two planar substructures. The magnetic properties of the substructures are remarkably interesting. For $Ni_{5.15}Sn_{0.85}(O_2BO_3)_2$, it is found a partial magnetic order at 180 K, while the other substructure seems not to be ordered. The structural, magnetic, and thermodynamic properties are presented.

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Weyl mediated helical magnetism in NdAlSi

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Weyl semimetals are topologically nontrivial phases of matter that sustain low energy excitations in the form of massless fermionic quasiparticles known as the Weyl fermions [1]. It is necessary to break either inversion or time-reversal symmetry to establish a Weyl semimetal. A rare occasion arises, however, if a material breaks both symmetries and offers an opportunity to study the interplay between magnetism and Weyl fermions [2]. Here we present an extensive experimental and theoretical study of a new Weyl semimetal, NdAlSi, that breaks both symmetries. Our neutron diffraction experiment reveals the leading instability of the Weyl semimetal is to long-wavelength incommensurate order followed by a lower temperature transition to commensurate ferrimagnetism. Using quantum oscillation measurements and density functional theory, we find that the incommensurate wavevector connects different branches of the Fermi surface that contain Weyl fermions. This raises the interesting possibility of a magnetic order driven by relativistic electrons in NdAlSi [3].

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QUOKKA, the Pinhole Monochromatic Small Angle Neutron Scattering (SANS) instrument for Magnetic Studies

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QUOKKA is a world-class 40 m SANS instrument with high flux and a state of the art high count rate detector. The instrument is designed to enable measurements at scattering vectors over three orders of magnitude, from 3 x 10^{-4} $Å^{-1}$ to 0.7 $Å^{-1}$ and features incident beam polarisation and polarisation analysis [1]. A wide range of sample environments is available including a 1 T vertical electromagnet, a 1.5 T closed cycle horizontal magnet, a 10 T wet horizontal field magnet and a newly commissioned 7 T asymmetric re-condensing vertical magnet with a maximum ramping rate of 0.5 T/min, the latter optimised for polarisation and analysis studies. Several examples of magnetic SANS performed on QUOKKA are presented [2-4].

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Rare-Earth-Free Permanent Magnets based on Exchange-Coupled and Decoupled Composites

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The theory on exchange-spring magnets was a breakthrough in the field of rare-earth-free permanent magnets. The model predicts a significant boost in the magnetic performance (BH_{max}) through combination of a hard and a soft magnetic phase, as long as the phases are magnetically exchange-coupled.[1] However, achieving an effective coupling in real systems has proven rather challenging in practice, preventing the proclaimed magnetic enhancement from being transferred from the theory into functional applications.[2]

The $CoFe_2O_4$(hard)/CoFe(soft) nanocomposite has drawn attention as it can be easily prepared in different compositions through partial reduction of $CoFe_2O_4$ nanoparticles.[3,4] In a recent study combining experiments and micromagnetic calculations, we obtained a 10-fold increase on BH_{max} for an weakly coupled sample.[5] On the other hand, maximizing exchange-coupling caused coercivity to collapse (and in turn, BH_{max}). Based on the calculations, this counterintuitive observation is a result of the soft phase having a size above the single-domain size. It appears that when the both magnetic phases (hard and soft) are exchange-coupled, soft particles in multi-domain configuration can demagnetize the hard phase. However, there has been no experimental evidence of this so far.

In the present work, we plan to investigate the core-shell nature of the particles and the magnetic interactions across the phase interfaces based on polarized small-angle neutron scattering (SANS) data. Additionally, electron energy loss spectroscopy (EELS-TEM) should allow identifying which of the magnetic compounds integrates the cores and which is conforming the shells.

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Investigation of structural and magnetic changes in transformer oil-based ferrofluids induced by electric field

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Dispersion of superparamagnetic nanoparticles (SPN) in transformer oils constitute an extraordinary cooling and electrical insulating medium (ferrofluid). The peculiar dielectric behavior and breakdown mechanism is still not clear. Recently, SPN aggregation in electric fields was deduced from dielectric measurements and formation of anisotropic structures was proved by SANS [1]. Thus, the aim of the experiment was to investigate the relation of the electric field induced structural changes in a ferrofluid in regard to their magnetic properties. SANSPOL intensities I+(q), I-(q) were measured depending on the magnetic field acting both, alone and simultaneously with the external electric field. It was found that the electric voltage acting on the ferrofluid causes a remarkable increase in scattering intensity at small q range. This increase is proportional to the strength of the field. The increase in the intensity originates from the presence of larger aggregates in the sample which were induced by the applied electric field. However there is no remarkable difference between the scattering intensity of up and down neutron spins, so pointing out the absence of any magnetic structure in the created aggregates. The identical SANSPOL curves are observed for both cases, in the absence and presence of the electric field. A noticeable difference in the SANSPOL curves has been detected in the case, when the sample is simultaneously exposed to both, electric and magnetic field. In magnetic field only, the SANSPOL curves indicate the well-known chain like anisotropy in the magnetic field induced aggregates. The most pronounced difference in the SANSPOL curves is seen in the case when both, magnetic and electric fields act on the ferrofluid sample. As the magnetic field was applied firstly on the sample and subsequently the electric voltage was switched on, one can assume that the electric field enhanced the magnetic anisotropy in the formed aggregates.

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Small-angle neutron scattering of nanomagnetic gyroid structures

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Gyroids are minimal-surface structures that can be formed by self-assembly of block co-polymers. Such soft matter structures, which also occur naturally in butterfly wings, have attracted recent research interest due to their interesting topological features and nanoscale local curvature, which can e.g. be interesting for photonic applications. In combination with a magnetic material their unique connectivity structure – with three legs meeting in each vertex – also makes gyroids also a three-dimensional artificial spin system with a high degree of geometrical frustration, which potentially could exhibit a classical spin-liquid phase.

Here, I will present small angle neutron scattering (SANS) measurements from a structurally-single-domain magnetic nickel network electroplated into a self-assembled block co-polymer gyroid template. Scattering from the three-dimensional structure with cubic lattice symmetry (space group $I4_132$) reveals a periodicity of ~62 nm. We used a polarised neutron beam (i.e. half-polarised SANS) to measure the scattering signal at applied fields of 1 T, 100 mT and 20 mT, and observed changes in the magnetic SANS signal, which becomes more diffusive at low fields. This indicates a higher degree of magnetic disorder and frustration.

To elucidate the relationship between the complex structure and emergent magnetism, we performed micromagnetic simulations and calculated the respective scattering intensities. We aim to compare the simulations to the observed SANS data to obtain an average nanomagnetic model at each applied magnetic field.

Magnetic Guinier Law

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Small-angle scattering of X-rays and neutrons is a routine method for the determination of nanoparticle sizes. The so-called Guinier law represents the low-q approximation for the small-angle scattering curve from an assembly of particles. The Guinier law has originally been derived for nonmagnetic particle-matrix-type systems and it is successfully employed for the estimation of particle sizes in various scientific domains (e.g. soft-matter physics, biology, colloidal chemistry, materials science). An important prerequisite for it to apply is the presence of a discontinuous interface separating particles and matrix.

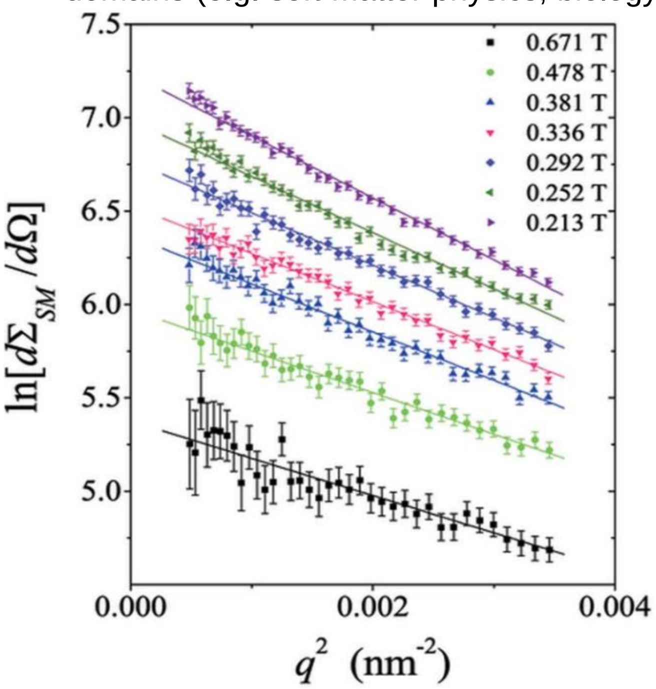

Figure 1: Guinier plot $\ln(d_{SM}/d\Omega)$ versus q^2 and fits (solid lines) at selected values of the internal magnetic field.

Here[1], the Guinier law is introduced for the case of magnetic small-angle neutron scattering and its applicability is experimentally demonstrated for the example of nanocrystalline cobalt. It is well known that the magnetic microstructure of nanocrystalline ferromagnets is highly nonuniform on the nanometre length scale and characterized by a spectrum of continuously varying long-wavelength magnetization fluctuations, i.e. these systems do not manifest sharp interfaces in their magnetization profile. The magnetic Guinier radius depends on the applied magnetic field, on the magnetic interactions (exchange, magnetostatics) and on the magnetic anisotropy-field radius, which characterizes the size over which the magnetic anisotropy field is coherently aligned into the same direction. In contrast to the nonmagnetic conventional Guinier law, the magnetic version can be applied to fully dense random-anisotropy-type ferromagnets.

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Coexistence of disorder and antiferromagnetism in $NdCu_2$ nanoparticles.

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Bulk Rare Earth intermetallics were object of an exhaustive scrutiny due to the rich variety of magnetic structures and the existence of crystal-field effects [1]. A family of those is constituted by binary systems of RX_2, where R = Rare Earth and X is usually a non-magnetic metal. In this, the magnetic coupling is assured by RKKY interactions. The study of metallic nanoparticles (NPs) of RCu_2 (R = Tb, Nd) revealed the presence of two magnetic environments (phases) with a disordered moment shell and an antiferromagnetic (AF) core via DC-magnetization as well as AC-susceptibility characterization. The amount of those phases is controlled by the NP size. It appeared clear that the magnetic structures are far from being trivial. In order to address the magnetic arrangements, we have used Neutron Diffraction (ND) and Small-Angle Neutron Scattering (SANS). The outcome for the $TbCu_2$ system showed that the AF structure in the bulk alloy (T_N = 48 K) remains in the NPs, and that there was a reduction of the ordered moment due to uncompensated AF chains [2]. The magnetic structure for $NdCu_2$ is more complex than that of $TbCu_2$, as ND analyses reveal the existence of two magnetic phases with an oscillating component of the Nd^{3+} moments. ND have also revealed that the bulk reorientation from a commensurate structure ($T<T_R$ = 4.5 K) to an incommensurate arrangement ($T_R<T<T_N$) is not maintained in the NP regime. Instead, a magnetically frustrated interacting Spin Glass phase takes place at $T<T_f$ = 5 K.

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Dipolar correlations in square arrays of magnetic nanoparticles

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Ordered arrays of magnetic nanoparticles have attracted great interest in fundamental research, e.g. in the study of dipolar and exchange coupling, as well as for technological applications in spintronics and information technology [1, 2].

Long-range ordered monolayer arrays of nanocubes on 1 x 1 cm² silicon substrates are routinely prepared by a drop-casting technique developed in our lab [3]. The nanoparticles have usually cubic edge lengths of ~10 nm, with an oleic acid surfactant shell of ~2 nm. The successful preparation of the ordered monolayers is confirmed by scanning electron microscopy. The in-depth structure can be obtained by reflectivity methods while the lateral structure can be revealed by grazing incidence small angle scattering. Low temperature macroscopic magnetization measurements reveal a systematic secondary magnetization reversal for the cobalt ferrite square lattice at low magnetic fields in the order of 100 mT. We attribute this effect to interparticle coupling in the array, as it is absent for the same, but non-interacting nanocubes in a dilute, frozen dispersion. Polarized SANS under grazing incidence is the method of choice for investigation of lateral magnetic dipolar interactions and the origin of the observed magnetic correlations in long-range ordered nanoparticle arrays.

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Kinetic small-angle neutron scattering of skyrmion lattice order in chiral magnets

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Skyrmions are topologically non-trivial spin textures that attract great interest, offering a possible avenue towards novel spintronics applications, e.g. in skyrmion-based racetrack memory [1]. A key feature that motivates this interest is related to the exceptionally efficient coupling of skyrmion lattice order to spin currents, notably spin-polarized charge currents and magnon currents as observed in MnSi, FeGe, and Cu2OSeO3, respectively [2,3,4]. This raises the question of the microscopic mechanisms that control the pinning and the elasticity modulus of the skyrmion lattice as well as the elasticity moduli of skyrmion lattices in chiral magnets, and how they depend on the topology, electronic structure, and disorder.

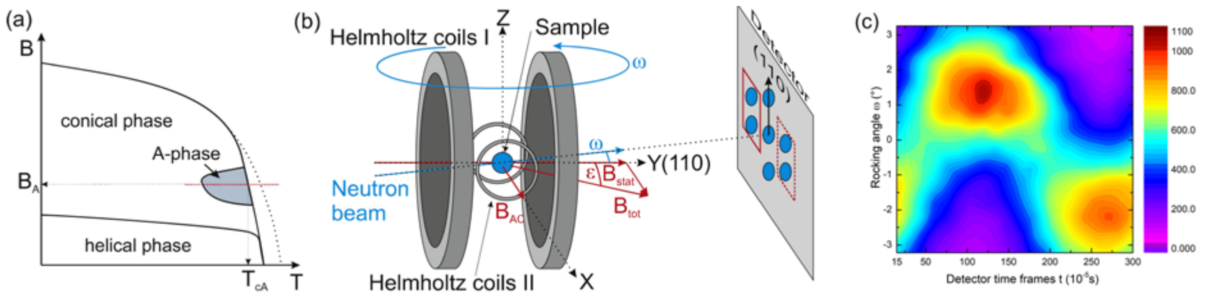

Fig. 1. (a) Schematic depiction of the magnetic phase diagram. (b) Illustration of the experimental setup with the orientation of the static and excitation magnetic fields. (c) Typical time resolved rocking maps of the unpinning of the skyrmion lattice in Cu_2OSeO_3.

In the following contribution, we report kinetic studies of skyrmion lattice order by means of Time-resolved Small Angle Neutron Scattering (TISANE) [5]. We compare the unpinning processes in different systems, such as $Mn_{1-x}Fe_xSi$ where spin-transfer torques are dominated by spin-polarized charge currents, insulating material Cu_2OSeO_3 with the spin transfer torques are due to magnon currents. This provides insights into the pinning mechanisms and elasticity moduli as a precondition for the development of spintronics devices.

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Investigating self-assembly of Au-Fe_3O_4 dumbbell nanoparticles using advanced scattering techniques

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We investigated parameters that affect self-assembly of magnetic dumbbell nanoparticles (DBNPs) in solution. The dumbbells consist of epitaxially grown magnetic Fe_3O_4 nanoparticles on the surface of spherical Au nanoparticles. Their structural, optical and magnetic properties are useful for variety of applications such as dual probes for drug delivery [1-2], catalysis [3], sensing [4], optics [5] and electronics [6]. However, fundamental understanding of mechanisms and parameters involved in self-assembly of DBNPs in solution is still missing. We studied several DBNPs coated with a mixture of oleic acid and oleylamine of different sizes: A13F14, A11F8, A10F14, A10F12, A9F11, where numbers indicate the diameters of Au (A) and Fe_3O_4 (F), respectively. Field-dependent DC magnetization reveals different shapes of hysteresis loops for our samples, which is presumably due to a Au/Fe_3O_4 interface and modification of magnetization profile of Fe_3O_4 [7-8]. Small-angle neutron scattering in applied magnetic field showed self-assembly of DBNPs in solutions, in contrast to zero-field measurements. We observed the onset of order beginning at 0.2 T for A10F14, A9F11 and at 1T for A13F14 (Figure 1). Surprisingly, we found no self-assembly for A10F12 and A11F8 even at 3T. We also performed a polarized SANS at 1T and 3T to separate nuclear and weak magnetic scattering.

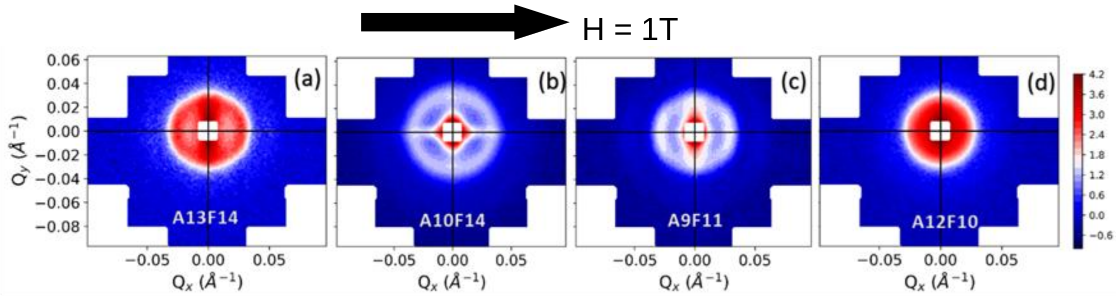

Figure 1: 2D SANS pattern of a) A13F14 b) A10F14 c) A9F11 d) A12F10

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Investigations of the magnetization reversal in Co nanowires bundles by Polarized SANS

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We are investigating the possibility of using the shape anisotropy to produce magnetic materials with a high coercivity which could be used for the fabrication of permanent magnets. This has recently been made possible by the fact that novel chemical processes allow the production of magnetic nanowires of Co which present both a high magnetization M_s = 1400 kA/m, a high Curie temperature T_c = 1360K, a high magneto-crystalline anisotropy Ku = 520 kJ/m^3 and high aspect ratios (AR>10).
These nanowires can be aligned to produce materials with high coercivities ($\mu_0 H_c$>0.75T) (Fang 2013) which in theory open the possibility of producing materials with $(BH)_{max}$ up to 300kJ/m^3. Such materials would exhibit performances equivalent to SmCo5 magnets and not too far for NdFeB magnets.
In this study we have investigated the magnetic reversal mechanisms in (Co nanowires-polymer) composites. The key tool for this investigation has been polarized SANS.

Spin-glass transition and magnetic properties in manganite perovskite $LaBiCaMn_2O_7$

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The manganite perovskite $LaBiCaMn_2O_7$ was synthesized by solid-state reaction route, and have been refined in space group I4/mmm using X-ray powder diffraction. The magnetic properties have investigated, the results obtained display two magnetic transitions: first for a spin-glass (SG) transition at blocking temperature T_B = 76 K and a second for the ferromagnetic-paramagnetic transition is found at Curie temperature T_C = 225 K. The Arrott plot analysis revealed that two transitions seemed to be of the second order type. On the basis of the Maxwell relation, the magnetic entropy variation ($-\Delta S_M$) induced by the magnetic field was assumed. Under a change in a magnetic field of 2T and around T_C, the value of ($-\Delta S_M^{max}$) is found to be 4.17 $J.Kg^{-1}.K^{-1}$ and the value of RC (refrigeration capacity) is of 397 $J.Kg^{-1}$. It should be noted that $LaCaBiMn_2O_7$ displays a relatively prominent magnetocaloric effect at 225K.

Effects of pyrolysis on the magnetic structure and dipolar interactions in iron oxide mesocrystals.

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Owing to their wide diversity and accessible synthesis, magnetic nanoparticles are promising for a variety of applications[1, 2] such as in biotechnology[3] or in material sciences[4]. Particularly interesting is the self-organization of nanoparticles into long-range ordered mesocrystals which incorporate the properties of individual nanoparticles as well as emergent effects. In face of rising demands for alternative materials in Li-ion batteries, mesocrystals of iron oxide nanoparticles have been suggested as nanostructured electrode host materials.[5] The self-assembly approach using nanoparticles as building blocks allows for tuning the magnetic and electrochemical behavior by variation of the nanoparticle size, morphology, composition as well as superlattice structure. In addition, iron oxide fulfills the criteria of cost-efficiency, abundance, and durability but it has the disadvantage of low electric conductivity.

In this contribution, we will highlight the potential of pyrolysis techniques to enhance the electrochemical properties of iron oxide mesocrystals. The organic surfactant covering the particles is decomposed during pyrolysis of mesocrystals, thus enhancing surface activity as well as overall electrochemical qualities. Grazing-incidence SAXS and macroscopic magnetization measurements were used to characterize the structure formation and magnetic properties in effect of the pyrolysis conditions. However, a thorough understanding of pyrolysis effects, electrochemical degradation processes and magnetic structure of iron oxide mesocrystals is needed to optimize their fabrication and realize novel electrode host materials with tailored properties. Magnetic SANS is the best-suited technique to obtain information about the magnetic nanoparticle morphology and dipolar interparticle interactions and has therefore great potential to give complementary insight into pyrolysis effects and electrochemical processes of mesocrystal electrode materials.

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Magnetic neutron scattering of nanoparticles: failure of the superspin model

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It is well known that beyond a certain size magnetic nanoparticles exhibit a nonuniform internal spin structure. This feature, which is relevance for many problem of practical interest (e.g., biomedical imaging and drug delivery), is commonly ignored when it comes to analysis of magnetic neutron scattering data on nanoparticle ensembles. By means of numerical micromagnetic computations we study the transition from single-domain to multi-domain behavior in nanoparticles and its implications for the ensuing elastic magnetic small-angle neutron scattering (SANS) cross section. Above the critical single-domain size we find that the magnetic SANS cross section and the related correlation function cannot be described anymore with the uniform particle model, resulting e.g in deviations from well-known Guinier Law. Independent of particle concentration, we identify a clear signature for the occurrence of a vortex-like spin structure at remanence. The micromagnetic approach to magnetic SANS offers greater flexibility than the structural-model-based superspin approach, and allows one to access the contributions of the individual Fourier components to the cross section and to obtain a deeper understanding of magnetic SANS

Keywords: Magnetic Small Angle Neutron Scattering, Micromagnetics, Numerical Simulation

Reference :

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Aggregation study of sodium ibuprofenate and 1-butyl-3-methilimidazolium ibuprofenate in aqueous solutions by SANS

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Ibuprofen is a non-steroidal anti-inflammatory drug widely used around the world. Its sodium salt is an amphiphilic molecule that forms micelles in water at molar concentration values higher than 0.18 M.[1] Throughout the years, several research groups tried to combine ibuprofen with amphiphatic molecules because ibuprofen shows poor solubility in water. In this regard, amphiphatic ionic liquids (ILs) are interesting candidates to incorporate in new pharmaceutical formulations in order to achieve better drug delivery and improved drug permeability, [2]. In particular, the 1-alkyl-3-methylimidazolium family was studied for its surface-active properties, because they are liquids at room temperature and present low vapor pressure.

In this work we studied the surfactant properties of sodium ibuprofenate (NaIbu) and 1-butyl-3-methyl-imidazolium ibuprofenate (BMImIbu) in aqueous solution by means Small-Angle Neutron Scattering (SANS). For this purpose, different aqueous solutions of both salts were prepared, ranging between 30 to 200 mM.

BMImIbu shows molecular aggregation starting from a concentration of 0.075 M, a concentration value lower than that obtained for NaIbu of 0.18 M. From SANS patterns it was observed that BMImIbu aggregates (radius of ~1.4 nm) are bigger than those for NaIbu (radius of 0.6 nm).

These results are compatible with studies based on dynamic light scattering.[3] At the same time, changes in fluorescence behavior of ibuprofen could be registered as a function of solution concentration and composition. Strong evidence was found that ibuprofen fluorescence increases when micelles are formed but it vanishes when BMIm is part of the aggregates.

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Interplay of proximity effects in Superconductor/Ferromagnet heterostructures

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Proximity effects in superconductor/ferromagnet thin film heterostructures are a highly topical issue due to their potential application in superconducting spin valves or fluxonic devices [1, 2]. Physical properties can be controlled by an applied magnetic field and emerge for example as stray-field generated domain-superconductivity or spin-triplet correlations. Our goal is to investigate their interplay and tunability by an external magnetic field. We use a heterostructure system of Nb/FePd with varying strength of magnetocrystalline anisotropy and a lateral domain structure, grown by molecular beam epitaxy.
On the one hand, macroscopic magnetoelectric transport measurements reveal a confined superconducting state due to the stray fields of $L1_0$-ordered FePd. On the other hand, direct proximity effects at the Nb/FePd interface with a non-collinear magnetization presumably lead to the generation of spin-triplet Cooper pair components with long penetration depth within the ferromagnetic layer [3]. Polarized Grazing-Incidence Small-Angle Neutron Scattering (GISANS) probe exchange mechanisms on the microscopic scale and reveal a change in the ferromagnetic domain pattern by an onset of domain-wall-superconductivity. This mechanism cannot be revealed by macroscopic magnetization measurements, which makes GISANS the method of choice for detecting inverse superconducting proximity effects.

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ENGINEERED Gd-Co BASED MULTILAYER STACK TO ENHANCED MAGNETO-CALORIC EFFECT AND RELATIVE COOLING POWER

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Magnetic refrigeration based on the magneto-caloric effect is one of the best alternatives to compete with vapor-compression technology. The viability of a magnetic refrigeration system for magnetic cooling can be tested by exploiting the materials in various forms, ranging from bulk to nanostructured materials. In order to achieve a wide refrigerating temperature range in magnetic refrigeration, we study in this paper a 100 nm-thick Gd-Co alloys-based multilayer stack. The stack is made of four individual Gd-Co alloy layers with different values of concentration and Curie temperature (T_C). A magnetic entropy change associated with the second-order magnetic phase transition was determined from the magnetic isotherms. Moreover, the relative cooling power (RCP) of the studied Gd-Co-based multilayer is enhanced compared to the one of bulk Gd, and reaches a value of 200 J/kg [1]. Such an enhancement of the RCP is not due to an enhanced maximum variation of entropy, but this is due to a much broader magnetic entropy peak. This study demonstrates the potential of nanostructured Gd-Co multilayer stack for magnetic cooling applications.

Keywords : magnetism, Thin films, Phase transition , Entropy

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Engineering Mesoscale Architecture in Superconductors via Block Copolymer Self-Assembly

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While the field of superconductivity is rich in mesoscale phenomena (vortex lattice structures, thermomagnetic flux avalanche behavior, and typical cooper pair coherence lengths as a few examples), to date there have been few investigations of superconductors with 3D periodic mesoscale lattice structures. The limitation of mesoscale structuring in superconductors largely to the thin film regime is a result of a scarcity of synthetic routes towards bulk, 3D structured materials. In this work, we make use of block copolymer (BCP) self-assembly (SA) to achieve mesoscale architectures in superconductors such as niobium nitrides (NbN), niobium carbo-nitrides (NbCN), and indium metal. Results indicate that BCP SA directed cubic co-continuous alternating (space group Q214) or double (Q230) gyroid structures of such superconductors affect macroscopic behavior by dictating quantum level properties. Findings suggest, e.g. that the gyroidal mesoscale networks induce vortex formation and flux pinning in Type I superconducting indium, and may serve as artificially defined pinning centers in Type II superconducting NbN or NbCN. These first examples showcase that emergent properties may be found at the interface of soft matter self-assembly science and quantum materials, while the use of facile solution based synthetic pathways holds technological promise for saleable and cost-effective approaches to such advanced materials.

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Antiferromagnetically coupled anti-phase domains under external magnetic fields

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Ni_2MnZ based Heusler compounds have attracted a considerable amount of attention due to their various appealing properties such as the ferromagnetic shape-memory effect or the magnetocaloric effect. The room temperature ground state structure is $L2_1$ order. Quenching a crystal from the B2 stable regime preserves its disordered structure at low temperatures, where atomic diffusion is inactive. During subsequent annealing, $L2_1$-ordered domains nucleate independently and grow, leading to a division of the crystal into antiphase domains (APDs) according to which sublattice is occupied by Mn atoms[1]. The magnetic moments in these systems are mainly carried by Mn atoms, with neighbouring Mn spins interacting anti-ferromagnetically, while next nearest neighbour Mn spins interact ferromagnetically. Using TEM and Lorentz TEM it has been found that the structural domains are identical with magnetic domains with the magnetization tending to reverse at structural antiphase domain boundaries, leading to atomically sharp ferromagnetic domain walls [1]. To clarify the reason of this relation we studied further the influence of coupling across antiphase domain boundaries (APBs) by applying small-angle neutron scattering under external magnetic fields.

We have investigated Ni_2MnAl and $Ni_2MnAl_{0.5}Ga_{0.5}$ powder samples in distinct ordering states via temperature-dependent magnetic small-angle neutron scattering, giving access to the magnetization microstructure. Without a magnetic field applied we observed a peak which broadens and shifts to lower q values with increasing annealing time demonstrating that structural order and magnetic order are positively correlated. We found their characteristic length scales being of the same size.

With an external magnetic field applied we observe a redistribution of intensity along the field direction, corresponding to the ferromagnetic domains coupling antiferromagnetically across APBs. Approaching the magnetic transition temperature of our sample with an external magnetic field applied we observe a change in the predominant spin orientation, turning them from perpendicular into parallel alignment to the B − field. This transition from antiferromagnetically coupled APDs into a field polarized state can be explained by the temperature dependent influence of the spin stiffness competing with the Zeeman energy.

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