13th International Conference on

Polarized Neutrons for Condensed Matter Investigations (PNCMI)

JULY 27 – 30, 2021

VIRTUAL

Welcome

The 13th international Polarized Neutrons for Condensed-Matter Investigations (PNCMI) Conference, organized by NIST, will be held online from July 27-30, 2021. This first short online PNCMI will feature 2 daily one-hour sessions from 9:00 am to 11:30 am US Eastern Time with a 30 minute break between sessions for 4 consecutive days and include both invited and poster presentations.

Despite the pandemic, 100 participants from more than 30 institutions and governments from Europe, Asia, Australia, and North America registered for the conference. We would like to thank all participants for joining us and hope you all to enjoy great scientific discussions and interactive gathering over the conference. We would also like add special thanks to the International Advisory Committee for guidance in developing extraordinary scientific program and NIST Conference Services for all their hard work and planning to help organize and host this meeting.

The next in-person PNCMI will take place in Annapolis, Maryland, USA in July, 2022.

PNCMI 2021 local organizing committee

Event Format

Our plenary sessions will be held on the BlueJeans Events platform virtual auditorium. Participants will have the opportunity to ask questions using the Q&A tab within the platform. A NIST AV technician will be available throughout the event to assist with troubleshooting technical issues.

The poster sessions and several of the breaks will be held on the GatherTown platform. This interactive platform consists of a map representing a conference center with different rooms/areas. An avatar will be created for you and placed in a large central room. You will be able to move your avatar to different rooms using your arrow keys. Movement will allow you to network with other conference attendees, view the posters and talk to the poster presenters.

About PNCMI

PNCMI started its long journey in Dubna, Russia in 1996 and has taken place biennially since then. The conference will cover the latest condensed-matter investigations using polarized neutrons and state-of-the-art methodologies and techniques of polarized-neutron production and utilization for novel instrumentation and experiments, with emphasis on prospects for new science and instrument concepts as well as combining neutrons with complementary techniques and in-situ secondary measurements.

PNCMI is the most comprehensive conference on the latest scientific research using polarized neutrons and on related instrumentation development. The topics will include:

- Multiferroics and chirality
- Strongly correlated electron systems
- Frustrated and disordered systems
- Quantum materials
- Magnetic nanomaterials
- Thin films and multilayers
- Soft matter
- Imaging
- Polarized neutron instrumentation
- Polarized neutron techniques and methods

Program Committees

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- Kathryn Krycka (NIST, USA)
- William Ratcliff (NIST, USA)
- Shannon Watson (NIST, USA)

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PNCMI 2021 Conference Schedule

USA, EST	Tuesday, July 27th	Wednesday, July 28th	Thursday, July 29th	Friday, July 30th
	1st Session (9:00 - 10:00 AM, USA Eastern Time)			
9:00 AM	**Welcome** *Dan Neumann*	***Magnetism Alexander Ioffe*** *Andrew Manning (ANSTO)*	***Poster Session***	***Poster Session***
9:05 AM	***Quantum Materials Kemp Plumb*** *Yixi Su (JCNS)*			
9:30 AM		***Magnetism Alexander Ioffe*** *Takashi Kurumaji (U. Tokyo)*		
9:35 AM	***Polarized Neutron Instrumentation Ross Stewart*** *Vasile Ovidiu Garlea (ORNL)*			
10:00 AM		**Break in GatherTown (10:00 AM - 10:30 AM Eastern Time)**		
10:05 AM	**Break in GatherTown (10:05 AM - 10:30 AM Eastern Time)**			
	2nd Session (10:30 - 11:30 AM, USA Eastern Time)			
10:30 AM	***Nanostructures Yumi Ijiri*** *Sabrina Disch (U. Cologne)*	***Polarized Neutron Instrumentation Thomas Gentile*** *Xin Tony Tong (CSNS)*	***Magnetism Rebecca Dally*** *Nikolaos Biniskos (JCNS)*	***Larmor Techniques Roger Pynn*** *Johanna Jochum (TUM)*
11:00 AM	***Nanostructures Yumi Ijiri*** *Deepak Singh (U. Missouri)*	***Polarized Neutron Instrumentation Thomas Gentile*** *Kathryn Krycka (NCNR)*	***Magnetism Rebecca Dally*** *Jennifer Graham (U. Birmingham/ILL)*	***Polarized Neutron Methods William Ratcliff*** *Iurii Kibalin (LLB)*
11:30 AM				
11:35 AM				**Concluding Remarks** *Wangchun Chen*

Time Zone

	US EST	UK	West Europe	China	Japan/Korea	Australia
Start time	9:00	14:00	15:00	21:00	22:00	1:00
End time	11:30	16:30	17:30	23:30	0:30	3:30

Welcome to PNCMI 2021 Gather

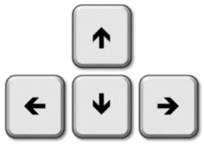
Gather is home to the PNCMI 2021 virtual meeting space for conference attendees to interact more effectively online. The conference poster sessions and breaks will be hosted in this space. The platform combines video-calling with a 2D map, allowing attendees to walk around and talk to other users right next to them and/or join other interactive spaces.

Getting Started

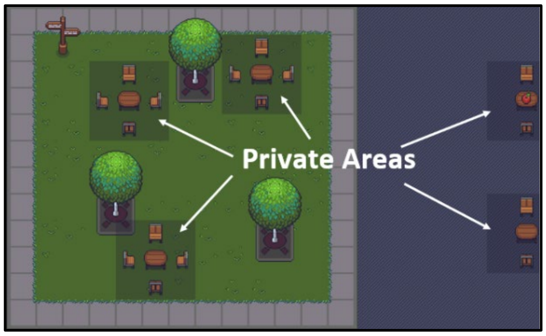
To join the PNCMI 2021 Gather click the invite link sent via email or copy and paste the link into a web browser. Right now, Gather is supported on Chrome, Firefox and Desktop Safari (in Beta).

Gather must request permission to use your microphone and camera from the web browser. For more information on how to enable your audio/video settings visit: https://support.gather.town/help/browser-settings-and-permissions

Tips for Using Gather



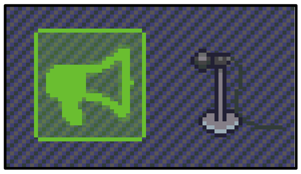
Use the keyboard arrow keys to navigate your avatar through the space. You can also use your mouse to move around in Gather. Double-click on a tile to walk to it. Clicking to move will automatically try and avoid private spaces.

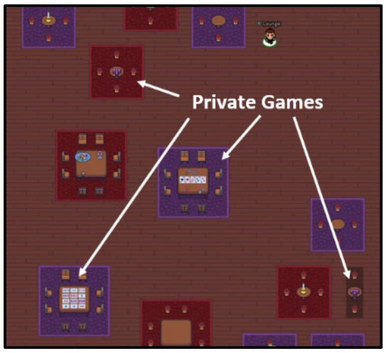


When your avatar approaches others, a video call automatically starts between you and the people you approach. All videos will initially appear at the top of your screen. In an open area, you will be connected to everyone within 5 tiles unless you activate Quiet Mode. When you are in a Private Area, you will be connected to everyone who is also inside of the private area.

Users can send and view messages in the Chat Panel, located above the participants tab, second from the bottom on the left of your screen. Here, you can view past messages, as well as send messages of your own.

You can share your screen with all of the people you are connected to on Gather if it is enabled in the space that you are in.



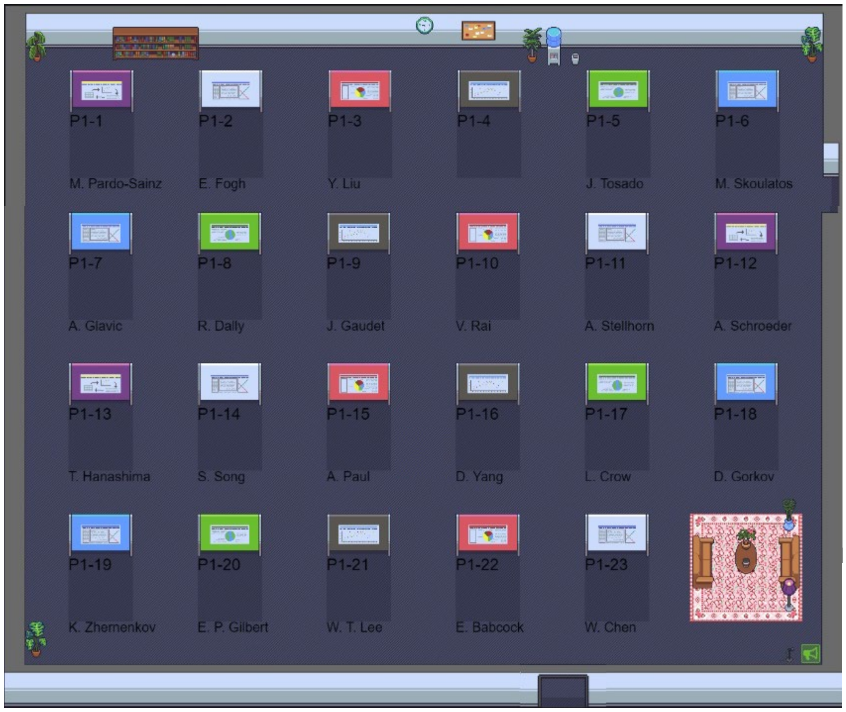


Spotlighting**:** Being spotlighted means having your video and audio broadcasted to up to 100 users in the same room. When you are spotlighted, you will be able to see the other users you are broadcasting to, however, their audio will be muted for you unless they are in the typical connection range to see and interact with you.

Several pre-set games have been incorporated into the lounge space. These games are set up so you can join private games within your Gather space while video chatting with friends.

Poster Sessions

The live poster sessions will take place on PNCMI 2021 Gather on **Thurs. July 29** and **Fri. July 30** from **9:00 – 10:00 AM, USA Eastern Time**. The sessions will take place in dedicated rooms where posters will already be pre-loaded and organized in a grid similar to an in-person conference. To interact with a poster, conference attendees will walk up to the poster and press the "x" key to enter a full screen viewing. While viewing the poster, they will also be able to interact with the presenter. An example poster room looks like this:



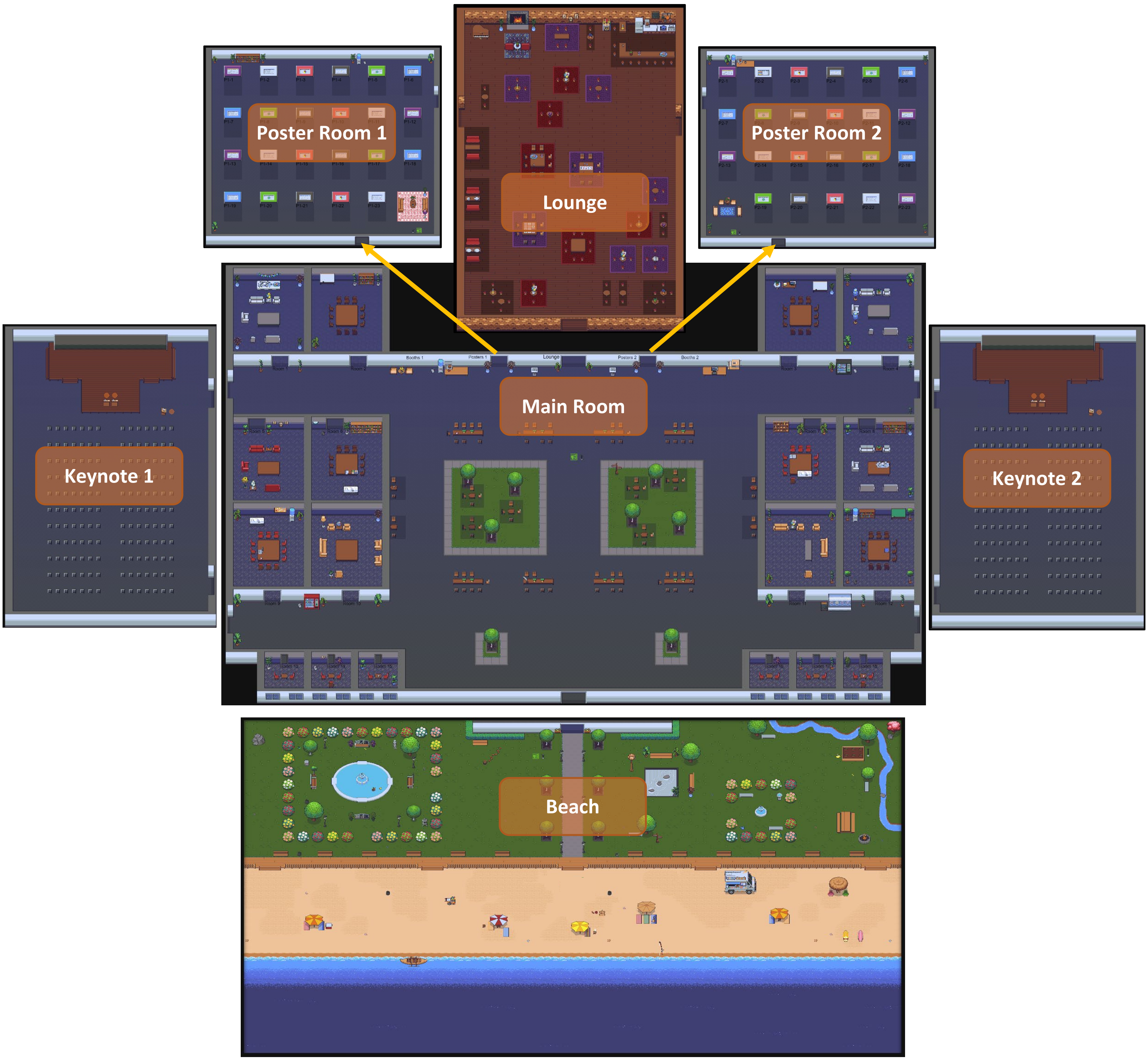
When your avatar is in the private space near a poster, all other conference attendees in that space will be able to see and hear you through your webcam and microphone. You will only be interacting with people in this space, and not the neighboring spaces. This promotes conversation with the presenter without interrupting conversation going on at other posters.

More Information

Additional information about the Gather platform and troubleshooting advice can be found at [Gather.Town's Help Center](). Feel free to direct other questions about the platform to the conference email at pncmi2021@nist.gov.

Gather Space Map

The PNCMI 2021 Gather space consists of a large Main Room equipped with several private meeting areas perfect for breakout sessions and smaller discussions. The poster sessions will take place in Poster Room 1 & 2 located above the Main Room. The deluxe lounge space is ideal for smaller video calls and includes several pre-set games for single and group entertainment. Feel free to explore the other conference spaces including two keynote rooms and an outdoor social area. Remember that users can send and view chat messages to coordinate meeting spaces via the Chat Panel, located above the participants tab, second from the bottom on the left of your screen.



Abstracts – Invited Talks

Tuesday, July 27th, 2021

Session 1-1: Quantum Materials, 9:05 – 9:35 am (EST)
Neutron scattering on correlated topological materials
Yixi SU

Session 1-2: Polarized Neutron Instrumentation, 9:35 – 10:05 am (EST)
Polarized neutron capabilities at the HYSPEC spectrometer at SNS
Ovidiu GARLEA, Melissa GRAVES-BROOK, Barry WINN

Session 2-1: Nanostructures, 10:30 – 11:00 am (EST)
Revealing Magnetic Morphologies and Spin Disorder in Ferrite Nanoparticles
Dominika ZÁKUTNÁ, Dirk HONECKER, **Sabrina DISCH**

Session 2-2: Nanostructures, 11:00 – 11:30 am (EST)
Investigation of Quantum Disordered State in Magnetic Honeycomb Lattice
Deepak K. SINGH

Wednesday, July 28th, 2021

Session 3-1: Magnetism, 9:00 – 9:30 am (EST)
Update on the neutron polarisation capabilities at the Australian Centre for Neutron Scattering, ANSTO
Andrew MANNING

Session 3-2: Magnetism, 9:30 – 10:00 am (EST)
Direct observation of cycloidal spin modulation in Néel-type skyrmion-hosting $VOSe_2O_5$
Takashi KURUMAJI, Taro NAKAJIMA, Artem FEOKTYSTOV, Earl BABCOCK, Zahir SALHI, Victor UKLEEV, Taka-hisa ARIMA, Kazuhisa KAKURAI, and Yoshinori TOKURA

Session 4-1: Polarized Neutron Instrumentation, 10:30 – 11:00 am (EST)
Polarized neutron R&D at the China Spallation Neutron Source
Xin TONG

Session 4-2: Polarized Neutron Instrumentation, 11:00 – 11:30 am (EST)
A survey of NCNR instruments equipped with polarized neutron analysis for studying magnetic systems
Kathryn KRYCKA, Shannon WATSON, Hannah BURRALL, Ross ERWIN, Alex GRUTTER, Julie BORCHERS, and Wangchun CHEN

Thursday, July 29th, 2021

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Investigating the spin excitation spectrum of Mn5Si3
N. BINISKOS, F.J. DOS SANTOS, S. RAYMOND, K. SCHMALZL, M. DOS SANTOS DIAS, S. BLÜGEL, S. LOUNIS, T. BRÜCKEL
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Session 5-2: Magnetism, 11:00 – 11:30 am (EST)
Local nuclear and magnetic order in the two-dimensional spin glass, $Mn_{0.5}Fe_{0.5}PS_3$
Jennifer N. GRAHAM, Matthew J. COAK, Suhan SON, Emmanuelle SUARD, Je-Geun PARK, Lucy CLARK and Andrew R. WILDES
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Friday, July 30th, 2021

Session 6-1: Larmor Techniques, 10:30 – 11:00 am (EST)
MIEZE@RESEDA: Spin-echo optimized for magnetic phenomena
Johanna K. JOCHUM, Christian FRANZ, P. BENDER, J. LEINER, O. SOLTWEDEL, C. FUCHS, P. BÖNI, C. PFLEIDERER
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Session 6-2: Polarized Neutron Methods, 11:00 – 11:30 am (EST)
Data analysis of polarized neutron single crystal and powder diffraction
Iurii KIBALIN, Arsen GUKASOV
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Session 1-1: Quantum Materials, 9:05 – 9:35 am (EST)

Neutron scattering on correlated topological materials

Yixi Su

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

Recent theoretical predictions and experimental realizations of exotic quasi-particles and topological excitations in condensed matter have led to tremendous research interests in topological quantum materials. Especially, correlated topological materials, such as e.g. magnetic Dirac and Weyl semimetals, and intrinsic magnetic topological insulators, in which both non-trivial topology of single-electron band structures and electron-electron correlations are essential ingredients, have emerged as an exciting platform to explore novel electronic and magnetic phenomena. In this talk, I will present a couple of selected examples of our recent neutron scattering studies along this line, with particular emphasis on the applications of polarized neutron scattering in disentangling complex magnetic orders.

[1] Fengfeng Zhu, *et al.*, Phys. Rev. Research **2**, 043100 (2020).

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Session 1-2: Polarized Neutron Instrumentation, 9:35 – 10:05 am (EST)

Polarized neutron capabilities at the HYSPEC spectrometer at SNS

Ovidiu GARLEA, Melissa GRAVES-BROOK, Barry WINN

Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831 USA

The HYSPEC spectrometer at the Spallation Neutron Source combines time-of-flight spectroscopy with focusing Bragg optics to allow for either unpolarized or polarized neutron scattering experiments. The incident neutron beam is monochromated using a Fermi chopper and is then vertically focused by Bragg scattering onto the sample position by either a highly oriented pyrolitic graphite or a Heusler crystal array. The polarization analysis of the scattered neutrons is carried out by a multi-channel array consisting of 960 FeCoV-based supermirror polarizers distributed over 60 degrees horizontally, with ±7.5 degrees acceptance vertically. The region around the sample is sufficiently configurable to accommodate a variety of polarization optics. Linear XYZ-polarization analysis is carried out by measurements of non-spin-flip and spin-flip cross sections for three orthogonal directions of the incident polarization vector with respect to the scattering vector. A Mezei flipper is used to reverse the incident neutron polarization, and the polarization vector is oriented by employing a guide field generated from a set of 3D coils situated around the sample position. Various upgrades have been made to improve the polarization analysis operations and effectiveness at HYSPEC. One such improvement is an elevator / oscillator system, which for the first time enables rapid change from an unpolarized or half polarized mode to a polarization analysis mode of operation, introducing significant flexibility and convenience. Additional upgrades include a newly built RF flipper and a new and compact 3D coil system. The current status of the polarization capability at HYSPEC will be illustrated by an overview of recent polarized elastic and inelastic scattering studies of several magnetic materials.

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Session 2-1: Nanostructures, 10:30 – 11:00 am (EST)

Revealing Magnetic Morphologies and Spin Disorder in Ferrite Nanoparticles

Dominika ZÁKUTNÁ[1,2], Dirk HONECKER[3], **Sabrina DISCH[1]**

[1]University of Cologne, Chemistry Department, Cologne, Germany

[2]Charles University, Department of Inorganic Chemistry, Prague, Czech Republic

[3]ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Didcot, United Kingdom

Being intrinsic to nanomaterials, disorder effects crucially determine the magnetization properties such as the heating performance of magnetic nanoparticles [1-4]. However, despite the considerable technological relevance and fundamental importance, a key challenge in magnetic nanoparticle research remains the quantitative interpretation of the three-dimensional magnetic configuration and the nanoscale distribution of magnetization and spin disorder. In this contribution, we will present our recent results on the magnetic morphologies and spin disorder in ferrite nanoparticles seen by magnetic SANS.

Polarized SANS is a versatile technique to investigate the chemical morphology and magnetization with nanoscale spatial resolution [5]. Physical and chemical properties of magnetic nanoparticles highly depend on their synthesis method and ageing behavior. Whereas the overall Fe:Co distribution in our as-prepared cobalt ferrite nanoparticles is homogeneous, the sensitivity of SANS to nanoscale density variations reveals a wuestite-like core and a spinel-type shell with different local magnetization. We further analyze the progressive oxidation of the core and the aging process into single-phase ferrite nanoparticles with nearly homogeneous magnetization distribution.

Single-phase magnetic nanoparticles are classically considered as a collinearly magnetized core with a structurally and magnetically disordered surface region. We have recently shown that this static idea needs revision as the intra-particle magnetization is more complex with a field-dependent magnetization process near the surface [6]. We have established a significant field-induced growth of the total particle moment by a magnetic ordering transition at the structurally disordered surface. Finally, we have elucidated the intra-particle spin-disorder energy, giving indirect insight into the structural defect profile in magnetic nanoparticles.

[1] P. Bender et al., J. Phys. Chem. C, **122**, 3068 (2018).

[2] A. Lak et al., Nano Lett., **18**, 6856 (2018).

[3] A. Lappas et al., Phys. Rev. X, **9**, 041044 (2019).

[4] A. Lak, S. Disch, P. Bender., Adv. Science, **8**, 2002682 (2021).

[5] S. Mühlbauer et al., Rev. Mod. Phys., **91**, 015004 (2019).

[6] D. Zákutná, D. Honecker, S. Disch et al., Phys. Rev. X, **10**, 031019 (2020).

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Session 2-2: Nanostructures, 11:00 – 11:30 am (EST)

Investigation of Quantum Disordered State in Magnetic Honeycomb Lattice

Deepak K. Singh

Department of Physics, University of Missouri. Columbia, MO 65211

Nanostructured magnetic materials with geometrically frustrated motif provides archetypal platform to study emergent phenomena in reduced dimension. [1, 2] Recently conceived magnetic honeycomb lattice of single domain nanoscopic element, with typical length of ~ 12 nm, stands out in this quest. [3] The spin ice type configuration of local magnetic moments in a honeycomb automatically generates magnetic charges of low (±Q) and high (±3Q) multiplicities on the vertices. The quantum mechanical nature of magnetic charges, represented by Pauli matrices, imparts unique advantage to explore new quantum state in the classical system. Thermal tunability of the lattice is a necessary requirement to this quest. The single domain element in our honeycomb lattice reduces the inter-elemental dipolar interaction energy to an unprecedented small value of ~ 10 K.[3] The new sample design enabled neutron-based exploration of emergent magnetic phases in two-dimensional honeycomb lattice.[4] More recently, we have discovered a quantum disordered state of magnetic charges, akin to the charge liquid state, in thermally tunable system.[5] Detailed experimental investigation of nanoengineered honeycomb lattice using spin polarized neutron reflectometry (PNR) and spin echo measurements have revealed massively degenerate magnetic charge configurations at low temperature that remain mostly unperturbed to external effect, such as large magnetic field application. The overall magnetization manifests a cooperative paramagnetic behavior as a function of temperature due to the charge correlation on honeycomb vertices. Most importantly, magnetic charges remain highly dynamic to the lowest measurement temperature of T = 5 K.[6] The experimental observations e.g. large degeneracy of ground state configuration, independence to external tuning parameter, paramagnetic characteristic and persistent dynamics are the hallmark of liquid-like quantum disordered state.[7] The new finding establishes the quantum mechanical characteristic of magnetic charge in artificial spin ice systems.

DKS thankfully acknowledges the support by the Department of Energy, Office of Science, Office of Basic Energy Sciences under the grant no. DE-SC0014461. Neutron scattering research works are performed at US DOE-BES supported facility at SNS-ORNL.

[1] S. Skjaerrvo, C. Marrows, R. Stamps and L. Heyderman, *Nat. Rev. Phys.* **2**, 13 (2020).
[2] C. Nisoli, R. Moessner and P. Schiffer, *Rev. Mod. Phys*. **85**, 1473 (2013)
[3] B. Summers, L. Debeer-Schmitt, A. Dahal, A. Glavic, P. Kampschroeder, J. Gunasekera and D. K. Singh, *Phys. Rev. B* **97***, 014401* (2018)
[4] A. Glavic, B. Summers, A. Dahal, J. Kline, W. Van Herck, A. Sukhov, A. Ernst and D. K. Singh, *Advanced Science* **5**, 1700856 (2018)
[5] G. Yumnam, Y. Chen, J. Guo, V. Lauter and D. K. Singh, *Advanced Science* **8**, 2004103 (2020).
[6] Y. Chen, G. Yumnam, J. Guo, L. Stingciau, P. Zolnierczuk, V. Lauter and D. K. Singh**,** *iScience* **24**, 102206 (2021)
[7] A. S. Wills, R. Ballou and C. Lacroix, *Phys. Rev. B* **66**, 144407 (2002)

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Session 3-1: Magnetism, 9:00 – 9:30 am (EST)

Update on the neutron polarisation capabilities at the Australian Centre for Neutron Scattering, ANSTO

Andrew Manning

ANSTO, Lucas Heights, Australia 2234

An overview of the neutron polarisation capabilities across the six compatible instruments at the Australian Centre for Neutron Scattering (ACNS) will be presented. This will include a discussion of the newly-acquired compensated 7 Tesla vertical magnet, which was designed specifically for neutron polarisation experiments on the SANS instrument Quokka in addition to other powder diffraction instruments, time-of-flight and triple-axis spectrometers.

Some recent experiments using these capabilities will be outlined, including a measurement of the chiral characteristics of a helimagnetic structure on the cold triple-axis spectrometer Sika.

An update on the current work to prepare XYZ polarisation capabilities for the time-of-flight spectrometer Pelican will also be given, along with an overview of the future directions of the polarisation efforts at ACNS.

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Session 3-2: Magnetism, 9:30 – 10:00 am (EST)

Direct observation of cycloidal spin modulation in Néel-type skyrmion-hosting $VOSe_2O_5$

Takashi Kurumaji[1,2], Taro Nakajima[1,3], Artem Feoktystov[4], Earl Babcock[4], Zahir Salhi[4], Victor Ukleev[1,5], Taka-hisa Arima[1,2], Kazuhisa Kakurai[1,6], and Yoshinori Tokura[1,7]

[1] *RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Japan,*

[2] *Department of Advanced Materials Science, The University of Tokyo, Kashiwa 277-8561, Japan,*

[3] *Institute for Solid State Physics, The University of Tokyo, Chiba 277-8581, Japan,*

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

[5] *Laboratory for Neutron Scattering and Imaging (LNS), Paul Scherrer Institute (PSI), CH-5232 Villigen, Switzerland,*

[6] *CROSS-Tokai, Research Center for Neutron Science and Technology, Tokai, Ibaraki 319-1106, Japan,*

[7] *Department of Applied Physics, The University of Tokyo, Tokyo 113-8656, Japan.*

Magnetic skyrmions are two-dimensional vortex-like spin state carrying a topological number. It is known that a skyrmion is described by the internal degrees of freedom in terms of the spin configuration, termed helicity and vorticity. Two main different types of skyrmions, Bloch or Néel type, are characterized by the helicity. As for the detection of Bloch-type skyrmions, Lorentz transmission electron microscopy is the most well-established technique, however, this method has a limited sensitivity to the Néel-type skyrmions due to the fundamental mechanism for the electron beam deflection via magnetic moments. Other techniques such as spin-polarized scanning tunneling microscopy can be used for local detection of a skyrmions regardless of the form of helicity, yet the probe pin is accessible to only on the surface of the sample. Observation of the spin configuration of Néel-type skyrmions in bulk materials has remained elusive. We investigate the spin rotational structure of magnetic skyrmions in a tetragonal polar magnet $VOSe_2O_5$ [1] via polarized small-angle neutron scattering. Spin polarization analysis of the scattered neutrons provides consistent evidence for the cycloidal spin modulation in all the incommensurate phases at zero and non-zero magnetic field along the *c* axis, including the triangular skyrmion-lattice phase [2].

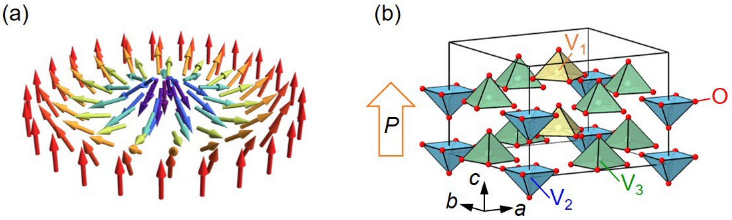

Figure 1 (a) Neel-type skyrmion. (b) Crystal structure of $VOSe_2O_5$.

[1] T. Kurumaji *et al.*, Phys. Rev. Lett. **119**, 237201 (2017).

[2] T. Kurumaji *et al.*, J. Phys. Soc. Jpn. **90**, 024705 (2021).

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Session 4-1: Polarized Neutron Instrumentation, 10:30 – 11:00 am (EST)

Polarized neutron R&D at the China Spallation Neutron Source

Xin Tong

[1]China Spallation Neutron Source, Dongguan, China

[2]Institute of high energy physics, Beijing, China

[3]Chinese Academy of Sciences, Beijing, China

China Spallation Neutron Source (CSNS) is a new accelerator-based neutron source located at Dongguan, China. There are currently 3 instruments in the general user program with a powder diffractometer, a SANS and a reflectometer. Eight new instruments are being constructed with 10 more coming along in the next few years. Polarization analysis, as an important and unique feature of neutron scattering technique, is one of the focuses of the future of CSNS. The polarized neutron team at CSNS has been developing in-house polarized neutron capabilities for the past two years, focusing on polarized 3He development, polarized neutron test beamline construction and polarized neutron devices including neutron flippers etc. In this talk I will present the recent progress of these R&D efforts.

[1] Z.C. Qin, et at., *Chin. Phys. Lett.* **38**, 052801, (2021)

[2] C.Y. Huang, et at., *Chin. Phys. Lett.* Accepted, (2021)

E-mail of the corresponding author: tongx@ihep.ac.cn

Session 4-2: Polarized Neutron Instrumentation, 11:00 – 11:30 am (EST)

A survey of NCNR instruments equipped with polarized neutron analysis for studying magnetic systems

Kathryn Krycka[1], Shannon Watson[1], Hannah Burrall[1], Ross Erwin[1], Alex Grutter[1], Julie Borchers[1], and Wangchun Chen[1,2]

[1]*National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA*
[2]*University of Maryland, College Park, Maryland 20742, USA*

Neutron polarization analysis is a powerful technique to separate magnetic from nuclear scattering. In addition, it can be used to resolve magnetic scattering components originating from spins parallel and perpendicular to the applied guide field, allowing for the study of nanoscale magnetic morphologies, magnetization density profiles, and magnetic excitations in a wide range of magnetic materials. For geometries involving a divergently scattered neutron beam, polarized ^{3}He neutron spin filters[1] can effectively polarize large areas and a broad range of neutron wavelengths; the ^{3}He polarization direction can be reversed at will using integrated NMR spin flipping. Here we shall discuss the current applications on the BT7 triple axis spectrometer[2], the multi-axis crystal spectrometer[3], and NG7 small-angle neutron scattering[4] instruments. Moreover, we shall cover new developments on CANDOR[5], including a new 15 cm x 6 cm, high efficiency neutron spin flipper, and VSANS where integration of four cross-section polarization analysis with a high-resolution detector yields polarized measurements down to a reciprocal space of 0.0003 Å^{-1}.

[1] W. C. Chen *et al.,* J. Phys.: Conference Series, **528,** 012014 (2014)
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We gratefully acknowledge the Center for High Resolution Neutron Scattering for providing funding.

Session 5-1: Magnetism, 10:30 – 11:00 am (EST)

Investigating the spin excitation spectrum of Mn_5Si_3

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Recently materials with non collinear spin arrangements and anomalous physical properties that do not consist from rare earth elements are exploitable for future spintronic and electronic devices and have attracted great scientific interest [1-3]. In this context Mn_5Si_3 is a promising material for applications since interesting thermodynamic and transport phenomena occur, such as the inverse magnetocaloric (MCE) [4] and the anomalous Hall effect [5]. Mn_5Si_3 undergoes two first order phase transitions towards a collinear and non collinear antiferromagnetic phase at T_{N2} =100K (AFM2) and T_{N1} =66K (AFM1), respectively. The inverse MCE and the large anomalous Hall effect are associated with the AFM1-AFM2 phase transition. A combination of polarized and unpolarized inelastic neutron scattering (INS) measurements in the collinear AFM2 phase (66<T<100K) suggested that the magnetic excitation spectrum consists of propagating spin waves and diffuse spin fluctuations, originating from the presence of magnetic and nonmagnetic Mn sites within this phase [4]. In contrast INS measurements indicate that the non collinear AFM1 phase (T<66K) consists only of propagating spin waves. An application of an external magnetic field in the AFM1 phase, restores the AFM2 phase and its associated spin fluctuations. Moreover, using density functional theory calculations we determined the magnetic exchange interactions of both AFM phases [6]. This provided the parameters for a Heisenberg model, from which we computed the spin-wave energies as a function of the external magnetic field. With this study we obtained the minimal magnetic model Hamiltonian and we investigated the role of the spin fluctuations in the AFM phases, and which Mn site may be responsible for them.

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[5] C. Sürgers et al; Nature Communications **5**, 3400 (2014).
[6] F.J. dos Santos et al; Phys. Rev. B **103**, 024407 (2021).

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Session 5-2: Magnetism, 11:00 – 11:30 am (EST)

Local nuclear and magnetic order in the two-dimensional spin glass, $Mn_{0.5}Fe_{0.5}PS_3$

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The *M*PS_3 compounds represent a diverse family of honeycomb layered van der Waals materials, where the physical properties are heavily reliant on the choice of transition metal ion, *M* [1]. These materials have been subject to significant interest over the years, for their ability to be intercalated or delaminated down to a monolayer, and have even been likened to magnetic graphene. In this study, we pay attention to the mixed compound, $Mn_{0.5}Fe_{0.5}PS_3$. Whilst a spin glass phase was known to exist in $Mn_{0.5}Fe_{0.5}PS_3$ [2] there are still a number of key details missing, in particular, the nature of its local nuclear and magnetic correlations. Here, we address these issues through a series of neutron scattering and magnetization measurements [3]. High resolution neutron powder diffraction data reveal a completely random distribution of magnetic ions throughout the honeycomb structure. Magnetization data confirm a spin glass phase, with the glass transition occurring at T_g = 35 K. Analysis of diffuse neutron scattering data show that within the honeycomb planes there are a mixture of satisfied and unsatisfied correlations, which we are able to explain by considering relationships between the magnetic structures of the two parent compounds. Correlations between the planes were found to be very weak, mirroring our observations of rod-like structures in single crystal diffraction measurements, and confirming that $Mn_{0.5}Fe_{0.5}PS_3$ is a near-ideal example of a two-dimensional magnetic material.

[1] F. Wang et al. Adv. Funct. Mater. **28**, 1802151 (2018), [2] T. Masubuchi et al. J. Alloys Compd. **460**, 668-674 (2007), [3] J. N. Graham et al. Phys. Rev. Mater **4**, 084401 (2020)

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Session 6-1: Larmor Techniques, 10:30 – 11:00 am (EST)

MIEZE@RESEDA: Spin-echo optimized for magnetic phenomena

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The MIEZE (Modulation of Intensity with Zero Effort) technique, is essentially 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. In combination with the possibility of performing measurements in a SANS configuration this makes MIEZE an excellent tool for studying fluctuations at (quantum) phase transitions as well as other dynamic magnetic phenomena, such as magnon dynamics, or the melting of superconducting vortex lattices [1-4].

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[3] Säubert et al., PRB 99, 184423 (2019)

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Data analysis of polarized neutron single crystal and powder diffraction

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Based on experiment with single crystal the polarized neutron diffraction (PND) is a well-established tool to investigate the spin density distribution in the magnetic compounds with quenched orbital moment. For such compounds, it is assumed that the direction of the spins is aligned by an externally applied magnetic field. This collinearity of induced moments with a magnetic field breaks due to the presence of orbital moment. Under such circumstances, PND technique can be used to retrieve a local atomic susceptibility, which models orientation of the induced atomic moments as a function of the applied field. Recently, this approach has been extended to study the magnetic anisotropy in powders, which opens large possibilities in the studies of local anisotropy in highly interesting powder materials, like frustrated magnets, multiferroics, molecular magnets or nanoscale systems [1].

In the report, recent studies using the polarized neutron powder diffraction to analyze the local magnetic anisotropy are presented. By this technique the quasyplanar (XY) local anisotropy of Dy ions has been for the first time revealed in hyperkagome dysprosium garnet Dy3Ga5O12 (Fig.1a) [2]. On an example of single-molecule magnet with Co(II) complex it was shown that the crystallites are oriented under a high external magnetic field (Fig.1b). Surprisingly, this effect improves the precision in the determination of the local susceptibility parameters in such a complex compound. Newly developed "CrysPy" library applied for the PND data analysis will be also presented (GitHub page is https://ikibalin.github.io/cryspy/).

[1] I.A. Kibalin, A. Gukasov. PRL, **1**, 033100 (2019).

[2] I.A. Kibalin et al. PRR, **2**, 033509 (2020).

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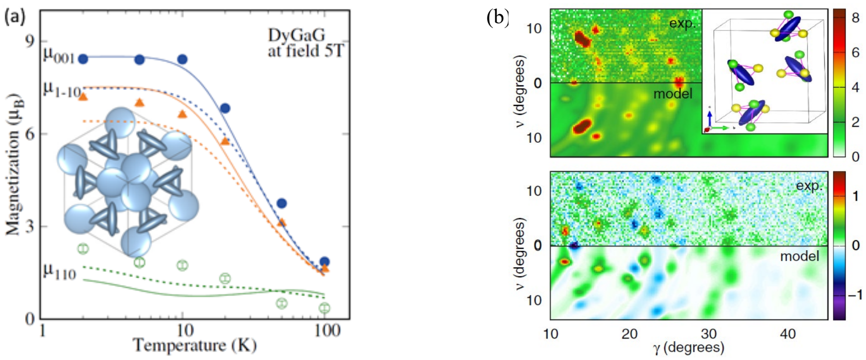

Fig.1: (a) Magnetization components versus temperature for DyGaG. Insets show magnetization ellipsoids. (b) The measured and calculated flipping sum (top) and difference (bottom) diffraction patterns collected on $Co([(CH_3)_2N]_2CS)_2Cl_2$ at 2K, 5T.

Abstracts – Posters 1

Thursday, July 29th, 2021
9:00 – 10:00 AM EST

Multiferroics and Chirality

<u>P1-1</u>: Incommensurate Magnetic Phases of the Multiferroic Compound $MnCr_2O_4$ Described with the Superspace Formalism
Miguel PARDO-SAINZ, Ayaka TOSHIMA, Gilles ANDRÉ, Juan BASBUS, Gabriel CUELLO, Takashi HONDA, Toshiya OTOMO, Katsuya INOUE, Yusuke KOUSAKA, Javier CAMPO
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<u>P1-2</u>: Tuning magnetoelectricity by mixing magnetic anisotropies
Ellen FOGH, Bastian KLEMPKE, Manfred REEHUIS, Philippe BOURGES, Christof NIEDERMAYER, Sonja HOLM-DAHLIN, Mark LAVER, Sebastian PAECKEL André SOKOLOWSKI, Alexandre PAGES, David VAKNIN, Niels B. CHRISTENSEN and Rasmus TOFT-PETERSEN
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<u>P1-3</u>: ferroelectric polarization controlled magnetic reconfiguration in ultrathin $La_{0.67}Sr_{0.33}MnO_3$ films
Chao LIU, **Yaohua LIU**, Bangmin ZHANG, Cheng-Jun SUN, Da LAN, Pingfan CHEN, Xiaohan WU, Ping YANG, Xiaojiang YU, Timothy CHARLTON, Michael R. FITZSIMMONS, Jun DING, Jingsheng CHEN, Gan Moog CHOW
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Strongly Correlated Electron Systems

<u>P1-5</u>: Higher order magnetic scattering with Spherical Neutron Polarimetry
Jacob TOSADO, Wangchun CHEN, Efrain E. RODRIGUEZ
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<u>P1-6</u>: Putative spin-nematic phase in $BaCdVO(PO_4)_2$
M. SKOULATOS, H. GABOLD, G. BRANDL, F. RUCKER, G.J. NILSEN, A. BERTIN, E. POMJAKUSHINA, J. OLLIVIER, A. SCHNEIDEWIND, R. GEORGII, O. ZAHARKO, L. KELLER, Ch. RÜEGG, C. PFLEIDERER, B. SCHMIDT, N. SHANNON, A. KRIELE, A. SENYSHYN, A. SMERALD
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<u>P1-7</u>: Spin correlations in triangular dipole coupled Ising spin lattices
Petai PIP, **Artur GLAVIC,** Kirill ZHERNENKOV
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Quantum Materials

Magnetic Nanomaterials

Thin Films and Multilayers

Polarized Neutron Instrumentation

P1-1: Multiferroics and chirality

Incommensurate Magnetic Phases of the Multiferroic Compound $MnCr_2O_4$ Described with the Superspace Formalism

Miguel PARDO-SAINZ[1,2], Ayaka TOSHIMA[3], Gilles ANDRÉ[4], Juan BASBUS[5], Gabriel CUELLO[6], Takashi HONDA[7], Toshiya OTOMO[7], Katsuya INOUE[3], Yusuke KOUSAKA[2], *Javier CAMPO[1]

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Nowadays, chromium-based normal spinel oxides ACr_2O_4 are one of the most studied materials in the condensed matter community due to the interplay between its magnetic, electric and structural properties [1,2].

In particular, for $MnCr_2O_4$, the ground state magnetic structure is still controversial because the magnetic structures reported by different groups and investigated by independent techniques are inconsistent [1-3].

The magnetic structure of this compound was reinvestigated by magnetization, specific heat and neutron diffraction experiments at different temperatures. The results suggested that a new magnetic phase, not previously reported, is developed under 18 K. The magnetic phases present in this sample were: ferrimagnetic order below T_C = 45 K; conical spin order with propagation vector $\vec{k}_{S1}$ = (0.62(1), 0.62(1), 0) below T_{S1} = 20 K; and conical spin order with propagation vector $\vec{k}_{S2}$ = (0.660(3), 0.600(1), 0.200(1)) below T_{S2} = 18 K.

Using the superspace group approach [4], the symmetry of the nuclear and magnetic structures is determined. Through simple theoretical calculations, we derive the directions along which the electric polarization lies for each magnetic phase.

[1] K. Dey *et al.*, Journal of Magnetism and Magnetic Materials **435**, 15 (2017).

[2] K. Tomiyasu *et al.*, Phys. Rev. B **70**, 214434 (2004).

[3] J. M. Hastings and L. M. Corliss, Phys. Rev. **126**, 556 (1962).

[4] J. Rodríguez-Carvajal and J. Villain, Comptes Rendus Physique **20**, 770 (2019).

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P1-2: Multiferroics and chirality

Tuning magnetroelectricity by mixing magnetic anistropies

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The ability to control magnetic and electric properties is attractive for tailoring materials for devices, data storage and sensor technology. In the so-called magnetoelectric (ME) materials, these two degrees of freedom are closely linked and this makes them particularly interesting [1]. Here we study one such system, $LiNi_{1-x}Fe_xPO_4$, using magnetometry, polarized neutron diffraction, pyrocurrent measurements and Monte Carlo simulations. The parent compounds of this mixed system, $LiNiPO_4$ and $LiFePO_4$, possess mismatched magnetic anisotropies and we demonstrate that by random magnetic anisotropy mixing it is possible to tune the magnetic and ME properties. Interestingly, the major spin component in the groundstate is along an intermediate anisotropy axis which is perpendicular to the plane spanned by the easy axes of the parent compounds. Such behavior was previously predicted with mean-field calculations and our study provides the first clear experimental evidence for such phase. The consequencing lowering of the magnetic symmetry unlocks additional ME couplings in the system. Most remarkably, we observe that the ME coupling strength may be enhanced by up to two orders of magnitude.

[1] W. Eerenstein, N. D. Mathur and J. F. Scott, Nature **442**, 759–765 (2006)

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P1-3: Multiferroics and chirality

ferroelectric polarization controlled magnetic reconfiguration in ultrathin $La_{0.67}Sr_{0.33}MnO_3$ films

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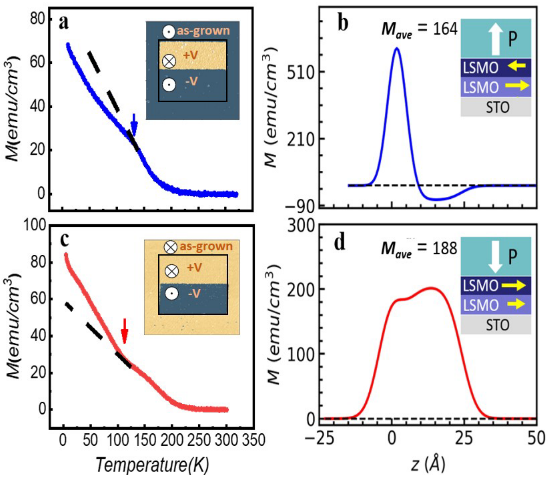

Multiferroic oxide heterostructures consisting of ferromagnetic and ferroelectric components hold the promise for nonvolatile magnetic control via ferroelectric polarization, advantageous for the low-dissipation spintronics. Modern understanding of the magnetoelectric coupling in these systems involves structural, orbital, and magnetic reconstructions at interfaces. Previous works have long proposed polarization-dependent interfacial magnetic structures; however, direct evidence is still missing, which requires advanced characterization tools with near-atomic-scale spatial resolutions. Here, extensive polarized neutron reflectometry (PNR) studies have determined the magnetic depth profiles of $PbZr_{0.2}Ti_{0.8}O_3/La_{0.67}Sr_{0.33}MnO_3$ (PZT/LSMO) bilayers with opposite self-polarizations. When the LSMO is 2−3 nm thick, the bilayers show two magnetic transitions on cooling. However, temperature-dependent magnetization is different below the lower-temperature transition for opposite polarizations. PNR finds that the LSMO splits into two magnetic sublayers, but the inter-sublayer magnetic couplings are of opposite signs for the two polarizations. Near-edge X-ray absorption spectroscopy further shows contrasts in both the Mn valences and the Mn−O bond anisotropy between the two polarizations. This work completes the puzzle for the magnetoelectric coupling model at the PZT/LSMO interface, showing a synergic interplay among multiple degrees of freedom toward emergent functionalities at complex oxide interfaces.

[1] C. Liu *et al.*, ACS Appl. Mater. Interfaces, https://doi.org/10.1021/acsami.1c02300, (2021).

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P1-5: Strongly correlated electron systems

Higher order magnetic scattering with Spherical Neutron Polarimetry

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Complex magnetic systems can be understood through the multipole expansion. In so doing, a magnetic system may then be conceptualized in terms of monopole, quadrupole, and torodapole moments that can each be distinguished by their respective symmetry. We will discuss the possibility of measuring these higher order moments using a polarized neutron scattering technique known as spherical neutron polarimetry. This technique both controls and measures the full three-dimensional neutron polarization to yield a magnetic property tensor of a material system. We will outline a novel approach for analyzing these Q-dependent tensors, demonstrating state-of-the-art calibration and visualization techniques.

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P1-6: Frustrated and disordered systems

Putative spin-nematic phase in $BaCdVO(PO_4)_2$

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We report neutron scattering and AC magnetic susceptibility measurements of the 2D spin-1/2 frustrated magnet $BaCdVO(PO_4)_2$ [1]. At temperatures well below $T_N \approx 1K$, we show that only 34% of the spin moment orders in an up-up-down-down strip structure. Dominant magnetic diffuse scattering and comparison to published µsr measurements indicates that the remaining 66% is fluctuating. This demonstrates the presence of strong frustration, associated with competing ferromagnetic and antiferromagnetic interactions, and points to a subtle ordering mechanism. On applying magnetic field, we find that at $T = 0.1K$ the magnetic order vanishes at 3.78T, whereas magnetic saturation is reached only above 4.5T. We argue that the putative high-field phase is a realization of the long-sought bond-spin-nematic state.

[1] M. Skoulatos et al., Phys. Rev. B **100**, 014405 (2019).

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P1-7: Frustrated and disordered systems

Spin correlations in triangular dipole coupled Ising spin lattices

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Ising spins on a triangular lattice are the textbook example for magnetic frustration that leads to a highly degenerate ground state. When the magnetic moments (or super-spins) are influenced not only to their nearest neighbor, as in a dipole-coupled system, the ground state can no longer be derived analytically. Monte-Carlo simulations of such systems show liquid behavior and a stripe magnetic order ground state at low temperatures [1]. The character of the magnetic phases and the ordering temperature was found to change when compressing the lattice in one direction, making the magnetic coupling asymmetric and reducing the frustration. While there are many simulations of such systems available it is challenging to manufacture and experimentally investigate the physics that occurs on the nanometer scale.

We have used samples of permalloy cylinders on a symmetric and 10% distorted lattice that were fabricated with electron beam lithography to physically implement the theoretical example. The shape anisotropy of the cylinders is out-of-plane and locks the single domain magnets (around 35 nm diameter) to behave Ising-like. To investigate the magnetic structure, we used Grazing Incidence Small Angle Scattering (GISANS) on the MARIA beamline at MLZ [2] with polarization analysis. With the high structural quality, single super-crystal samples we managed to measure diffuse magnetic scattering for the two samples. Magnetic correlations were short range and there was a clear difference between symmetric and distorted lattice.

For quantitative analysis of the magnetic structure factor in our samples we used the Distorted Wave Born Approximation as implemented in BornAgain [3] and extended it with a custom structure factor model that empirically describe the short-range correlations modeled with the Monte-Carlo simulations [1]. With a single fit parameter of reduced temperature (normalized by coupling energy) we can well replicate the measured magnetic scattering on the Yoneda line in two independent directions.

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P1-8: Quantum materials

Chirality preference deduced via polarized neutron diffraction in the centrosymmetric kagome helimagnet YMn_6Sn_6

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YMn_6Sn_6 exhibits topologically protected characteristics which are uncommon given the underlying centrosymmetric crystal lattice (*P*6/*mmm*). The crystal structure comprises Mn atoms on a kagome lattice in the *ab*-plane, which are then stacked along the *c*-axis with the layers separated either by three Sn layers or a mixed Y and Sn layer. Mn atoms in-plane are at equivalent positions and are strongly coupled ferromagnetically via nearest neighbor exchange and have the spins in the *ab*-plane due to easy-plane anisotropy. This stacking pattern has an important magnetic implication, mainly, that within a unit cell there are two unequal interlayer exchange pathways with opposite signs. A short-lived commensurate collinear antiferromagnetic phase, with an onset of $T_N \sim 340$ K, transitions below 333 K to an incommensurate double-flat-spiral magnetic structure due to the exchange competition. At elevated temperatures and modest in-plane magnetic fields, a topological Hall effect (THE) emerges [1, 2] despite a null scalar spin chirality; dynamic chiral fluctuations are thought to be responsible, thus making YMn_6Sn_6 a prototype material for a fluctuation based THE mechanism. [1] Here, we present results obtained via a polarized neutron diffraction study. [3] Unexpectedly, unequal chiral domain populations of the zero-field spiral state were found despite the underlying centrosymmetric crystal symmetry. This could be a significant finding as it implies that the spiral state can energetically favor one domain over the other, possibly in a controlled manner. This is another example, along with the THE, of YMn_6Sn_6 displaying unusual behavior for a structure with inversion symmetry.

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P1-9: Quantum materials

Spin structure determination of the topological Weyl semi-metal candidates Mn_3Ge and Mn_3Sn

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The recent discovery of anomalous Hall effect in Mn_3X (X=Sn, Ge) suggests the existence of Weyl nodes in the electronic band structure of these non-collinear antiferromagnets [1,2]. The details of the magnetic structure of Mn_3X are crucial to Weyl physics, but are still under debate due to the lack of experimental studies. Here, we report polarized neutron diffraction studies on Mn_3X, which provide crucial information on their magnetic structure. In Mn_3Ge, a 2D $\mathbf{k} = 0$ anti-chiral spin structure was determined [3], which naturally explains the origin of a net in-plane magnetization along the [110] direction. In Mn_3Sn, concomitant with the disappearance of the anomalous Hall effect, an additional magnetic phase was discovered at low temperature for which our polarization analysis reveals both an in-plane and an out-of-plane incommensurate spin component [4]. The magnetic ground state selection of Mn_3X will be discussed in terms of long-range exchange, Dzyaloshinskii-Moriya, and crystal electric field interactions.

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P1-10: Quantum materials

Polarized neutron diffraction of Hexagonal-$(Mn_{0.78}Fe_{0.22})_3Ge$

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Topological quantum materials have attracted enormous attention since their discovery due to the observed anomalous transport effects (ATE), which originate from the non-zero Berry curvature. Mn_3Ge has gained special attention because anomalous transport effects can be studied below the Néel temperature (365 K), down to 2 K [1]. Since ATE emerge from the robust topological band structure, it is interesting to study the effects of Fe doping on ATE in $(Mn_{1-x}Fe_x)_3Ge$. Our transport measurements show the existence of an anomalous Hall effect (AHE) in the intermediate temperature range for the 22% Fe doped sample. However, the origin of the AHE cannot be attributed to Weyl points without knowledge of the ground state magnetic structure of doped samples. Therefore, we have performed polarized neutron diffraction from the $(Mn_{0.78}Fe_{0.22})_3Ge$ sample using the D3 CRYOPAD setup at ILL, France. Our analysis concludes that the magnetic structure of the 22% Fe doped sample remains the same as Mn_3Ge in the temperature range where AHE is observed. This suggests that the physics behind AHE observed in doped samples is most likely the same as in Mn_3Ge. Therefore, it can be argued that the Weyl Fermions do not vanish by suitable doping of the sample, as long as the magnetic structure of the doped samples remains the same.

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P1-11: Magnetic nanomaterials

Inverse proximity effects in superconductor/ferromagnet heterostructures: a study by GISANS with polarization analysis

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Proximity effects in superconductor(S)/ferromagnet(F) heterostructures with perpendicular magnetic anisotropy can manifest in various forms such as domain-wall-superconductivity [1] and the generation of long-ranged spin-triplet Cooper pairs [2]. Understanding the origin of such phenomena is the key for an application in fluxonic devices and in spintronics, respectively [3, 4]. Especially a modification of the ferromagnetic domain structure by the onset of superconductivity is barely studied, due to only small variations of the ferromagnetic state with much higher Curie temperature compared to the critical temperature of BCS superconductors.

Grazing-Incidence Small-Angle Neutron Scattering (GISANS) with polarization analysis is the method of choice to study depth-resolved lateral magnetic structures on the mesoscopic length-scale, and enables to investigate the proximity effects in S/F systems with high sensitivity to changes in the magnetic orientation of the ferromagnetic domain pattern.

This work presents a combined study of the macroscopic superconducting and ferromagnetic parameters, and a mesoscopic investigation of the lateral magnetic depth-profile as function of temperature in a model system of Nb(S)/FePd(F) grown by molecular beam epitaxy.

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P1-12: Magnetic nanomaterials

Revealing magnetic correlations close to quantum critical point in the disordered ferromagnetic alloys Ni-V with polarized SANS

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We present a small-angle neutron scattering (SANS) analysis of the alloy $Ni_{1-x}V_x$ with random atomic distribution [1] where the ferromagnetic (FM) order is destroyed towards a paramagnetic phase by sufficient substitution of Ni by V. The critical temperature T_c vanishes at $x_c = 0.116$ indicating a quantum critical point (QCP) with signatures of disorder [1]. We collected full polarized SANS data on different $Ni_{1-x}V_x$ polycrystalline samples close to x_c (with $T_c < 50K$) at NG7SANS, NCNR, NIST utilizing a ^3He cell within the wave vector regime Q = 0.06-1nm^{-1}. Through the angular dependence of the different magnetic cross sections with the magnetic field transverse to the beam we succeed to resolve the small magnetic scattering at diverse length scales within the FM state well below T_c [2]. Besides isotropic magnetic short-range correlations that remain at very low temperatures we find an anisotropic magnetic contribution that reveals large scale magnetic domains below T_c. High field data support the coexistence of short-range fluctuations and long-range order. In addition, we notice local magnetic defects that relate to the V concentration. The polarized SANS study reveals how these different contributions evolve with V concentration x, characterizing a disordered FM alloy, close to the QCP.

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P1-13: Thin films and multilayers

Magnetic structural analysis in $[Fe_3Si/FeSi_2]_{20}$ superlattice using polarized neutron reflectivity

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We report the temperature dependence of in-plane magnetic structures of $[Fe_3Si/FeSi_2]_{20}$ superlattice in the applied in-plane magnetic field. The macroscopic magnetization measurements on the superlattice reveals an anomalous decrease of the magnetization at low temperatures for the applied in-plane magnetic fields below 3 Tesla. For example, at 1 Tesla, the magnetization decrease anomalously for temperatures T < 250 K. Polarized neutron reflectivity measurements under an applied field of 1 Tesla clarify that non-collinear ferromagnetic structures with a transverse antiferromagnetic order are induced at low temperatures below 240 K. These low-temperature structures are characterized by the symmetric and alternate tilting of the Fe_3Si layer magnetization to the in-plane magnetic field direction separated through non-magnetic spacer layers of $FeSi_2$. The tilting angle increases with decreasing temperature causing the anomalous decrease of the magnetization. Above 240 K, the moments are aligned ferromagnetically along the applied field. Figure 1 shows each magnetic structures. Due to the semi-conducting property of the non-magnetic $FeSi_2$ space layer, as the temperature decreases, the biquadratic interlayer coupling term J_2 becomes relatively stronger than the bilinear interlayer coupling term J_1. This might explain the temperature-dependent non-collinear magnetic structures in this magnetic metal/non-magnetic semiconductor superlattice and its anomalous magnetization behaviors at low temperatures.

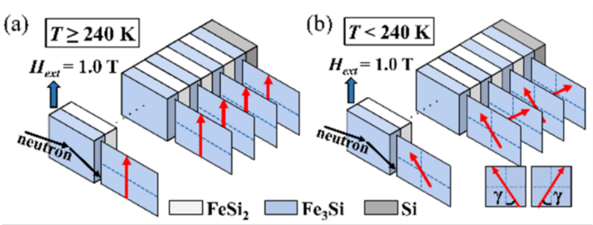

Fig 1. (a) Schematic figure of collinear ferromagnetic structure of $Fe_3Si/FeSi_2$ superlattice, and (b) one of non-collinear ferromagnetic structure with transverse anti-ferromagnetic order.

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P1-14: Thin films and multilayers

Characteristics of the residual ferromagnetic ordering in the antiferromagnetic state of FeRh film

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B2-phase FeRh shows metamagnetic first-order phase transition from antiferromagnetic to ferromagnetic above 370 K[1]. The transition shows a volume expansion of about 1% and variation of electrical resistivity due to the increasing density-of-state at the Fermi level [2, 3]. Unlike bulk, unexpected ferromagnetic (FM) characteristics have been observed in a thin-film form [4].

This presentation shows the detailed origin of the residual FM state by examining temperature-dependent physical properties. First, the residual ferromagnetic induce thermomagnetic irreversibility (e.g., spin-glass-like behavior) and negative magnetoresistance. Second, the non-uniform distribution of the magnetic profile at low temperature (i.e., below the transition temperature) is observed from the temperature-dependent polarized neutron reflectometry. Interestingly, the bottom and top interfaces exhibit an FM state while the middle region is an AFM state. Furthermore, the bottom (top) interface shows a temperature-independent (-dependent) FM state, indicating that the FM origin of the interface between substrate and film (bottom interface) and capping layer (Al) and film (top interface) are due to structural distortion and Fe-defect state, respectively.

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In situ polarized neutron reflectivity (*i*-PNR) in determining the evolving magnetic moments of Fe monolayers: a perspective w.r.t ex situ X-ray magnetic circular dichroism (XMCD)

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We have combined two complementary techniques, element sensitive ex situ X-ray magnetic circular dichroism (XMCD) and in situ polarized neutron reflectivity (*i*-PNR), to determine the values of evolving magnetic moments obtained from a low symmetry system of hetero-epitaxial Fe monolayers (MLs), as a function of thickness [1].

The samples were grown by magnetron sputtering on face-centered-cubic (fcc) Cu(001)/Si(001). Within experimental errors, we found a corroboration of the modulated moments from the XMCD and of the magnetic anisotropies from magnetization measurements with those obtained earlier from layer-by-layer i-PNR measurements. The modulation was attributed to initial island-like growth morphology assisted monolayer-magnetism during sputtering. Furthermore, analyzing the depth sensitive i-PNR profile of a bulk-like film, we developed a model characterized by monotonic magnetism involving collinear spins. The model is further described by a higher magnetization for the deeper layers, which decreases gradually for the upper layers before attaining saturation at its bulk value within a few MLs. This model contradicts the earlier proposed non-collinear model involving antiferromagnetic units, thus clarifying the long-standing ambiguity in the coverage regime. The results have been compared with those existing, following the theoretical parameterized tight-binding model with satisfactory agreement.

This study distinguishes the variation of monolayer-magnetism owing to the growth morphology from the layer-by-layer investigation vis-à-vis depth-profiling of bulk-like film. At the same time, it also promises the general possibility of depth-profiling using i-PNR in other complex multilayered systems on high flux neutron sources.

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P1-16: Thin films and multilayers

Interfacial reconstruction in epitaxial $CoFe_2O_4/\alpha\text{-}Al_2O_3$ thin-film systems

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Oxide interfaces, characterized by the distinctively strong interaction and reconstruction among charge, spin, orbital and structural degrees of freedom, have served as versatile platforms to study emergent novel states and phenomena in the last decade. Spinel oxides are natural candidates for studies on interfacial emergent phenomena, because their inter-site cation migration, potentially as the driving force for interfacial reconstruction, can be enhanced if parameters such as temperature and lattice constants are adjusted. Among them, inverse spinel $CoFe_2O_4$, of large magnetocrystalline anisotropy, superior mechanic hardness and excellent physical and chemical stability, has been widely studied and applied in high-density magnetic storage, magnetoelectric transducers and spin filters. And $CoFe_2O_4$ films of (111) normal direction can be epitaxially grown on α-Al_2O_3 (0001) substrates of the rhombohedral corundum structure. The large difference in crystal structures and lattice parameters between these two materials implies potential strong interfacial reconstruction. Here we report an interfacial layer potentially dominated by CoO/FeO formed between $CoFe_2O_4$ thin films and sapphire substrates corroborated by the analysis of structure and magnetism.

We have epitaxially grown $CoFe_2O_4$ (111) films on Al_2O_3 (0001) substrates by pulsed laser deposition [1]. X-ray and reflection high-energy electron diffraction (RHEED) demonstrate an interfacial layer of a different crystal structure from the “bulk” part of the $CoFe_2O_4$ film. As a result of this interfacial reconstruction, colossal intrinsic exchange bias up to 7 ± 2 kOe was observed, whose interfacial origin is indicated by the power-law thickness-dependence relation of exchange bias. The temperature dependence of exchange bias reveals the exchange interaction between the interfacial layer and the ferrimagnetic $CoFe_2O_4$ disappear at about 250K, close to the Néel temperature of CoO(~290 K) and FeO(~190 K). And the lattice constant of the interfacial layer extracted from thickness-resolved RHEED patterns matches those of CoO and FeO. X-ray reflection and polarized neutron reflection data further support the emergence of the interfacial layer and imply the complexity of the interfacial components and the mechanism of interfacial reconstruction. This work suggests a path for enhancing intrinsic exchange bias using a combination of film and substrate of large structural differences, highlighting the role of interfacial atomic and electronic reconstructions.

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P1-17: Polarized neutron instrumentation

Beamlines for Polarized Neutron Development at the High Flux Isotope Reactor

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At Oak Ridge National Laboratory, the neutron optics and polarization group currently operates two development beamlines at the High Flux Isotope Reactor (HFIR).

The newest is the "Larmor" cold neutron polarization development beamline at the CG4B guide position, commissioned in 2018. The first experiment on this beamline imaged He ions in turbulent flow. More recent measurements include tests of resonant spin echo with superconducting rf flippers, and quantum entanglement using Wollaston prisms. We also tested new apparatus for spherical polarimetry.

The HB-2D polarized beamline in the beam room has also hosted many prototypes and components. These beamlines provide necessary resources for instrumentation development at both the Spallation Neutron Source and HFIR, as well as technique demonstration for future instruments.

In about 2024, HFIR will be shut down for replacement of its permanent beryllium reflector, which will necessitate removal of the instruments. This offers an opportunity to replace many instruments, and planning is in progress for the future development positions.

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P1-18: Polarized neutron instrumentation

KOMPASS – the polarized cold neutron triple-axis spectrometer at the FRM II

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KOMPASS is a polarized cold-neutron three axes spectrometer (TAS) currently undergoing its final construction phase at the MLZ in Garching. The instrument is designed to exclusively work with polarized neutrons and optimized for zero-field spherical neutron polarization analysis for measuring all elements of the polarization matrix. In contrast to other TASs, KOMPASS is equipped with a unique polarizing guide system. The static part of the guide system hosts a series of three polarizing V-cavities providing a highly polarized beam. The exchangeable straight and parabolic front-end sections of the guide system allow adapting the instrument resolution for any particular experiment and provide superior energy- and ***Q***-resolution values when compared with the existing conventional guide and instrument concepts [1, 2]. In combination with the end position of cold neutron guide, the large doubly focusing HOPG monochromator and analyzer, the V-cavity for analysis of polarization of scattering beam, the KOMPASS TAS will be very well suited to study various types of weak magnetic order and excitations in variety of complex magnetic structures.

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P1-19: Polarized neutron instrumentation

MARIA – The high-intensity polarized neutron reflectometer of JCNS – overview of current research and developments

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MARIA of JCNS [1] is a state of the art high-intensity polarized neutron reflectometer that provides the opportunity to investigate 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. In the case where dynamic ranges in order of 4-5 orders need to be accessed, the measurement time is in few minutes range. MARIA installed in the neutron guide hall of the FRM II reactor in Garching. A velocity selector (4.5Å<λ<40Å) is used as a primary wavelength filter with resolution of 10% and in combination with the optional Fermi-Chopper the wavelength resolution can be increased to 3% or 1%. The full cross section of the beam is polarized by a double-reflecting super mirror (4.5Å<λ<12Å) and in the vertical direction the elliptically focusing neutron guide significantly increases the flux at the sample position that permits to reduce 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 measurements of Oxide MBE samples[2] and with various soft matter solid/liquid interface cells connected to a “sample robot” allowing automatic solvent contrast exchange and remote heating/cooling. Together with the 400x400 mm^2 position sensitive detector and a time-stable ^3He polarization spin filter based on in-situ Spin-Exchange Optical Pumping (SEOP) covering the whole detected beam [3] the instrument is well equipped for investigating (off-)specular scattering from magnetic structures down to monolayer regime [4]. Furthermore, GISANS option can be used to investigate lateral structural and magnetic correlations in the nm range [5] with full polarization analysis. Due to large detector area even grazing incidence diffraction measurements are possible

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P1-20: Polarized neutron instrumentation

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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P1-21: Polarized neutron instrumentation

Polarised neutrons for European Spallation Source instruments

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Polarised neutrons will be a prominent feature in many ESS instruments. Of the currently approved 15 instruments [1], 12 instruments aim to have polarised neutron capabilities. They include 7 of 8 "first-instruments" that will soon begin hot-commissioning upon beam-on-target: diffractometers DREAM and MAGiC, spectrometers BIFROST and CSPEC, SANS instrument LoKI, reflectometer ESTIA, and imaging instrument ODIN. Depending on the instrument configuration, there will be combinations of different types of polariser, analyser and spin-flipper technologies to get the optimal performance and cost-effectiveness. They include MEOP and SEOP based polarised ^{3}He neutron spin filters, polarising supermirrors, radio-frequency gradient-field spin flippers, and we will adopt innovative designs where applicable for these components. Even at an early stage of ESS operation, the neutron flux is expected to be on par with some of the polarised-neutron-capable instruments at major facilities. The polarisation developmental effort is therefore underway in parallel to instrument construction, with the aim of delivering polarised neutrons for first-science experiments as instruments are entering operation.

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Polarized instrumentation of the JCNS at the MLZ

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The JCNS at MLZ operates 10 neutron instruments and a test beamline at the FRM II research reactor in Garching, and two more will come into operation with the new guide hall under construction. Of these over 80% have polarization "P" options, and many with polarization analysis "PA" capability. The polarized diffraction suite consists of three SANS instruments, KWS1, KWS2, KWS3, two reflectometers MARIA, TREFF and hot diffractometer POLI. The polarized spectroscopy suite currently contains cold triple axis PANDA, DNS wide angle spectrometer, neutron spin echo J-NSE and in the future a thermal spectrometer TOPAS. Some such as MARIA, DNS, J-NSE, TREFF, PANDA and POLI are in routine operation with P and PA. KWS-1 and KWS-2 have routine P but are waiting for commissioning of their in-situ polarized ^{3}He PA systems, work which has been delayed due to the pandemic and reactor technical delays. In the meantime KWS-3 has commissioned a super mirror (SM) polarizer as well as off-line polarized ^{3}He cells for PA. Other instruments continually work towards upgrades and new options. POLI is constructing two new in-situ ^{3}He SEOP polarizers for P and PA which are nearing completion. Upcoming instruments such as TOPAS will be commissioned with P and PA when that guide hall comes into operation. Polarization components of TOPAS have already been used for P on POLI and PA on NEAT.

JCNS also makes significant instrument contributions to the ESS*: providing P for the DREAM instrument including an in-situ ^{3}He polarizer similar to the TOPAS and POLI devices and novel permanent magnet guide fields to minimize shadowing of the DREAM back-scattering detectors in work partially funded by the Röntgen-Ångstrom Cluster**, and planning another similar in-situ ^{3}He polarizer for the thermal wavelength band of the T-REX instrument.

*We thank Hal Lee's contributions for integration of polarization devices and polarizers to the ESS, and **Sabrina Disch as co-proposer for the scientific part of the German portion of the Röntgen Ånström Cluster grant.

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P1-23: Polarized neutron instrumentation

QENS measurements with polarization analysis

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A polarized neutron capability with wide-angle polarization analysis has been developed for studies of hard condensed matters on the Multi-Axis Crystal Spectrometer (MACS) at the National Institute of Standards and Technology Center for Neutron Research (NCNR) [1]. Here we report an expansion of the wide-angle polarization analysis capability for QENS studies of soft matters. The incident beam is polarized by a cylindrical ^{3}He spin filter cell in a radio frequency-shielded solenoid and neutron polarization is flipped at will by inverting the ^{3}He polarization using the adiabatic fast passage nuclear magnetic resonance technique. The scattered neutron polarization is spin-analyzed by a "horseshoe"-shaped ^{3}He cell with wide-angle coverage of 240 degrees. The capability provides one of the most intense polarized cold neutron beams in neutron spectroscopy with a polarized incident neutron flux of 1x10^8 cm^{-2}s^{-1} at 10 meV. This capability has recently been employed to unambiguously separate the coherent and spin incoherent signal from the QENS spectra for the investigation of both the collective and single-particle dynamics in partially deuterated (CH_3OD, D 99.5 % purity) methanol [2]. Yet, the energy resolution in FWHM (≈0.18 meV at 3.4 meV and ≈0.255 meV at 4.2 meV) on MACS might unfortunately represent the main limiting factor for soft matter applications. We are exploring ways to deploy the wide-angle polarization analysis capability on MACS to the Disk Chopper Spectrometer at NCNR that has much better energy resolution. We present the results of the first QENS study of partially deuterated methanol and advancement of the wide-angle polarization analysis capability for QENS measurements of both collective and single-particle dynamics.

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Abstracts – Posters 2

Friday, July 30th, 2021
9:00 – 10:00 AM EST

Polarized Neutron Techniques and Methods

Polarized Neutron Instrumentation

P2-1: Polarized neutron techniques and methods

Polarization system for a proposed small- and wide-angle neutron scattering diffractometer/spectrometer, CENTAUR, at the Second Target Station of SNS

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CENTAUR is an instrument concept proposed for the Second Target Station (STS) of the Spallation Neutron Source at ORNL. The instrument will leverage the STS source and large detector coverage to deliver a capability that will enable assessment over a wide range of length scales with excellent resolution, measurements on smaller samples, and time-resolved investigations of evolving structures in soft matter, polymer sciences, geology, biology, quantum condensed matter, and other materials sciences. The addition of the polarized neuron capability and a high-resolution chopper will enable detailed structural and dynamical investigations of magnetic materials and quantum materials.

We will present the polarization system at CENTAUR (shown in the figure below). Based on the science cases, the required Q range for polarization analysis is 0.002 Å-1 to 0.3 $Å^{-1}$. A supermirror polarizer in the optics system will provide polarized neutron. For simplicity and practicality, an ex-situ polarized ^{3}He analyzer system will be used after the sample position. In the ex-situ system[1], multiple ^{3}He cells with different diameters of up to 15 cm can be dropped in and swapped easily during the experiment as needed.

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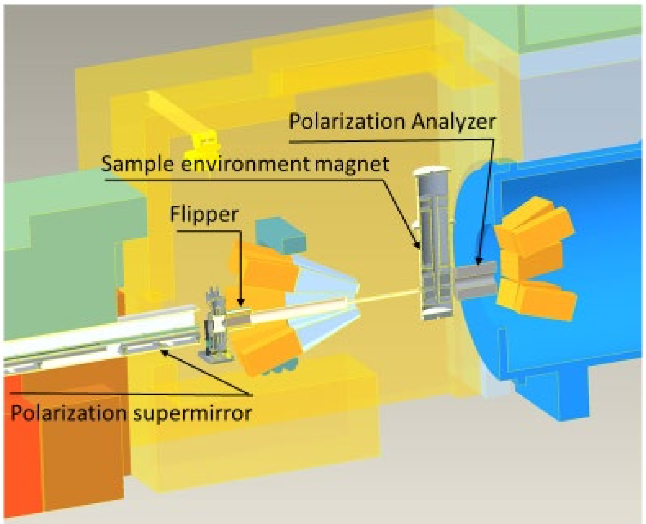

P2-2: Polarized neutron techniques and methods

High performance hot neutron polarizer based on in-situ polarized ^{3}He

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We have developed compact and high performance in-situ ^{3}He polarizers based on spin-exchange optical pumping for the polarization and polarization analysis of hot (wavelengths from 0.3 to 1.1 Å, and energy from 0.06 to 1 eV) neutrons. Efficient polarization of neutrons of these wavelengths/energies is difficult to perform by means of other methods. Therefore, ^{3}He technique is of major interest. Our ^{3}He polarizers have been commissioned and used for 0.9 Å neutrons where neutron polarizations in excess of 97% with over 24% neutron transmission are achieved[1]. The performance can easily be extended to 0.3 Å neutrons as would be available on the POLI instrument at the MLZ in Germany[2] by utilizing a higher pressure ^{3}He cell. Consequently we are in the processes of completing an upgraded polarizer design optimized for this neutron instrument that can also operate in the vicinity of the available 8 T sample magnet[3]. These polarizers will be used for studies of magnetism in single crystal neutron diffraction as well as in fundamental and particle physics. Using the double focused beam of POLI they enable one of the most intense polarized hot neutron beams available.

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PASTIS on NEAT: polarization analysis with ^{3}He on a high performance TOF neutron spectrometer

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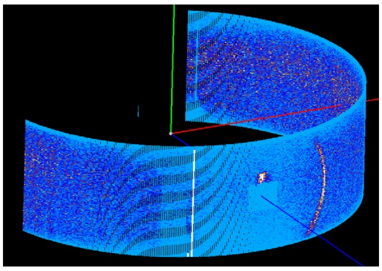
The NEAT spectrometer is a high performance, low background, time-of-flight (TOF) neutron spectrometer that was operated and developed at the former medium flux BERII reactor in Berlin[1]. Few inelastic neutron scattering instruments with large area detectors have been able to achieve polarization analysis, partly due to low intensity of the scattering signals coupled with the losses in neutron flux due to the addition of polarization that can reduce flux at the detectors by an order of magnitude. However, the unique chopper system and final upgrades to the instrument resulted in detector count rates using polarization analysis that remained about an order of magnitude higher than the pre-upgrade values, giving NEAT a world class polarized neutron performance for an instrument of this type. The polarization is performed by a V-type supermirror[2], and the analysis by a wide angle SEOP-polarized ^{3}He spin filter cell in a PASTIS style magnetic environment[3]. This PASTIS system, originally developed for XYZ polarization on the thermal TOF spectrometer TOPAS to be operated on the FRM II reactor at the MLZ in Garching[4], provided good polarization analysis performance for the full detector coverage of 240° horizontal and 40° vertical for incident wavelengths of 2 Å to 6 Å. The ^{3}He lifetime was up to 100 hours in one horizontal direction “X” and about 40 hours in the vertical “Z” and other horizonal direction “Y” with a 4 cm outer diameter cryostat installed for the sample. The incident neutron polarization was guided into this compact system with a special XYZ guide-coil system without adverse effects on either the neutron polarization or ^{3}He lifetime. We present the performance of the PASTIS system and experiences gained from this work.

JCNS PASTIS on NEAT showing the cryostat and ^{3}He PASTIS cell installed providing large scattering angles.



NEAT Detector map showing complete detector coverage of 240° by 40° from the ^{3}He cell.

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P2-4: Polarized neutron techniques and methods

^{3}He system at China Spallation Neutron Source (CSNS)

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The China Spallation Neutron Source (CSNS), as one of the major neutron facilities in China, has committed resources to the development of a polarized ^{3}He NSF program to support its growing polarized neutron research. A spin-exchange optical pumping (SEOP) station based polarized ^{3}He system and other necessary hardware for NSF transport has been recently developed.

The performance of the system is benchmarked using an in-house developed cell named ``Trident" [1] at the neutron technology development beamline (BL-20) at the CSNS. The cell was fully polarizing using the off-situ SEOP station then transported to the BL-20 for neutron transmission measurement to quantify the polarization of the ^{3}He gas. Neutron beam measurements yield a ^{3}He polarization of 77% with over 200 hours of on beam relaxation time.

Combining this newly developed SEOP system with the recently reported cell fabrication station, CSNS is now capable of fully self-sustained production of ^{3}He NSFs that shall support its future neutron polarization research.

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P2-5: Polarized neutron techniques and methods

At last, an *in-situ* polarized ^{3}He neutron spin filter has been installed on POLANO at J-PARC

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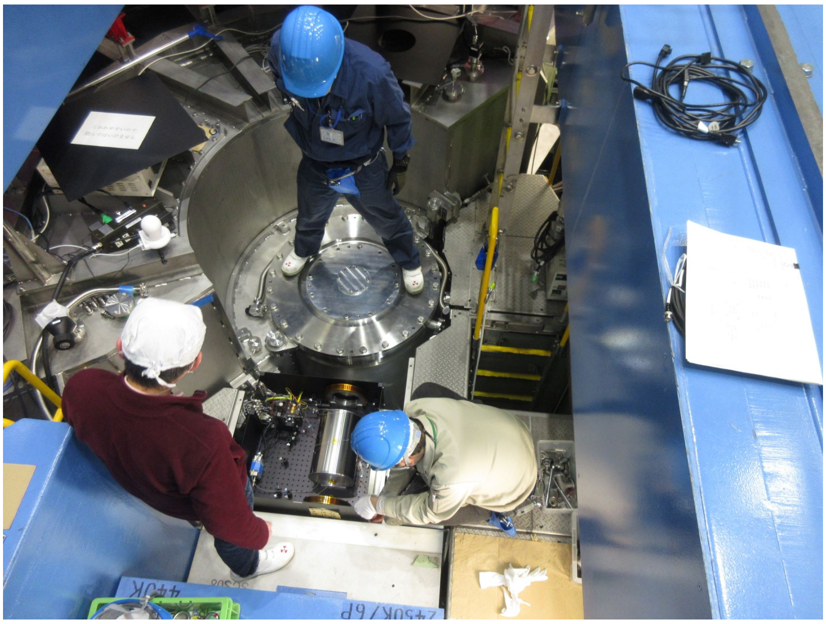
An *in-situ* polarized ^{3}He neutron spin filter (NSF) for incident neutron beam polarization has been installed recently on POLANO - Polarized Neutron Spectrometer - at Materials and Life Science Experimental Facility, J-PARC [1]. POLANO is an inelastic neutron scattering instrument that enables polarization analysis of inelastic scattering experiments to investigate dynamical properties of multiple degrees of freedom [2]. Incident neutrons up to 100 meV are to be polarized with the newly installed *in-situ* ^{3}He NSF, and scattering neutrons up to 40 meV can be spin-analyzed by m = 5.5 supermirrors. The commissioning of the ^{3}He NSF is now underway, and the first polarized neutron beam will soon be delivered on POLANO.



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P2-6: Polarized neutron techniques and methods

The Larmor phase correction of MIEZE

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Modulation of Intensity Emerging from Zero Effort (MIEZE) is a neutron resonant spin echo technique which allows one to measure the time correlation functions in materials by modulating the neutron beam using radio-frequency (RF) neutron spin flippers. The technique avoids neutron spin manipulation between the sample and the detector, and thus could find applications in cases where the sample depolarizes the neutron beam. However, the finite sample size creates a variance in the neutron path length between the locations where scattering and detection happens, which causes the aberrations in Larmor phase. Such aberrations greatly limit the contrast in the intensity modulation in particular towards long correlation times or large scattering angles. We propose two approaches to correct such aberrations, which will enable us to extend those detection limits to longer times and larger angles. One approach involves the physical tilting of the RF flippers in the primary spectrometer with respect to the beam direction [1] and the other approach involves two magnetic Wollaston prisms in addition to the two RF flippers [2]. Both approaches can shape the wave front of the intensity modulation at the sample position to compensate for the path variance from the sample and the detector. The simulation results indicate that both approaches enable one to operate a MIEZE instrument at much increased RF frequencies, thus improving the effective energy resolution of the technique.

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P2-7: Polarized neutron techniques and methods

A cylindrical miniaturised polarisation analysis device (MiniPAD)

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Spherical neutron polarimetry (SNP) has been systematically developed and applied over the last decades since the Cryogenic Polarisation Analysis Device (CryoPAD) presented by Tasset et al. in 1989 [1-3]. This technique gives access to all nine components in the polarisation matrix and therefore allows solving the Blume-Maleyev equations describing the spin evolution in the neutron magnetic scattering [4,5]. The biggest advantage of SNP over conventional polarisation analysis methods is its ability to separate nuclear and magnetic contributions even in the presence of finite nuclear-magnetic interference terms. Hence, the magnetic properties, e.g. magnetoelectricity, non-collinear magnetic structures and different types of magnetic domains in antiferromagnetic structures, can be finely determined. Inspired by the previous devices [6,7], the MiniPAD is designed to have a very compact form with the precession coils bent into a cylindrical shape around the sample, allowing scattering angles up to 140°. Thanks to its size, it is simple to handle and can be easily inserted into a standard cryostat. We would like to report on the latest development of MiniPAD including the newest measurements and the subsequent optimisations.

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P2-8: Polarized neutron techniques and methods

Progress on ^{3}He NSF cell filling station and magnetic holding field for polarized neutron scattering experiments at China Spallation Neutron Source

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Polarized neutrons are unique probe for the investigation of magnetic properties in the materials. Polarized neutron scattering experiments require control of neutron polarization and its polarization analysis. Owing to its spin dependent strong absorption and negligible scattering cross sections with neutrons, polarized ^{3}He gas in a suitable glass cell is used as a wide band neutron spin filter (NSF) at most of the neutron sources. Recently, CSNS has started successfully producing ^{3}He NSF cells and has developed related techniques on site.

^{3}He glass cells and tubing for NSF applications are blown in-house in a dedicated lab area. Filling station equipped with gas purifiers and residual gas analyzer (RGA) is used for filling the mixture of high purity $^3He/N_2$ gases and K/Rb alkali metals in the cell [1]. ^{3}He gas up to 3 bar can be sealed in the glass cell using liquid N_2 bath. ^{3}He filled cells, to be used for NSF applications, are polarized using Spin Exchange Optical Pumping (SEOP) method [2]. Polarized ^{3}He cell can be used for NSF applications either in-situ [3] or off-situ conditions at the polarized neutron scattering instruments (beamlines). Life time of ^{3}He cell is very sensitive to the magnetic field inhomogeneity. So, off-situ (^{3}He cell not being continuously pumped at the beamline) use of ^{3}He NSF cells must be transported and kept in homogeneous magnetic field environment avoiding any interference with stray magnetic field.

In this poster I will be introducing our newly built filling station and shielded solenoid based homogeneous magnetic field cavity to hold ^{3}He polarization. The cell was transported to the test beamline (BL-20) at CSNS in the magnetic holding field to check its performance. Obtained results will be discussed in the poster.

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[3] Junpei Zhang et. al., to be submitted

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P2-9: Polarized neutron techniques and methods

Novel type polarization analysis using multi-analyzer setup @ PUMA, FRM II

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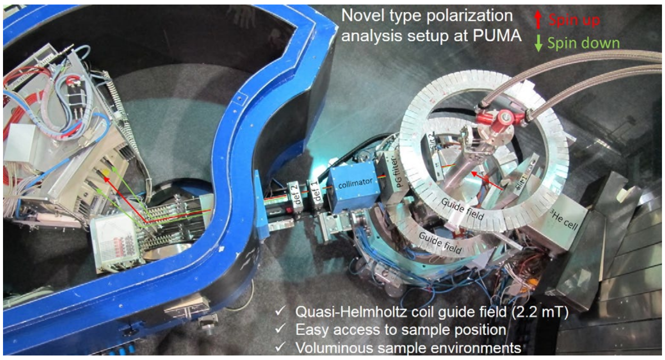
The thermal triple-axis-spectrometer PUMA at the neutron research reactor FRM II (MLZ) is one of the most robust and yet extremely flexible instruments worldwide of its kind. To meet the ever-growing demands of the scientific community worldwide, PUMA delivers a good number of unique features in addition to its "*normal triple axis*" setup. Multiplexing using eleven arbitrarily configurable analyzer-detector channels of the multi-analyzer-multi-detector setup is one of such available features. In particular, single shot kinetic experiments are well suited as the setup allows the measurements of an entire ($\boldsymbol{Q}$,$\boldsymbol{\omega}$)-scan within a time scale even less than a minute as a function of any external stimulant [1]. Moreover, the same setup can be very efficiently used for polarization experiments. By directing the spatially separated different spin-states of the scattered neutrons into the different analyzer channels, the spin flip (SF) and the non-spin flip (NSF) components can be simultaneously determined [2], and to best of our knowledge none of the conventional existing neutron instruments collects both spin-states at the same time. Especially in case of kinetic time-resolved experiments, where both spin states need to be registered synchronously at the same state of the sample, this set up is of absolute necessity. To allow an easy and efficient operation of this sophisticated polarization setup and provide support for subsequent data analysis, we have also developed GUI based MAX-PA software. I will present the current status of this novel type polarization analysis setup at PUMA, including results from the pilot experiments [3].



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P2-10: Polarized neutron techniques and methods

Development of a compact wide-angle neutron spin-echo device

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Neutron Spin Echo (NSE) is well established as a high energy resolution technique. However, most NSE instruments accept only a narrow range of scattering angles from the sample, limiting their application in short length-scale materials and increasing measurement times. We present a design and prototype of a compact, modular NSE device with a ~10° angular acceptance. A key obstacle in wide-angle NSE is the maintenance of a constant field integral as a function of scattering angle, which we address by changing the field shape to approximate a circle centered on the sample position. The precession field region is well defined using high-temperature superconducting (YBCO) films as Meissner screens while the angular dependence of the magnetic field integral is cancelled by shaped pole caps on the superconducting magnets that provide the precession field. This half-meter long device can achieve a ~1 ns spin echo time for cold neutrons. The device includes two magnetic Wollaston prisms that can accomplish linear field-integral corrections. In addition, the inclusion of these prisms allows the device to be used easily for spin-echo code of scattering angles for applications such as SESANS, SEMSANS, Larmor diffraction and phonon focusing. We have designed the device so that all components can have their magnetic fields either vertical or horizontal, allowing for the creation of spin textured beams, including orbital angular momentum states.

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P2-11: Polarized neutron techniques and methods

Simulation and optimization of a polarizing bender for Flexx at MLZ

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The cold neutron triple-axis spectrometer Flexx at the BER2 reactor in Berlin will be transferred to the FRM2 reactor in Munich. The original polarizing solid state S-bender in the neutron guide is not suitable for the guide system at FRM2 and a new bender after the monochromator is needed. To design and optimize the bender, we performed Monte Carlo ray tracing simulations using the McStas software and compared several polarizing benders. We explored the methods to improve the performance of the transmission C-bender for a larger wavelength range and proposed a transmission C-bender with the two remnant polarizing collimators, which shows a high performance.

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P2-12: Polarized neutron techniques and methods

Demonstration of contextuality in neutrons and entangled neutron scattering

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The non-locality of physical reality is a well-known and rigorously tested consequence of quantum mechanics. *Contextuality*, a generalization of non-locality, essentially states that the measurements of quantum systems do not reveal pre-existing values: the observed result depends on the *context*, the set of all compatible (simultaneously measurable) observables [1]. Entanglement is the cause of the nonclassical correlations that are responsible for contextuality, as well as many other phenomena in complex materials, such as superconductivity and quantum spin liquids. Confirmation of contextuality implies confirmation of a mode-entangled (intraparticle entangled) neutron beam.

We have demonstrated contextuality in a bipartite-entangled (spin and path) and tripartite (spin, path, and energy) neutron beam using magnetic Wollaston prisms and radio-frequency flippers at both a continuous reactor source and a pulsed spallation source [2,3]. Analogous to the violation of the Bell inequality, we constructed the Clauser-Horne-Shimony-Holt (CHSH) contextuality witness and observed the maximal violation of the classical bound of the CHSH inequality. Maximal entanglement was verified down to path separations below 100 nm, even when the wavepackets of the two paths significantly overlapped.

We expect these entangled beams to be sensitive to samples with entanglement at similar length scales to the separation of the two paths. An ongoing theoretical investigation has already shown the existence of unique scattering signatures with entangled samples in idealized models [4].

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P2-13: Polarized neutron techniques and methods

Spin textured neutron beams

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The technique of spin echo modulated small angle neutron scattering (SEMSANS) was suggested several years ago and has been implemented at polarized beam lines both at reactor and pulsed neutron sources [1]. The method uses inclined neutron spin flippers to create a well-defined spatial modulation of the neutron polarization which, when analyzed, yields a pattern of intensity stripes on a position sensitive neutron detector. A scattering sample blurs these stripes, and the degree of blurring yields direct information about the real-space correlation function for the scattering entities in the sample. One method that we have successfully used to produce such a striped intensity pattern involves the use of superconducting magnetic Wollaston prisms. Using McStas simulations and analytic calculations, we show that various combinations and orientations of Wollaston prisms can be used to prepare more complex spatial spin structures, including "checkerboards" and vortex lattices that carry orbital angular momentum (OAM). We show that it is possible to set up an OAM echo experiment in which the full neutron polarization is retrieved when no scattering sample is used. We discuss potential uses for spatially textured beams.

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P2-14: Polarized neutron techniques and methods

Neutron polarimetry using a polarized ^{3}He cell for the aCORN experiment

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The neutron polarization of the unpolarized NG-C beamline at the NIST Center for Neutron Research was measured as part of the aCORN neutron beta decay experiment. Neutron transmission through a polarized ^{3}He spin filter cell was recorded while adiabatic fast passage (AFP) nuclear magnetic resonance (NMR) reversed the polarization direction of the ^{3}He in an eight-step sequence to account for drifts. The dependence of the neutron transmission on the spin filter direction was used to calculate the neutron polarization. The time dependent transmission was fit to a model which included the neutron spectrum, and ^{3}He polarization losses from spin relaxation and AFP-NMR. The method, analysis, and result of $|P_n| \leq 4 \times 10^{-4}$ with 90% confidence will be presented.

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P2-15: Polarized neutron techniques and methods

A new phase-correction method using complete ellipsoidal focusing mirrors for neutron resonance spin-echo spectroscopy: Double-focusing method

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Neutron resonance spin-echo (NRSE) spectroscopy is a technique for measuring intermediate scattering functions of samples using resonance spin flippers (RSFs) [1]. NRSE geometries with focusing mirrors have been proposed in previous studies [2, 3]. NRSE spectrometers with focusing mirrors enable experiments with a high energy resolution and signal-to-noise ratio simultaneously. Only a limited circumference of a complete ellipsoidal mirror to reflect the neutron beam was used in previous studies. Therefore, the neutron spin phase was aligned by tilting the RSFs which are set to be perpendicular to the diagonal of the right triangle determined by the semi-major and semi-minor axes of the ellipse. The effect of this tilt was numerically evaluated [3]. This tilt increased the MIEZE contrast in an experiment [4] using developed ellipsoidal focusing supermirrors [5]. However, the utilization of larger divergent beams using the entire circumference of an ellipsoidal focusing mirror is impossible via this tilt method because the RSFs can only be tilted in one direction. Thus, a new phase-correction method is required to conduct NRSE experiments using a complete ellipsoidal focusing mirror.

We propose a double-focusing method in which two identical ellipsoidal mirrors are arranged in series [6]. This arrangement enables us to correct the path length differences for large divergent beams using a complete ellipsoidal focusing mirror. In this study, we evaluated the effectiveness of this geometry both analytically and numerically. A Fourier time of 1 μs is achievable using this method.

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P2-16: Polarized neutron techniques and methods

An introduction of the TOF-MIEZE spectrometer at J-PARC MLF BL06

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We present an introduction of the neutron spin-echo spectrometer at BL06 [1] at Materials and Life Science Experimental Facility (MLF), Japan Proton Accelerator Research Complex (J-PARC). The beamline has two spin-echo instruments using RF spin flippers: NRSE (neutron resonance spin-echo) and MIEZE (Modulation of intensity with zero effort [2]). We have tested features of MIEZE technique using time-of-flight of pulsed neutrons (TOF-MIEZE) [3]. This spectroscopy was applied to a long-range magnetic order in MnSi in a small angle scattering geometry [4]. The fine wavelength resolution of the pulse beam allows us to analyze the spin dynamics in a precise region of interest in (Q_x, Q_y) space. Such measurements can provide information for interpreting a microscopic model of transformation of the magnetic structure.

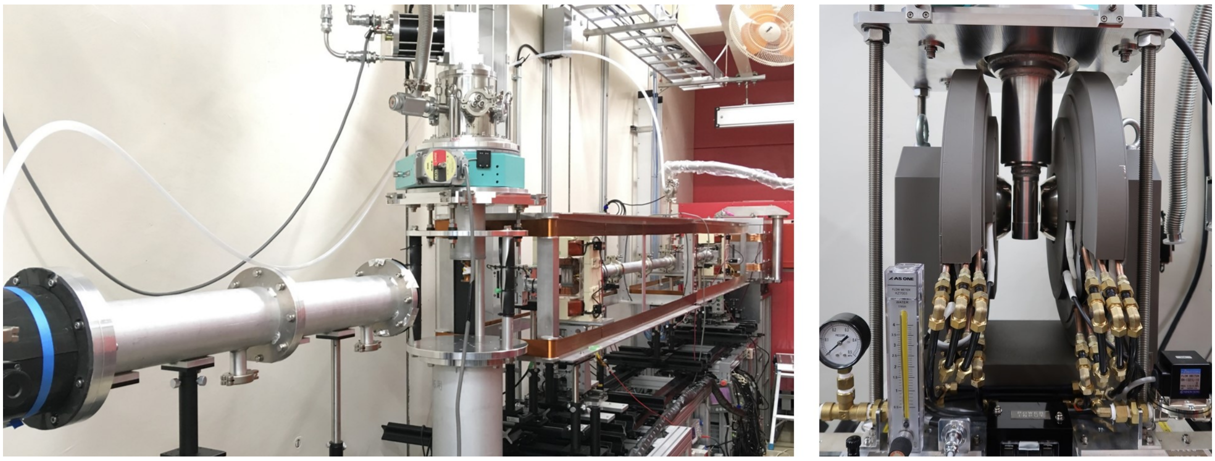

Figure: (left) MIEZE spectrometer at BL06. (right) Newly installed magnet and cold head.

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P2-17: Polarized neutron techniques and methods

Development of a large beam high efficiency radio-frequency neutron spin flipper for the polychromatic reflectometer CANDOR

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The capability for performing longitudinal polarization analysis is important in studies of magnetic thin films and multilayers and is being developed for both specular and off-specular reflectivity measurements on the polychromatic reflectometer CANDOR.at the National Institute of Standards and Technology Center for Neutron Research (NCNR). A critical component to such a capability is a large beam high efficiency radio-frequency (RF) neutron spin flipper. We report the design, simulation, and experimental characterization and optimization of the flipper. Unlike a conventional RF flipper, three permanent magnet guide field sections with air gaps are employed to provide a linear field gradient along the beam propagation direction over a large cross-sectional area. An RF oscillator based on coupling the resonant coil of a Hartley oscillator to the excitation coil was developed and provided a higher current, and thereby a larger RF amplitude, as compared to a conventional RF power amplifier. In addition, a neutron guide insert is necessary to be placed inside the RF coil to prevent loss of the intensity of the incident beam. An experimental means using two opaque ^{3}He neutron spin filters was developed to allow for measurements of the flipping probability of the flipper at very high precision (10^{-4}). The RF spin flipper (together with the two opaque ^{3}He NSFs) has yielded a spatially uniform flipping ratio as high as 853(55) over a 6 cm by 15 cm ^{58}Ni-coated neutron guide with a flipping probability of 0.9999(2).

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P2-18: Polarized neutron techniques and methods

Status of the ^{3}He Program at the NCNR

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^{3}He neutron spin filters (NSFs) continue to be an integral part of the NIST Center for Neutron Research (NCNR) as the program continues to improve NSF performance on current instruments, such as the Small Angle Neutron Scattering (SANS) and Thermal Axis Spectrometer (TAS) instruments. The implementation of a Ge180 toroid cell has produced significant data on the Multi-Angle Crystal Spectrometer (MACS). These results are due to further improvements in polarized neutronic performance, improved cell lifetimes, neutron spin transport, and minimization of ^{3}He polarization loss occurred during the adiabatic fast passage (AFP) NMR based ^{3}He polarization inversion. The use of NSFs at the NCNR have been expanded to the Very Small Angle Neutron Scattering (VSANS) instrument followed by the Chromatic Analysis Neutron Diffractometer Or Reflectometer (CANDOR) and a new magnetostatic cavity for each.

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P2-19: Polarized neutron instrumentation

Polarization Analysis Capability on vSANS at NCNR

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Polarization analysis capability using a ^{3}He neutron spin filter (NSF) as a spin analyzer has been developed on the very small-angle neutron scattering (vSANS) instrument at the National Institute of Standards and Technology Center for Neutron Research (NCNR). The polarized beam apparatus consists of a double-V supermirror polarizer, a radio-frequency (RF) spin flipper, and a ^{3}He analyzer. A ^{3}He analyzer cell is polarized offline by spin-exchange optical pumping and stored in a magnetically shielded solenoid that provides a homogeneous magnetic field along the neutron beam axis. Neutron spin flipping of the scattered beam is accomplished by inverting the ^{3}He polarization using the adiabatic fast passage nuclear magnetic resonance technique. Key features of practical applications for a ^{3}He NSF in polarization analysis on vSANS are large angular coverage, long ^{3}He polarization storage times even in the presence of stray fields from strong sample magnetic fields, and versatility of the sample field desired for an experiment.

We will present significant improvements in spin-analyzed SANS capabilities. The recently achieved high ^{3}He polarizations, together with a double-V supermirror cavity polarizer and a home-designed RF flipper allow us to achieve a flipping ratio as high as 100 with a neutron transmission of 50 % for the desired spin state of the ^{3}He analyzer. We have significantly improved the relaxation times of the ^{3}He analyzer up to 350 h even when the solenoid is placed close to a 1.6 T sample magnet, which has been achieved with an improved design of the magnetically shielded solenoid. The capability is fully integrated with a variety of sample field configurations to accommodate user's needs. The new polarization analysis capability on vSANS is creating opportunities for studies of hard matter investigations such as magnetic nanoparticle assemblies and magnetic nanowires.

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The following lists includes the names of those who registered for the conference by July 26, 2021 at 10:00 AM EST and answered “yes” to be included in the participant list during registration.

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