

14<sup>th</sup> International Conference on

# Polarized Neutrons for Condensed Matter Investigations (PNCMI)

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July 25 – 29, 2022 ANNAPOLIS, MD, USA





## **Welcome**

The 14th international Polarized Neutrons for Condensed-Matter Investigations (PNCMI) Conference, organized by NIST, will be held in-person from July 25-29, 2022 in Annapolis, Maryland at the Graduate Annapolis Hotel. The conference will not only accommodate the majority of conventional PNCMI topics, but also include a new scientific session, “Polarized QENS”. There will be 11 oral and 1 poster session on a wide range of topics.

Despite the pandemic, 60 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 will enjoy great scientific discussions and interactive gatherings during the conference. We would also like to add a special thanks to the International Advisory Committee for guidance in developing an extraordinary scientific program and the University of Maryland Conference Services for all their hard work and planning to help organize and host this meeting. Finally, we would like to extend our gratitude to all sponsors for making the conference possible.

Conference proceedings will be published in the Open Access Journal of Physics: Conference Series, published by IOP publishing. In addition, attendees of the virtual PNCMI 2021 may submit a manuscript as well.

PNCMI 2022 local organizing committee

## **Event Format**

The Welcome Reception will be held Monday July 25<sup>th</sup> in the Atrium from 6:00 - 8:00 pm. The Keynote Lunch will be Tuesday, July 26<sup>th</sup>, in the Regatta Ballroom, at the hotel from 12:10 – 2:00 pm.

Our oral sessions will be held in the Regatta Ballroom. The first two days will be comprised of four oral sessions followed by one poster session. There will be three sessions the third day with time to explore Annapolis before the Conference Dinner that evening. The last day will have presentations from the next PNCMI candidates followed by closing remarks and finish with a bus ride to NIST for a tour of the NIST Center for Neutron Research facility.

Each oral session will be an hour and a half with a 30-minute break between sessions. Each invited talk includes a 25-minute presentation and a 5-minute Q&A. Each contributed talk includes a 17-minute presentation and a 3-minute Q&A. An AV technician will be available throughout the event to assist with troubleshooting technical issues.

The poster sessions and breaks will be held in the Atrium.

## **About PNCMI**

PNCMI started its long journey in Dubna, Russia in 1996 and has taken place biennially until 2018. PNCMI in the year of 2020 was postponed due to the pandemic and instead held online in 2021. 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

### International Advisory Committee

- Ken Andersen (SNS, USA), **Chair**
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- Julie Borchers (NIST, USA)
- Rob Briber (University of Maryland, USA)
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- Antonio Faraone (NIST, USA)
- Jonathan Gaudet (NIST/University of Maryland, USA)
- Alexander Grutter (NIST, USA)
- Kelly Hedgepeth (University of Maryland, USA)
- Kathryn Krycka (NIST, USA)
- Lisa Press (University of Maryland, USA)
- William Ratcliff (NIST, USA)
- Shannon Watson (NIST, USA)

## **Polarized Neutron School**

It is tradition that a polarized neutron school be associated with the PNCMI conference. The school this year will be held preceding the conference from July 24th to July 25th, 2022 at the NIST Center for Neutron Research (NCNR) in Gaithersburg, Maryland. The Polarized Neutron School will provide a comprehensive introduction to polarized neutrons, techniques and scientific applications. Staff will give a series of lectures focused on neutron scattering techniques and applications for a variety of scientific fields. These lectures will cover small-angle scattering, reflectometry, diffraction/inelastic scattering, and instrumentation. The lectures will be followed by virtual experiments in polarized neutron reflectometry and triple axis spectrometry in small groups and the relevant data reduction process. This will provide a useful background before the PNCMI conference.

The school is intended for graduate students and young postdoctoral researchers familiar with scattering techniques.

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## Venue and Accommodation



**Graduate Annapolis Hotel**  
126 West Street  
Annapolis, Maryland 21401  
United States  
Ph: (410) 263-7777  
Email: [info@graduateannapolis.com](mailto:info@graduateannapolis.com)





## Welcome Reception

The PNCMI 2022 welcome reception will be held from 6:00 to 8:00 PM on **Monday, July 25<sup>th</sup>** in the Graduate Annapolis Hotel Atrium. Attendees will be provided 1 drink ticket. A cash bar will also be available, accompanied by a selection of Hors d 'Oeuvres. We hope to see you there!



*Graduate Annapolis Atrium*

## Keynote Lunch



Dr. Charles F. Majkrzak is currently the Leader of the Surface and Interface team at the NIST Center for Neutron Research and is recognized for his creative contributions in the development of measurement and interpretive methods for neutron reflectometry in the study of the microstructures of layered condensed matter systems of interest in physics, chemistry, biology and polymer science. These methods include polarized beam applications and phase-sensitive measurements leading to the direct inversion of scattering data. Of particular relevance to this Conference are the investigations of Dr. Majkrzak and colleagues on a variety of magnetic materials, including a seminal polarized neutron scattering study of Gd/Y

superlattices that revealed unexpected oscillatory exchange coupling across non-magnetic layers. This research was cited in the Nobel Prize for Physics in 2007 as it provided a context for interpreting giant magnetoresistance (GMR) in transition-metal multilayers, a phenomenon that revolutionized magnetic recording.

Dr. Majkrzak has received many distinguished awards including, to name only a few, the Bertram E. Warren Diffraction Physics Award in 2006, the Clifford G. Shull Prize from the Neutron Scattering Society of America in 2016, and a presidential Rank Award in 2021.

Lunch with Keynote Speaker Dr. Majkrzak will be provided on **Tuesday, July 26<sup>th</sup>** at the Graduate Annapolis Hotel. The Keynote Lunch is included with conference registration and will be held in the Regatta Ballroom. Please identify any dietary restrictions in your conference registration (e.g., vegetarian, vegan, allergies), or contact [PNCMI2022@nist.gov](mailto:PNCMI2022@nist.gov).



## Conference Schedule

### PNCMI 2022 Conference Schedule

	Monday, July 25	Tuesday, July 26	Wednesday, July 27	Thursday, July 28	Friday, July 29
8:00 AM			Breakfast		
9:00 AM		Nanostructures 1 9 - 10:30AM	Polarized QENS 9 - 10:40AM	Nanostructures 2 9 - 10:30AM	PNCMI 2024 candidate presentation
10:00 AM			Refreshments		
11:00 AM		Magnetism 1 11 AM - 12:10 PM	Magnetism 2 11 AM - 12:30 PM	Magnetism 3 11:00 AM - 12:40 PM	Bus departs hotel to NIST
12:00 PM		Keynote Lunch			Box lunch at NIST
1:00 PM			Lunch on own		
2:00 PM	Registration (Atrium)		Instrumentation: Facility Reports 2 - 3:30 PM	Instrumentation: Soft Matter 2 - 3:30 PM	NIST Tour
3:00 PM			Refreshments		
4:00 PM		Larmor Techniques 4 - 5:40 PM	Techniques and Methods 4 - 5:30 PM		Bus departs NIST to Shady Grove
5:00 PM			Posters		
6:00 PM	Welcome Reception (Atrium)			Conference Dinner (Buddy's Crabs & Ribs)	
7:00 PM					
8:00 PM					

## Oral Sessions

Tuesday, July 26<sup>th</sup>, 2022

### Session O1: Nanostructures 1

9:00 – 10:30 am

Chair: Christy Kinane

O1-1 9:00 – 9:30 am: **Substrate-dependent hydrogen incorporation and magnetic changes at surfaces of freestanding manganite thin films (INVITED)**

Purnima BALAKRISHNAN (NCNR)

O1-2 9:30 – 9:50 am: **Probing structural and magnetic depth profiles in magneto-ionic heterostructures by polarized neutron reflectometry**

Christopher J. JENSEN (Georgetown University)

O1-3 9:50 – 10:10 am: **Reversible Hydrogen-Induced Phase Transformations in La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> Thin Films Characterized by In Situ Neutron Reflectometry and Drop in Polarization for the Liquids Reflectometer**

Timothy R. CHARLTON (ORNL)

O1-4 10:10 – 10:30 am: **In-situ GHz Dynamics of Skyrmions Probed with SANS**

Nan TANG (University of Tennessee)

### Session O2: Magnetism 1

11:00 am – 12:10 pm

Chair: Junjie Yang

O2-1 11:00 – 11:30 am: **Optically induced magnetization in 2D superlattice perovskite film established by circularly polarized orbital polarization ordering effects (INVITED)**

Bin HU (University of Tennessee)

O2-2 11:30 – 11:50 am: **Case for a U(1) $\pi$  Quantum Spin Liquid Ground State in the Dipole-Octupole Pyrochlore Ce<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub>**

Evan SMITH (McMaster University)

O2-3 11:50 am – 12:10 pm: **Long-range order, re-entrant spin glass and spin liquid correlations in Anion disordered Gd<sub>2</sub>Hf<sub>2</sub>O<sub>7</sub>**

Jianhui XU (RWTH Aachen University)

**Session O3: Instrumentation: Facility Reports**

**2:00 – 3:30 pm**

**Chair: Markus Strobl**

O3-1 2:00 – 2:30 pm: **Recent science highlights from polarization analysis experiments on the LET spectrometer at ISIS (INVITED)**

Gøran J. NILSEN (STFC)

O3-2 2:30 – 2:50 pm: **Polarized Instrumentation for the HBS Facility**

Jörg VOIGT (JCNS)

O3-3 2:50 – 3:10 pm: **The Future of Polarized Neutron Development Beamlines at the High Flux Isotope Reactor**

Lowell CROW (ORNL)

O3-4 3:10 – 3:30 pm: **Update on the neutron polarisation capabilities at the Australian Centre for Neutron Scattering, ANSTO**

Andrew MANNING (ANSTO)

**Session O4: Larmor Techniques**

**4:00 – 5:40 pm**

**Chair: Thomas R. Gentile**

O4-1 4:00 – 4:30 pm: **Polarized neutron dark-field imaging (INVITED)**

Markus STROBL (PSI)

O4-2 4:30 – 5:00 pm: **Development of real space scattering technique: spin echo modulated small angle neutron scattering (INVITED)**

Fankang LI (ORNL)

O4-3 5:00 – 5:20 pm: **Advancements toward an NRSE instrument: Performance of a transverse RF Flipper**

Stephen KUHN (Indiana University)

O4-4 5:20 – 5:40 pm: **Development and prototyping of a zero-net-field, field-integral-correction device for neutron resonance spin echo**

Sam McKAY (Indiana University)

## Wednesday, July 27<sup>th</sup>, 2022

### Session O5: Polarized QENS

9:00 – 10:40 am

Chair: Péter Falus

O5-1 9:00 – 9:30 am: **The coherent dynamic structure factor of water from the meso- to the inter-molecular scale: neutron spectroscopy with polarization analysis and molecular dynamics simulations (INVITED)**

Juan COLMENERO (CFM-MPC, CSIC-UPV/EHU)

O5-2 9:30 – 10:00 am: **Coherent, incoherent and magnetic quasielastic scattering and the phonon-liquid electron-crystal concept in AgCrSe<sub>2</sub> (INVITED)**

David J. VONESHEN (STFC)

O5-3 10:00 – 10:20 am: **Coherent and Incoherent Scattering of Tetrahydrofuran from Meso- to Inter-molecular Scales by Neutron Spectroscopy with Polarization Analysis and Spin Echo**

Arantxa ARBE (CFM-MPC, CSIC-UPV/EHU)

O5-4 10:20 – 10:40 am: **Coherent dynamics of acyl tail correlations in a lipid bilayer**

Michihiro NAGAO (NIST/University of Maryland/University of Delaware)

### Session O6: Magnetism 2

11:00 am – 12:30 pm

Chair: Javier Campo

O6-1 9:00 – 11:30 am: **Observation of the spin-current carrier with Px polarized neutrons (INVITED)**

Yusuke NAMBU (Tohoku University)

O6-2 11:30 – 11:50 am: **Polarized Inelastic Neutron Scattering Study of the Kitaev Material D<sub>3</sub>LiIr<sub>2</sub>O<sub>6</sub>**

Thomas HALLORAN (Johns Hopkins University)

O6-3 11:50 am – 12:10 pm: **Polarized SANS & GISANS studies on condensed matter systems**

Annika STELLHORN (Lund University)

O6-4 12:10 – 12:30 pm: **Mixed magnetic phases in Al<sub>x</sub>CoCrNiFe high entropy**  
Cameron JORGENSEN (University of Tennessee)

**Session O7: Instrumentation: Soft Matter**

**2:00 – 3:30 pm**

**Chair: Arantxa Arbe**

O7-1 2:00 – 2:30 pm: **WASP the Wide Angle Spin Echo instrument at ILL is in user operation (INVITED)**  
Péter FALUS (ILL)

O7-2 2:30 – 2:50 pm: **Simulations and concepts for a 2D spin-echo modulated SANS (SEMSANS) instrument**  
Steven R. PARNELL (T.U. Delft)

O7-3 2:50 – 3:10 pm: **Capability of Ultra-High-Resolution Lattice Structure Measurements at Oak Ridge National Laboratory\***  
Kaleb BURRAGE (ORNL) \*(Hard Matter)

O7-4 3:10 – 3:30 pm: **Towards realization of nmr-modulated polarized neutron scattering from hyperpolarized solutes**  
George THURSTON (Rochester Institute of Technology)

**Session O8: Techniques and Methods**

**4:00 – 5:30 pm**

**Chair: TBD**

O8-1 4:00 – 4:30 pm: **<sup>3</sup>He polarization work at the JCNS (INVITED)**  
Earl BABCOCK (JCNS)

O8-2 4:30 – 4:50 pm: **Neutron polarimetry using <sup>3</sup>He neutron spin filters**  
Thomas R. GENTILE (NIST)

O8-3 4:50 – 5:10 pm: **Generation and detection of spin-orbit coupled neutron beams**  
Connor KAPAHI (University of Waterloo)

O8-4 5:10 – 5:30 pm: **Wide bandwidth neutron polarizing supermirror due to ferromagnetic interlayer exchange coupling**  
Ryuji MARUYAMA (J-PARC)

**Thursday, July 28<sup>th</sup>, 2022**

**Session O9: Nanostructures 2**

**9:00 – 10:30 am**

**Chair: Purnima Balakrishnan**

O9-1 9:00 – 9:30 am: **Using Bayesian model selection for interpreting PNR data (INVITED)**  
Andrew CARUANA (STFC)

O9-2 9:30 – 9:50 am: **The 3-dimensional depth profile of magnetic skyrmion tubes**  
W.L.N.C. LIYANAGE (University of Tennessee)

O9-3 9:50 – 10:10 am: **Skyrmion lattice formation and destruction mechanisms probed with SANS**  
Dustin A. GILBERT (University of Tennessee)

O9-4 10:10 – 10:30 am: **The Development of Transverse Neutron Polarimetry at NIST and Its Application in Neutron Scattering of Magnetic Topological Materials**  
Melissa HENDERSON (University of Waterloo)

**Session O10: Magnetism 3**

**11:00 am – 12:30 pm**

**Chair: Yusuke Nambu**

O10-1 11:00 – 11:20 am: **New Incommensurate Magnetic Phases in the Multiferroic Compound MnCr<sub>2</sub>O<sub>4</sub>**  
Javier CAMPO (Aragón Nanoscience and Materials Institute (CSIC-University of Zaragoza))

O10-2 11:20 – 11:40 am: **Anisotropic non-collinear spin densities revealed in non-centrosymmetric multiferroics by advanced maximum-entropy reconstruction**  
Henrik THOMA (Institute of Crystallography (RWTH Aachen))



O10-3 11:40 am – 12:00 pm: **Neutron polarization analysis of the anisotropic spin wave excitations in multiferroic BiFeO<sub>3</sub>**  
Masaaki MATSUDA (ORNL)

O10-4 12:00 – 12:20 pm: **Magnetic chirality induced by chemical substitution in a chiral magnet New Incommensurate Magnetic Phases in the Multiferroic Compound MnCr<sub>2</sub>O<sub>4</sub>**  
Junjie YANG (New Jersey Institute of Technology)

O10-5 12:20 – 12:40 pm: **Field and polarization dependence of magnons in collinear CuFeO<sub>2</sub>**  
Duncan MOSELEY (ORNL)

**Session O11: Instrumentation: Diffraction & Spectroscopy** **2:00 – 3:30 pm**

**Chair: Jörg Voigt**

O11-1 2:00 – 2:30 pm: **Wide Angle Polarization Analysis and first results with PASTIS-3 for IN20 (INVITED)**  
Ursula B. HANSEN (ILL)

O11-2 2:30 – 2:50 pm: **Design of the PoLAR Cold Neutron Spectrometer at the NCNR**  
Leland HARRIGER (NCNR)

O11-3 2:50 – 3:10 pm: **New options on the polarized neutron single crystal diffractometer POLI at MLZ**  
Jianhui XU (RWTH Aachen University)

O11-4 3:10 – 3:30 pm: **Latest Development in Spherical Neutron Polarimetry at ORNL**  
Jacob TOSADO (ORNL)

3:30 pm – 6:00 pm Free Time to explore Annapolis

6:00 pm – 8:00 pm Dinner at Buddy's Crab and Ribs  
100 Main St, Annapolis, Md 21401

## Friday, July 29<sup>th</sup>, 2022

Closing Remarks	9:00 – 10:30 am
NCNR Tour Bus Departure	10:30 am
Lunch (NIST)	12:00 – 1:00 pm
NIST Tour	1:00 – 4:00 pm
Bus to Metro	4:00 pm

**Substrate-dependent hydrogen incorporation and magnetic changes at surfaces of freestanding manganite thin films****Purnima BALAKRISHNAN<sup>1</sup>**<sup>1</sup>NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

Complex oxide thin films have highly tunable magnetic properties, not only due to the correlated degrees of freedom within these materials, but also due to the constraints imposed by limited choice of substrate material. For example, the magnetic properties of the manganites depend heavily on subtle induced changes to crystallographic structure, resulting in a dead layer at the substrate/film interface which can inhibit technological applications [1,2,3]. Recently, exciting new techniques have been developed using water-soluble intermediate layers to separate oxide thin films from the substrate after growth, decoupling structural and chemical degrees of freedom at the interface [4]; this technique may both enable development of more magnetically uniform films as well as enable their integration with previously incompatible materials.

In this work, a combination of polarized neutron reflectometry supplemented with other depth-sensitive measurement techniques such as secondary ion mass spectroscopy provide a detailed understanding of both the chemical composition – with particular sensitivity to light elements such as hydrogen – and in-plane magnetization of freestanding  $\text{LaMnO}_{3+\delta}$  (LMO) films as a function of depth. By investigating the effects of film thickness and choice of final substrate – in particular, Si/SiO<sub>2</sub> or LSAT – on the magnetic and chemical uniformity of the films, we find substrate-dependent changes in magnetic anisotropy [5] correlated with significant hydrogen incorporation into the surfaces of transferred LMO thin films [6]. Specifically, LMO films transferred onto Si/SiO<sub>2</sub>, but not onto LSAT, develop surface regions with increased hydrogen content, causing a non-uniform magnetic anisotropy through the film. Despite elimination of chemical bonds with the substrate surface, the choice of substrate can still affect the magnetic properties of freestanding films through chemical effects, which may have implications for their integration into existing silicon-based technologies.

[1] X. Zhai *et al.*, Nature Communications, **5**, 4283 (2014).

[2] E. J. Moon *et al.*, Nano Letters, **14**, 2509-2514 (2014).

[3] Z. Liao *et al.*, Journal of Applied Sciences, **9**, 144 (2019).

[4] D. Lu *et al.*, Nature Materials, **15**, 1255-1260 (2016).

[5] Q. Lu *et al.*, ACS Nano, **16** (5), 7580-7588 (2022).

[6] P. P. Balakrishnan *et al.*, in preparation.

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**Probing structural and magnetic depth profiles in magneto-ionic heterostructures by polarized neutron reflectometry**

**Christopher J. JENSEN**<sup>1</sup>, Peyton D. MURRAY<sup>2</sup>, Alberto QUINTANA<sup>1</sup>, Alexander J. GRUTTER<sup>3</sup>, Brian J. KIRBY<sup>3</sup>, Patrick QUARTERMAN<sup>3</sup>, Junwei ZHANG<sup>4</sup>, Xixiang ZHANG<sup>4</sup>, Huairuo ZHANG,<sup>3</sup> Albert DAVYDOV,<sup>3</sup> and Kai LIU<sup>1,2</sup>

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<sup>4</sup>King Abdullah University of Science & Technology, Thuwal, Saudi Arabia

Polarized neutron reflectometry (PNR) is ideally suited to extract both structural and magnetic depth profiles in thin film heterostructures. This is particularly relevant for magneto-ionic studies where ionic motion under buried interfaces can be used to modulate physical properties in an energy-efficient manner. We have used PNR to study Pd/Gd/NiCoO and Pd/Ta/CoFe/MnN/Ta heterostructures, where the exchange bias (EB) can be electrically controlled via O and N ions migration. In the Pd/Gd/NiCoO system, upon deposition of Gd, a thin interfacial region of antiferromagnetic (AF) NiCoO is spontaneously reduced to ferromagnetic NiCo [1,2]. The formation of NiCo is indicated by the presence of spin asymmetry between the non-spin-flip cross sections of the reflectivity data. Bulk magnetometry and electron energy-loss spectroscopy (EELS) were also used to confirm this observation. Upon field cooling the samples to induce EB, the magnetic layer thickness increases and the real ( $\rho_N$ ) and imaginary components of the scattering length density (SLD) indicate intermixing of Gd-Ni. After applying a voltage bias, PNR shows that oxygen ions migrate from NiCoO toward Gd and the NiCo and GdNi layers undergo changes in thickness and magnetization. The combined changes lead to an increase in EB. In the Pd/Ta/CoFe/MnN/Ta system, nitrogen initially migrates out of the AF MnN layer into both Ta layers during the field cooling process, indicated by a reduction of  $\rho_N$  in the MnN layer and increase of  $\rho_N$  in the Ta layers. A reduction in the initial EB has been observed as the amount of nitrogen removed increases [3]. By applying a voltage bias such that N migrates from the Ta seed layer toward MnN,  $\rho_N$  decreases in the Ta seed layer and increases in the MnN layer near the CoFe interface. These changes indicate that the increase in N in the MnN layer contributes to the increase in EB observed by magnetometry. Our findings highlight the viability of the solid-state magneto-ionic approach to achieve electric control of exchange bias, with potentials for energy-efficient magneto-ionic devices.

This work has been supported in part by NSF, SRC/NIST nCORE SMART center and KAUST.

[1] P.D. Murray et al., ACS Appl. Mater. Interfaces, **13**, 38916-38922 (2021).

[2] C. J. Jensen et al, J. Magn. Magn. Mater. **540**, 168479 (2021).

[3] P. Quarterman et al., Phys. Rev. Mater., **3**, 064413 (2019).

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**Reversible Hydrogen-Induced Phase Transformations in  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  Thin Films Characterized by In Situ Neutron Reflectometry and Drop in Polarization for the Liquids Reflectometer**

Alessandro R. MAZZA<sup>1</sup>, Qiyang LU<sup>1</sup>, Guoxiang HU<sup>2</sup>, Haoxiang LI<sup>1</sup>, James F. BROWNING<sup>3</sup>, Timothy R. CHARLTON<sup>3</sup>, Matthew BRAHLEK<sup>1</sup>, Panchapakesan GANESH, Thomas ZAC WARD<sup>1</sup>, Ho Nyung LEE<sup>1</sup>, and Gyula ERES<sup>1</sup>

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We will present a description of a drop-in polarization option for the Liquids Reflectometer and its first usage investigating the mechanism for hydrogen-induced topotactic phase transitions in perovskite oxides using  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ [1]. Hydrogenation starts with lattice expansion confirmed by X-ray diffraction (XRD). The strain and oxygen-vacancy-mediated electron-phonon coupling in turn produces electronic structure changes that manifest through the appearance of a metal insulator transition accompanied by a sharp increase in resistivity. The ordering of initially randomly distributed oxygen vacancies produces a perovskite to brownmillerite phase ( $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_{2.5}$ ) transition. This phase transformation proceeds by the intercalation of oxygen vacancy planes confirmed by in situ XRD and neutron reflectometry (NR) measurements. Despite the prevailing picture that hydrogenation occurs by reaction with lattice oxygen, NR results are not consistent with deuterium (hydrogen) presence in the  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  lattice at steady state. The film can reach a highly oxygen-deficient  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_{2.1}$  metastable state that is reversible to the as-grown composition simply by annealing in air. Theoretical calculations confirm that hydrogenation-induced oxygen vacancy formation is energetically favorable in  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ . The hydrogenation driven changes of the oxygen sublattice periodicity and the electrical and magnetic properties similar to interface effects induced by oxygen-deficient cap layers persist despite hydrogen not being present in the lattice.

[1] A. R. Mazza, *et. al.*, ACS Appl. Mater. Interfaces, **14**, 10898 (2022)

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## In-situ GHz Dynamics of Skyrmions Probed with SANS

Nan TANG<sup>1</sup>, Sergio MONTOYA<sup>2</sup>, W.L.N.C. LIYANAGE<sup>3</sup>, Sheena PATEL<sup>2,4</sup>, Lizabeth J. QUIGLEY<sup>1</sup>, Alexander J. GRUTTER<sup>5</sup>, Michael R. FITZSIMMONS<sup>3,6</sup>, Sunil K. SINHA<sup>4</sup>, Julie A. BORCHERS<sup>5</sup>, Eric E. FULLERTON<sup>2,7</sup>, Lisa DEBEER-SCHMITT<sup>8</sup>, Dustin A. GILBERT<sup>1,3</sup>

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Magnetic skyrmions present interesting and unique pseudo-particle behaviors which arises from their topological protection [1]. Key among these behaviors is their resonant dynamics, under microwave fields, which include both breathing and gyration modes. Due to their small size, and magnetic-only contrast of skyrmions, coupled with high frequency dynamics – in the GHz regime – it is challenging to do in-situ measurements on these excitations. This work reports the use of small angle neutron scattering (SANS) to capture the dynamics of hybrid skyrmions stabilized in Fe/Gd multilayers by means of dipolar interactions. Using perpendicular DC fields and in-plane RF fields, we explored the gyration modes of hybrid skyrmions away, below, at, and above resonance. We find the dynamic modes of hybrid skyrmions contribute to the SANS signal in two ways: first, the scattered neutrons incur additional transverse momentum as a result of scattering from a moving source, and second, the gyration skyrmions disrupt ordering of the lattice giving rise to enhancement form-factor scattering. Ferromagnetic resonance measurements confirm the RF and DC field conditions for these gyration modes. Our results offer new insights into the nanoscale dynamics of magnetic skyrmions and present a unique use of SANS to probe magnetization dynamics.

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**Optically induced magnetization in 2D superlattice perovskite film established by circularly polarized orbital polarization ordering effects**

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This presentation reports an optically induced magnetization within 2D superlattice perovskite film at room temperature by establishing circularly polarized orbital polarization ordering stabilized on the surface of ferromagnetic Co film by using depth-resolved neutron magnetoreflexivity measurement. 2D superlattice perovskites are known as strong-orbital semiconducting materials simultaneously carrying spin-orbital coupling and Rashba effects. We found that an incident circularly polarized photoexcitation can generate circularly polarized excitons with prolonged mutual orbital interaction. Our laser spectroscopy studies indicate that the prolonged mutual orbital interaction between circularly polarized excitons can be essentially established between magnetic dipoles of circularly polarized orbitals in coherent manner when inter-exciton distance is reduced upon increasing photoexcitation intensity. Furthermore, we found that, when placing 2D superlattice film on the Co surface, the ferromagnetic spin dipoles on Co surface can directly interact with the circularly polarized orbitals within 2D superlattice perovskite in the hybridized 2D/Co film. Consequently, magnetically switching the direction of ferromagnetic dipoles can swap the circularly polarized orbitals between left-hand and right-hand polarization, identified by magnetic field effects of circularly polarized photoluminescence. Interestingly, an optically induced magnetization was observed within 2D superlattice perovskite in the hybridized 2D/Co film under circularly polarized photoexcitation at room temperature and steady state.

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**Case for a  $U(1)\pi$  Quantum Spin Liquid Ground State in the Dipole-Octupole Pyrochlore  $Ce_2Zr_2O_7$**

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The  $Ce^{3+}$  pseudospin-1/2 degrees of freedom in the pyrochlore magnet  $Ce_2Zr_2O_7$  are known to possess dipole-octupole character, making it a candidate for novel quantum spin liquid ground states at low temperatures. We report new polarized neutron diffraction at low temperatures, as well as heat capacity ( $C_p$ ) measurements on single crystal  $Ce_2Zr_2O_7$ . The former bears both similarities and differences with that measured from the canonical dipolar spin ice compound  $Ho_2Ti_2O_7$ , while the latter rises sharply at low temperatures, initially plateauing near 0.08 K, before falling off toward a high temperature zero beyond 3 K. Above 0.5 K, the  $C_p$  dataset can be fit to the results of a quantum numerical linked cluster calculation, carried out to fourth order, that allows estimates for the terms in the near-neighbor XYZ Hamiltonian expected for such dipole-octupole pyrochlore systems. Fits of the same theory to the temperature dependence of the magnetic susceptibility and unpolarized neutron scattering complement this analysis. A comparison between the resulting best-fit numerical linked cluster calculation and the polarized neutron diffraction shows both agreement and discrepancies, mostly in the form of zone-boundary diffuse scattering in the non-spin-flip channel, which are attributed to interactions beyond near neighbors. The lack of an observed thermodynamic anomaly and the constraints on the near-neighbor XYZ Hamiltonian suggest that  $Ce_2Zr_2O_7$  realizes a  $U(1)\pi$  quantum spin liquid state at low temperatures, and one that likely resides near the boundary between dipolar and octupolar character.

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**Long-range order, re-entrant spin glass and spin liquid correlations in  
Anion disordered Gd<sub>2</sub>Hf<sub>2</sub>O<sub>7</sub>**

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Pyrochlore antiferromagnets (AFM) Gd<sub>2</sub>T<sub>2</sub>O<sub>7</sub> (*T*: tetravalent metal elements) are prototypical materials for realizing classical spin liquid states. However, all of them have been observed to show long-range magnetic order [1-3]. Previous specific heat data of Gd<sub>2</sub>Hf<sub>2</sub>O<sub>7</sub> show a tiny sharp peak on the top of a large broad maximum indicating a long-range AFM order [4]. However, our sample does not show that sharp peak in specific heat, but the ac susceptibility evidences an ordering transition followed by a spin-glass transition. Using neutron diffraction, we found that the sample has oxygen Frankel defects and undetectable Gd/Hf anti-site defects. The polarized neutron diffuse scattering pattern shows liquid-like scattering without any magnetic Bragg peaks. The subtle long-range order and re-entrant spin glass are attributed to bond disorder due to oxygen anion disorder.

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**Recent science highlights from polarization analysis experiments on the LET spectrometer at ISIS**

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The combination of time-of-flight spectroscopy with polarization analysis provides unprecedented information on the dynamics of condensed matter systems in both space and time. Since the implementation of uniaxial polarization analysis on the LET direct geometry time-of-flight spectrometer at ISIS in 2019, it has been used to separate the collective (coherent) and self (incoherent) scattering contributions in a number of non-magnetic molecular liquids, energy materials, and biological systems. Recently, the method has also been extended to magnetic samples via the pixilation of the LET detector. In this presentation, I will briefly summarize the technical implementation of uniaxial polarization analysis [1] on the LET spectrometer and show some recent science highlights spanning the above fields. Among these are a recent experiment on the organic solvent THF, a preliminary study of the solid-state battery electrolyte material  $\text{Li}_{6.75}\text{La}_3\text{Nb}_{0.25}\text{Zr}_{1.75}\text{O}_{12}$ , as well as the first full separation of the neutron scattering cross section in  $\text{Ho}_2\text{Ti}_2\text{O}_7$ . Some future perspectives beyond LET will also be discussed.

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**Polarized Instrumentation for the HBS Facility**

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The shutdown of many research reactors has triggered strong research activities worldwide on compact accelerator driven neutron sources. These employ nuclear reactions well below the spallation threshold to release free neutrons. Traditionally this technique has been used for small scale neutron sources, but projects such as the SONATE project in France or the HBS project push the limits of this approach to provide neutron instrumentation on the level of today's national neutron facilities. These High Current Accelerator driven Neutron Sources (HiCANS) can host the full range of neutron instrumentation, including high resolution instruments and other flux hungry techniques. For the entire instrument suite, we consider PA as an essential tool to optimize the signal-to-noise ratio by making specific measurements e.g. of magnetic thin films on diamagnetic substrates or studying hydrogen motions by separation of spin-incoherent scattering.

Here we present concepts to realize polarization analysis for different types of neutron scattering instrument including SANS machines, diffractometers, chopper spectrometers and indirect geometry spectrometers.

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**The Future of Polarized Neutron Development Beamlines at the High Flux Isotope Reactor**

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The High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory currently host two beamlines for polarized neutron development and one for neutron detector development. These will run in their present form until 2024 or 2025. After that time, all HFIR instruments will be temporarily removed to allow replacement of the reactor's beryllium reflector, possibly in conjunction with replacement of the reactor pressure vessel.

The planned future HB-2D instrument in the thermal beam room will have a shorter wavelength than the present 4.25 Å, and is expected to have higher intensity. It will also provide a side beam for detector development, since the present cold guide hall CG1A position will not be available. In the new cold guide hall configuration, an alignment instrument at NB-2A will have some availability for development. The long lead time for the proposed NB2 Spin Echo instrument will also allow interim development of a cold neutron development beamline to support continuing development of Larmor techniques.

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

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An update on neutron polarisation activities at the Australian Centre for Neutron Scattering (ACNS) over the last 12 months will be given. This includes a new setup for a 0.5 T horizontal magnetic field applied to a sample on a triple-axis spectrometer for measurements over an extended  $Q$  range, a project to design and build a new laser system for our metastable-exchange optical pumping (MEOP) station, and a discussion of some recent measurements on the cold triple-axis spectrometer Sika including a study of 2D triangular lattice Heisenberg antiferromagnet.

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## Polarized neutron dark-field imaging

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Polarized neutron imaging [1] and neutron dark-field contrast imaging [2] are two powerful advanced neutron imaging methods providing access to spatially resolved studies of magnetic structures and microstructures. Polarized neutron imaging utilizes contrast induced by the local interaction of a polarized incident beam with a sample and enables to reconstruct magnetic field and/or structure distributions like e.g. the trapped field in a superconductor [1] or the distribution of ferromagnetic phases in steel. Dark-field contrast on the other hand is sensitive to microstructures that induce small angle scattering and provides maps of the small angle scattering characteristics and thus varying microstructures of materials. Scanning of instrumental parameters allows for quantitative local structural analyses [3]. Application in microstructural investigations cover a wide range of fields from energy research [4], engineering [5,6] to soft matter [7,8], like examples from fuel cell research, additive manufacturing and food science are suited to underline. However, a particularly strong field of application is magnetism, due to the sensitivity of the contrast mechanism to magnetic domain walls [9].

Here the combination of both, polarized neutrons and dark-field contrast imaging in a grating interferometer set-up including polarization analyses [10] shall be presented. While such set-up first enabled to investigate the nature of dark-field contrast induced by a magnetic field gradient, it is demonstrated that it particularly enables spatially resolved polarized SANS measurements including analyses of spin-flip and non-spin flip scattering [11].

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**Development of real space scattering technique: spin echo modulated small angle neutron scattering**

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To investigate long length scale structures beyond 200nm using neutron scattering, real space techniques have shown certain advantages over the conventional methods working in reciprocal space. As one of the real space measurement techniques, spin echo modulated small angle neutron scattering (SEMSANS) has attracted attention [1], due to its relaxed constraints on sample environment and the possibility to combine SEMSANS and a conventional small angle neutron scattering (SANS) instrument [2]. By modulating the neutron beam spatially, SEMSANS allows the scattering signal of the sample to be encoded into a change in the neutron beam polarization via Fourier transform, which increases the accessible Q range and therefore extends the real space length scale to several microns. The implementation and data reduction of SEMSANS using the superconducting magnetic Wollaston prisms (MWPs) at both constant wavelength and time-of-flight neutron sources will be presented [3-5]. Additionally, the applications of MWP to further increase the resolution and contrast of conventional neutron scattering techniques will be presented and discussed.

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**Advancements toward an NRSE instrument: Performance of a transverse RF Flipper**

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Neutron Resonance Spin Echo (NRSE), a high-energy resolution technique which uses four radio-frequency (RF) flippers, is being developed as a potential alternative to Neutron Spin Echo, which uses static fields. Some potential advantages of NRSE are an increase to the resolution and a reduction to the overall length of the instrument. In order to reach similar performance as contemporary NSE instruments, the RF flippers must flip efficiently up to about 4 MHz.

We have constructed a boot-strapped resonant RF flipper using high temperature superconducting (HTS) technology and tested it up to 1.2 MHz. The transverse flipper has the static field perpendicular to the beam and the RF field parallel to the beam. 300-nm-thick HTS films on 0.5-mm-thick sapphire substrates sharply define the flipper field region and ensure a spatially homogenous static field. The HTS films and their substrates are the only material in the neutron beam, guaranteeing very low beam attenuation. Measurements show a flipper efficiency above 98% for a 25-mm-diameter neutron beam without significant RF heating at a neutron wavelength of 0.55 nm. We anticipate being able to increase the RF frequency of this device by at least a factor of two in the future.

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**Development and prototyping of a zero-net-field, field-integral-correction device for neutron resonance spin echo**

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*Neutron spin echo* is a well-established polarized neutron scattering technique which is often used to study long time-scale dynamics. A traditional spin echo experiment consists of two arms of equal-magnitude static magnetic fields that straddle a sample. In the absence of scattering, the Larmor phase accumulated in the first arm is canceled by the second arm. Scattering from the sample results in a non-zero net phase at the detector; this encoding of the scattering in the polarization is referred to as *Larmor labeling*.

*Neutron resonance spin echo* (NRSE) is a similar technique that replaces each static field with two radio-frequency (RF) spin flippers, which increases the resolution and eliminates the need for an extremely long and homogeneous magnetic field region. However, NRSE introduces aberrations from travel differences between the two RF flippers in each arm due to the scattering from the sample.

We show analytically and with numerical simulations that this aberration can be corrected with a series of three *NRSE correction devices* in each arm; each device generates a quadratic field-integral dependence in both the horizontal and vertical transverse directions. We have fabricated a prototype device that consists of two square, high-temperature superconducting (HTS) coils wrapped around soft-iron pole pieces. The field is well-contained in the device by HTS films. The spatial variation of the field-integral across the neutron beam is achieved by using shaped pole pieces and by tuning the separation between one HTS film and the edge of the pole pieces. The device has been tested at the HFIR with encouraging results that we present in this communication.

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**The coherent dynamic structure factor of water from the meso- to the inter-molecular scale: neutron spectroscopy with polarization analysis and molecular dynamics simulations**

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The collective dynamics of water in the terahertz range has been a topic of intense activity since the 1970's. Although the first experimental investigations were carried out using inelastic neutron scattering, since the 1990's most studies were performed using inelastic X-ray scattering (IXS) [1]. However, in principle, quasi-elastic neutron scattering (QENS) is the ideal technique with which to directly observe the collective relaxation of water in a wide Q-range (Q: momentum transfer) due to the high energy resolution currently available. The problem is that the measured intensity always contains a combination of coherent and incoherent contributions. By means of the recently implemented neutron polarization analysis on a wide time-of-flight spectrometer (LET @ ISIS), we have separately measured coherent and incoherent dynamic structure factor of heavy water with sub-meV resolution in a wide Q-range [2]. The results obtained have been interpreted with the help of massive atomistic molecular dynamics (MD) simulations [3]. These simulations nicely explain why the relaxation part of the measured coherent dynamic structure factor hardly depends on Q in the low Q-range and how it crosses over to a diffusion-driven process in the Q-range of the first maximum of the static structure factor. They also give support to the main assumptions of the model previously used to fit the experimental data in the crossover range [2].

This work opens a new way of approaching the unknown territory of coherent scattering -from meso- to inter-molecular scales- not only in water but also in H-bonded liquids, glass-forming liquids and biological systems. It also convincingly proves the power of neutron spectroscopy with polarization analysis that can hugely impact the progress of microscopic dynamic investigations in different fields.

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**Coherent, incoherent and magnetic quasielastic scattering and the phonon-liquid electron-crystal concept in AgCrSe<sub>2</sub>**

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Superionic materials have garnered much interest as thermoelectrics due to their ultra-low thermal conductivity. The proposed origin, the Phonon-Liquid Electron-Crystal (PLEC) [1] picture can be tested by inelastic neutron scattering [2]. Recent work on AgCrSe<sub>2</sub> has found contradictory evidence about the validity of the PLEC in this material. The first neutron study found extremely fast diffusion and concluded that this was a true PLEC [3] but subsequent work found slower diffusion and the persistence of the transverse phonons [4] suggesting it is not.

These two very different pictures are somewhat surprising given that there is no controversy about the sample purity or phase. The structure is well understood and all the samples appear to be nominally the same.

We have performed unpolarized neutron scattering on these samples and our results are broadly consistent with the previous studies. However, we also have polarized data from ThALES. With polarized neutrons, we find that the timescale from self-diffusion, as measured in the spin-incoherent channel, is much longer than in either of the previous reports. Instead the previously reported broader QENS signals come from other cross sections. One arises from coherent scattering and is rather localized in Q while the second is very much faster and from magnetic fluctuations. Our results explain the apparent contradiction and confirm that AgCrSe<sub>2</sub> is not a phonon liquid.

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**Coherent and Incoherent Scattering of Tetrahydrofuran from Meso- to Inter-molecular Scales by Neutron Spectroscopy with Polarization Analysis and Spin Echo**

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We have extended our previous investigations on self- and collective dynamics of liquid water [1,2] to the case of tetrahydrofuran (THF). Neutron polarization analysis on a wide-angle time-of-flight spectrometer (PLET @ ISIS) has allowed measuring separately coherent and incoherent dynamic structure factor of deuterated THF with sub-meV resolution in a wide scattering vector (Q) range. The combination with Neutron Spin Echo (WASP @ ILL) experiments on deuterated and protonated THF with higher resolution has allowed to fully characterize the contributions to self- and collective dynamic structure factors. We compare results on both liquids, water and THF, to address the question of the impact of H-bonds on the dynamics.

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[2] A. Arbe, G. Nilsen, J. R. Stewart, F. Alvarez, V. García-Sakai and J. Colmenero, *Physical Review Research* **2**, 022015 (2020).

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## Coherent dynamics of acyl tail correlations in a lipid bilayer

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Membrane fluidity plays an important role in cell functions such as active permeation, deformation and migration. One of the quantitative determinants of the fluidity is the membrane viscosity, which characterizes the transport of materials within the membrane. For example, cell membranes tightly regulate their viscosity in two-dimensions in order to facilitate the transport of constituent molecules to their sites of action in the membrane while simultaneously ensuring a retained structure. Therefore, experimental, theoretical and computational studies to measure membrane viscosity have attracted significant research attention. Measuring two-dimensional membrane viscosity is, however, an on-going experimental challenge. Based on the previous neutron studies that relate the center of mass structural relaxation and viscosity in three-dimensional simple liquid systems, we have estimated the membrane viscosity from the acyl tail correlation dynamics of the two-dimensional lipid bilayers by using neutron spin echo spectroscopy. [1] This line of study will provide new insights into molecular origins of membrane viscosity.

To accurately determine the relaxation dynamics from neutron spectroscopy measurements, separating coherent and incoherent scattering signals is key as they contribute almost evenly to the total signal at the acyl tail correlation peak. Here, we employed the polarized neutron option of the LET chopper spectrometer at ISIS to separate coherent and incoherent relaxation dynamics occurring in lipid bilayers in the 10s to 100s of ps timescales. At the correlation peak lengthscale, the relaxation time of the coherent and incoherent dynamics were similar to each other. In this presentation, we will also report the temperature and wave vector transfer dependencies of the measured relaxation behavior for both coherent and incoherent signals.

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## Observation of the spin-current carrier with $P_x$ polarized neutrons

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Spin current, a flow of the spin degree of freedom in matter, is fundamental in spintronics research. Creation, annihilation, and control of the spin current have been one of the main topics. Spin currents can be generated electromagnetically, optically, and thermally, and their propagation spans the whole momentum ( $Q$ ) space. However, the detection has been limited to the long-wavelength limit ( $Q = 0$ ) by voltage measurement through the inverse spin Hall effect. The measured voltage is the macroscopic sum of the induced spin currents; hence, only the overall propagation direction and relative intensity can be discriminated. To gain microscopic views of the spin current, information at the characteristic  $Q$ /energy ( $E$ ) positions is required.

The spin current in magnetic insulators is carried by the transverse component of spin waves (quantized magnons) [1]. Magnons can be polarized, and the magnon polarization, i.e., the direction of the precessional motion of the spin, affects the thermodynamics of spintronic materials, governing the magnitude and the propagation direction of the spin current. However, the magnon polarization of magnon modes has eluded experimental observation. We show the first observation of the magnon polarization through polarized neutron scattering [2,3].

The target compound,  $Y_3Fe_5O_{12}$  (YIG), is a ferrimagnetic insulator with a complex structure and is a quintessential material for spintronics research. There exist major two magnon modes, and the energy gap separating optical and acoustic modes is of the order of the thermal energy at room temperature. A maximum of the spin Seebeck signal near room temperature [4] has been interpreted in the competition between magnon modes with opposite polarization between the two modes. From our experiment at IN20, ILL with  $P_x$  polarized neutrons, we found negatively polarized optical modes over the exchange gap and the positively polarized acoustic mode. Our experimental findings are well accounted for by atomistic spin dynamics calculations and indicate that thermal excitation of the optical mode will limit the amplitude of the induced spin current.

In this talk, we briefly review neutron scattering studies on YIG [3], and then show the methodology and results for the observation of the magnon polarization.

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## Polarized Inelastic Neutron Scattering Study of the Kitaev Material $D_3LiIr_2O_6$

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The Kitaev model is a rare example of an exactly solvable Quantum spin-liquid (QSL) beyond one dimension. In this model, spins on a honeycomb lattice interact through bond-dependent Ising-like interactions resulting in a QSL ground state with Majorana fermion and  $Z_2$  gauge flux excitations. The honeycomb iridates were proposed as a physical realization of this model, where the bond anisotropy originates from the strong spin-orbit coupling of the  $5d$   $Ir^{4+}$  ions. These materials take the chemical form of  $X-Li_2IrO_3$  ( $X=\alpha,\beta,\gamma$ ) or  $X_3LiIr_2O_6$  ( $X=Ag, H$ ) and feature honeycomb lattices of  $Ir^{4+}$  ions. All magnetically order at low temperatures into incommensurate spiral phases, precluding the possibility of a true QSL phase [1]. The sole exception is the case of  $H_3LiIr_2O_6$ , for which heat capacity and NMR studies find no evidence of long-ranged order or spin freezing down to temperatures of  $T=50$  mK with evidence of strong interactions from the Curie Weiss temperature of  $-113$  K [2]. Though this suggests a possible QSL ground state, very little is known regarding the excitations in  $H_3LiIr_2O_6$ .

We first performed unpolarized inelastic neutron scattering studies to probe the dynamics of  $D_3LiIr_2O_6$ . This is experimentally difficult, as only powder samples exist, both Li and Ir are strong neutron absorbers, and D/H have a relatively strong incoherent cross section. By means of isotopic enrichment, a custom annular sample can, and temperature dependent scattering, we have overcome these issues and found a magnetic excitation spectrum at low energies which is consistent with the nearest neighbor spin correlations expected in the KSL. The extraction of this spectra from our unpolarized measurements requires the removal of background contributions that far exceed the intensity of the proposed magnetic signal, potentially casting doubt on its validity.

Polarized inelastic neutron scattering was the natural choice to isolate these large background contributions which originate from multiple scattering effects. We separate these from the purely magnetic component, which we expect to match the excitation spectra in the unpolarized data. These measurements were performed on the HYSPEC instrument, which allowed for a full 3D polarization analysis of the scattering in  $D_3LiIr_2O_6$ . Alone, neither the unpolarized nor polarized datasets would be enough to confirm the excitations in this material. However, the clear separation of contributions to the signal using the 3D polarized scattering provides a direct verification of the extracted magnetic excitation spectra, providing new information on an exciting KSL candidate material.

[1] Stephen M Winter et al, J. Phys. Condens. Matter, **29**, 493002 (2017) [2] Kitagawa K, *et.al.*, Nature **554**: 341–345, (2018)

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**Polarized SANS & GISANS studies on condensed matter systems**

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Small-Angle-Neutron-Scattering (SANS) and Grazing-Incidence-SANS (GISANS) techniques have seen a remarkable growth in their application in magnetic material studies. One example for this is condensed-matter system with complex spin textures such as magnetic chirality, which offers great potential for applications in spintronic devices. Together with neutron polarization analysis, *polarized* SANS investigates systems with magnetic periods on the mesoscopic scale, being complemented by its surface-sensitive counterpart, polarized GISANS. These techniques rely on proper data reduction and analysis to extract the physics.

My research focuses on using and establishing suitable data reduction and analysis methods in these techniques. First, our research on magnetic chiral structures occurring in magnetoelectric single crystal  $Ba_{2-x}Sr_xMg_2Fe_{12}O_{22}$  [1], and in magnetic-domain-hosting compound FePd thin film will be presented. Second, magnetic field simulations of polarized GISANS setups, to optimize the neutron spin-transport, will be discussed. Third, current developmental efforts on polarized SANS data analysis in software SASView [2] will be reported. Polarization analysis has been incorporated as an integral part of the European Spallation Source instrument suite [3]. An introduction of its current scope will also be provided.

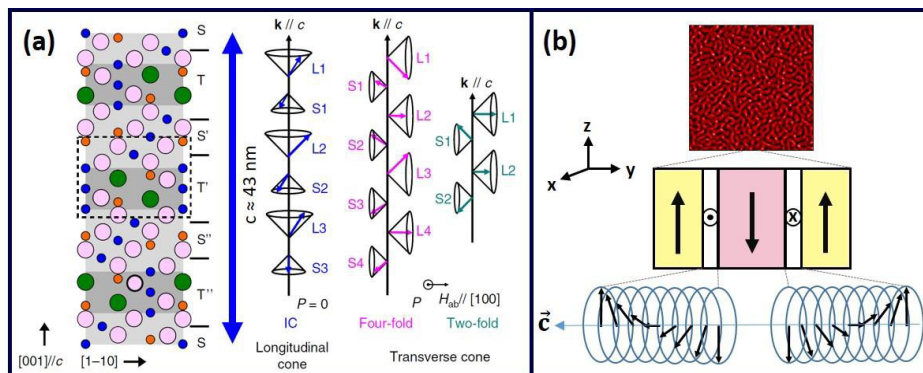


Figure 1 (a): chiral magnetic spin structures in magnetoelectric  $Ba_{2-x}Sr_xMg_2Fe_{12}O_{22}$  [1]. (b)

Ferromagnetic FePd thin films with perpendicular magnetic anisotropy, forming a maze domain structure and chiral Bloch domain walls.

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[2] [www.sasview.org](http://www.sasview.org)

[3] W. T. Lee *et al.*, Report on ESS Polarisation Workshop, ESS-3549713 (2020).

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## Mixed magnetic phases in $\text{Al}_x\text{CoCrNiFe}$ high entropy

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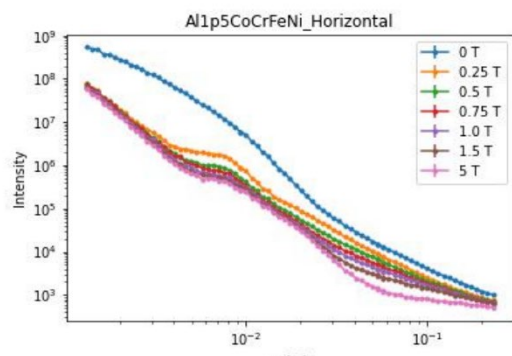
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The large distribution in atomic sizes and masses in high-entropy alloys results in extreme local environments, which manifests strongly in the thermal and magnetic properties. In this work, high-entropy alloys of  $(\text{Fe,Co,Cr,Ni})\text{Al}_x$ ,  $0 < x < 2$ , are prepared and their temperature-dependent magnetic and electronic properties determined. Magnetometry results show that all the samples are ferromagnetic, with a high-temperature phase,  $T_C > 200$  K, and a second low-temperature phase with  $T_C \approx 20$  K. However, the high-temperature phase is not associated with an open hysteresis loop, suggesting superparamagnetic behavior. The closed hysteresis loop suggests the ferromagnetism appears as small clusters, a theory explored with small-angle neutron scattering (SANS). SANS helps confirm soft ferromagnetic properties with alignment occurring with as little as 0.25 T in the Al  $x=1.5$  sample as can be seen in Figure 1, as well as smaller features that we predict to be associated with chromium frustrations localized in a matrix of Al, Ni, and Fe. The samples also show downturn in the magnetization at  $T < 10$  K which can be associated with an antiferromagnetic phase. Recent works have suggested that extreme strain distributions can induce antiferromagnetic ordering<sup>1</sup>. This research used resources at the High Flux Isotope Reactor and the Spallation Neutron Source, as appropriate, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory, and was funded by the DOE DE-SC0021344.

Figure 1



[1] Jorgensen, Cameron, et al. "In-Situ Study of Microstructure Evolution of Spinodal Decomposition in an Al-Rich High-Entropy Alloy." *Frontiers in Materials* 9 (2022).

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**WASP the Wide Angle Spin Echo instrument at ILL is in user operation**

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The first Neutron Spin Echo (NSE) instrument, IN11, was in user operation for 40 years. The newest spin echo instrument WASP took the relay and just had its first full year of user operation. I will use this occasion to review how the design of the wide angle NSE spectrometers has developed. The technical and scientific capabilities of the new instrument will be presented as well.

All functioning Neutron Spin Echo spectrometers use the basic IN11A design where the precession field is generated by long solenoids along the neutron beam. This construction limits the angular coverage and count rate of the instruments. Last century there have been two attempts to make a wide-angle coverage neutron spin echo instrument. IN11C at ILL was equipped with a flattened solenoid downstream of the sample and was in use until recently. It had a 30 degree-wide angular coverage but a very limited resolution. This instrument was practically trading intensity for resolution. The SPAN instrument [1] at HZB used a pair of coils in the anti-Helmholtz configuration creating an azimuthally symmetric magnetic field, which, in theory, could allow a nearly 360 degree detector coverage. WASP uses an improved SPAN construction, and it aims to have a 500 times higher detected intensity than IN11A while the resolution remains the same.

The long construction has finished in 2018, and the instrument has seen 4 full cycles of user operation. The detailed characteristics of the instrument and the first scientific results [2][3] will be presented.

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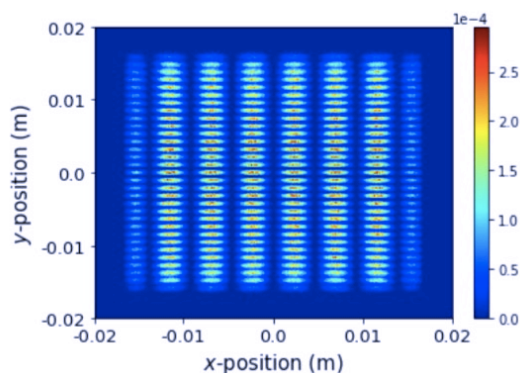
## Simulations and concepts for a 2D spin-echo modulated SANS (SEMSANS) instrument

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The spin-echo small-angle neutron scattering (SESANS) technique utilises a series of inclined magnetic fields before and after the sample to encode the scattering angle into the polarisation to obtain a much higher resolution than in conventional SANS. The analogous technique (spin echo modulated SANS (SEMSANS)) [1] implements spin manipulations before the sample only to encode the scattering into an intensity modulation. The technique can be combined with SANS to expand the length scale range probed from  $\sim 1$  nm to microns [2].

Using McStas [3] we show that using a series of four Wollaston prisms [4] in two orthogonal pairs with a  $90^\circ$  rotation can be utilised to create SEMSANS modulations in 2D. The figure below shows such modulations at the detector. These modulations can also be different in each encoding direction. This method can be applied to anisotropic scattering samples. Also this allows for the simultaneous measurement at two orthogonal independent spin-echo lengths. This technique yields directly information about the structure of oriented samples.



*Intensities on a PSD screen from McStas simulation.  $\lambda = 2.36 \text{ \AA}$   $\Delta\lambda = 0.05 \text{ \AA}$  and magnetic field strength of  $\Delta B = 7.5 \text{ mT}$  between the two Wollaston prisms. The magnetic field difference between the prisms in the first set was  $\Delta B = 30.0 \text{ mT}$ , whereas the difference between the prisms in the second prism set was  $\Delta B = 6.9 \text{ mT}$ . As a result, the spatial period in the x- and y-directions are different.*

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**Capability of Ultra-High-Resolution Lattice Structure Measurements at Oak Ridge National Laboratory**

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The inverse relationship between resolution and useable flux for neutron beams creates limitations in data collection from conventional neutron scattering techniques to determine accurate sample mosaics and inherent sample quality. The Larmor precession of neutron spin, however, provides a method of ultra-high resolution measurements by encoding the neutron velocity after interaction with a sample and observing small shifts in the total Larmor phase. This can be used to measure crystal mosaics, thermal expansion, and relative lattice distortion ( $D/d$ ) to a resolution of  $1 \cdot 10^{-6}$ . The high achievable resolution ensures beneficial diffraction capabilities for material and other scientific studies while also making the best use from all neutrons, even in large or divergent beams. In this study, we will report a newly developed technique using magnetic Wollaton prisms to investigate the crystal mosaic spread of samples on the HB-1 polarized triple axis spectrometer at the High Flux Isotope Reactor (HFIR), Oak Ridge National Laboratory, TN. Such technique would allow us to characterize the mosaic of the sample over a large volume simultaneously.

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**Towards realization of nmr-modulated polarized neutron scattering from hyperpolarized solutes**

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We use molecular dynamics (MD) simulations of hyperpolarizable solutes in solvent to study candidate pilot cases which are aimed towards experimental realization of polarized neutron scattering from NMR spin-manipulated samples. We evaluate the ability of MD using a ReaxFF force field [1] to reproduce published neutron scattering cross-sections for solvent methanol, analyze MD predictions for methanol restructuring around solute methyl nicotinate and other candidate hyperpolarizable solutes, and use published expressions for polarized neutron scattering cross-sections from spin-manipulated samples [2] to calculate the contributions of hyperpolarized solute nuclei. With use of the site-site pair correlation functions of each type resulting from the MD simulations, we study signal-to-noise considerations and estimate measurement durations needed to permit determination of intramolecular distances between specific methyl-nicotinate protons, as they depend on polarized neutron flux, sample size, and other instrumental parameters. To do so, we include the influence of known solute NMR longitudinal relaxation parameters on selected scattering measurement protocols. We apply these considerations to estimate needed measurement durations at existing polarized neutron scattering sources.

This work is supported by the National Science Foundation under Award No. 2108977.

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### <sup>3</sup>He polarization work at the JCNS

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An in-situ polarization analyzer has been in operation for the MARIA magnetic reflectometer. Here it provides a continual polarization and a wide angle of  $\pm 6^\circ$  for a cold neutron beam that is fully decoupled for the sample environment conditions and magnetic field. This device has been used as the basis for additional polarizer devices, using what has been learned to develop improved devices. A polarizer for thermal-energy beams, such as on the planned TOPAS spectrometer, has been completed and tested on POLI for 0.89 Å neutrons. Consequently, two new polarizers for neutron polarization and analysis have been constructed specifically for the POLI hot-beam diffractometer, and work is underway to adapt designs for both DREAM and TREX at the ESS. Further a compact device based on a 50% reduced scale of the MARIA polarizer is in testing for KWS1 (SANS) as is make a very high angular coverage,  $\pm 17^\circ$ , device based on a compensated solenoid geometry for KWS2 (SANS). Work done toward wide angle polarization analysis will also be presented where much experience was gained through work with NEAT at HZB. This work continues for the TOPAS spectrometer at MLZ, and TREX at ESS. The status of the various projects and device performance including scientific examples where available will be presented.



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## Neutron polarimetry using $^3\text{He}$ neutron spin filters

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$^3\text{He}$  neutron spin filters have been employed for various forms of neutron polarimetry. We present their use for four different applications: accurate determination of the neutron polarization produced by a supermirror in a monochromatic beam for a neutron interferometry experiment to determine the spin dependence of the neutron scattering length for  $^3\text{He}$  [1], polarization and polarization analysis of a monochromatic beam for an experiment to directly observe neutron spin rotation in Bragg scattering due to the spin-orbit interaction in silicon [2], sensitive transverse polarization analysis employed to image electric fields with a polychromatic neutron beam [3], and null measurement of an unpolarized polychromatic beam for a determination of the electron-antineutrino angular coefficient in neutron beta-decay [4].

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**Generation and detection of spin-orbit coupled neutron beams**

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Structured waves and spin-orbit coupled beams have become an indispensable probe in both light and matter-wave optics [1-2], for neutron specifically, showing distinct scattering dynamics for some samples [3-4]. We present a method of generating neutron orbital angular momentum (OAM) states utilizing <sup>3</sup>He neutron spin filters along with four specifically oriented triangular coils and magnetic field shielding. These states are verified via their spin-dependent intensity profiles [5]. The period and OAM number of these spin-orbit states can be altered dynamically via the magnetic field strength within the coils and the total number of coils to tailor the neutron beam towards a particular application or specific material [6].

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## Wide bandwidth neutron polarizing supermirror due to ferromagnetic interlayer exchange coupling

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A neutron polarizing supermirror is one of the most important optical devices to polarize a neutron beam. It is a stack of alternating layers of ferromagnetic (FM) and non-magnetic materials with a variation in bilayer thickness to extend the bandwidth of the neutron polarization. We have developed Fe/Ge polarizing supermirror by using ion-beam sputtering technique. A wide bandwidth is important especially for time-of-flight instruments installed at spallation neutron sources such as the J-PARC MLF since it determines the available wavelength-range of polarized neutrons. It is important to increase the ratio  $m$  of the critical momentum transfer of the supermirror to that of nickel to extend the bandwidth. The spontaneous magnetization of the ion-beam sputtered Fe/Ge multilayer, however, disappears when the Fe layer thickness is reduced to 2-3 nm because the Curie temperature becomes to be less than room temperature. This limits the  $m$ -value of the polarizing supermirror because the multilayer fails to form a high and low contrast in the scattering length density profile for spin- up and -down neutrons. The polarized neutron off-specular scattering measurement of Fe/Ge periodic multilayers revealed that the FM interlayer exchange coupling between neighboring Fe layers grew with decreasing Ge thickness less than 2 nm [1]. The FM interlayer exchange coupling observed here contributed to the presence of the saturation magnetization comparable to the bulk and to smaller coercivity and larger initial permeability than the multilayer without the FM interlayer exchange coupling. This offers a possibility to keep the spontaneous magnetization for the multilayer with a thin bilayer thickness and hence to increase the  $m$ -value of the polarizing supermirror. We proposed a modified layer sequence of the neutron polarizing supermirror, where the minimum Fe thickness was set to 3.5 nm, whereas the Ge thickness was reduced. A performance test of the neutron polarizing supermirror showed that the FM interlayer exchange coupling contributed to the presence of the magnetization comparable to the bulk and resulted in a marked enhancement in the  $m$ -value larger than 6.

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## Using Bayesian model selection for interpreting PNR data

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Magnetic thin film devices and the phenomena that are exhibited in these systems, have wide ranging applications for future technologies such as low powered/novel computation, waste heat recovery to name a few. Understanding of phenomena such as novel magnetic ordering (e.g., helical phases), or proximity induced magnetization, is often essential for device optimization. As such, many of these systems require quantification of the depth dependent magnetization.

Polarized neutron reflectivity (PNR) has the ability to structurally and magnetically depth profile thin film systems [1,2]. Providing information about the layered structure, such as: layer thicknesses, roughness(s), densities, while also providing depth dependent magnetometry on the in-plane moment. PNR analysis typically involves parametric modelling to interpret the data by modelling a real space scattering length density profile (SLD).

Magnetic features of interest can manifest themselves as non-trivial (sometimes subtle) perturbations on the magnetic profile. Attempts to model these effects can lead to increasingly complicated models, which run the risk of overinterpreting the data – i.e., does the data have enough information content (encoded in properties such as the statistical error bars or the resolution the data were taken with) to support the modelling? Typically, multiple models are required to compare against null or other hypotheses, often resulting in multiple models that can describe the data with very similar goodness of fit (likelihood). While additional external information can help in breaking this dead lock, there can be cases where more than one physical model can describe the data well. In these situations, some form of model selection is required.

Bayesian model selection considers the model complexity (Occam's razor) in addition to the information in the data for a given model-data combination - this can be quantified by calculating the model evidence [3]. By comparing the model evidence for multiple models given the same data, it is possible to quantify the model that is most consistent with the data.

Here, we show examples of where Bayesian model selection (in conjunction with external data) has been used to investigate proximity induced magnetism, and in the determination of the existence of helical phases in thin film CoZn. We will explain the process and methodology of applying Bayesian methods to PNR data analysis, including the limitations in the framework presented.

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### The 3-dimensional depth profile of magnetic skyrmion tubes

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Magnetic skyrmions have been the focus of intense research recently. These chiral spin textures are frequently presented as a 2D projection, inherently ignoring their three-dimensional tube-like structure. Recently, we have demonstrated the realization of skyrmions stable at ambient condition in Gd/Fe multilayers. These skyrmions are stabilized by magnetic dipolar interactions. [1]. Given the Fe/Gd multilayers possess flux-closure domains are favored at the top and bottom surfaces of the film; TEM results reveal an azimuthal winding along the center of the film. The dipole skyrmions exhibit a hybrid structure with Neel-type spin structure on the top and bottom, with chirality defined by the dipole fields, and a Bloch-type structure around the equatorial belt. In this work, we use grazing-incidence small-angle neutron scattering (GISANS) and polarized neutron reflectometry (PNR), both performed on a single Fe/Gd specimen, to determine the depth-dependent profile of the hybrid skyrmion. Specifically, in the GISANS and PNR patterns, the specular data captures the depth-dependent structure of the skyrmions, which averages to zero across the sample plane since the structure is highly symmetric. While the off-specular GISANS data captures the in-plane periodic structure. Together, these datasets provide a full depth-dependent profile of the hybrid skyrmions. To interpret the data, micromagnetic simulations of the hybrid skyrmions were performed using the object-oriented micromagnetic framework (OOMMF), then the specular and off-specular patterns were calculated and compared to the experimental results. Through iterative modification of the model, a simulated pattern is generated which accurately reproduces our experiments. This work was supported by U.S. DOE, Office of Science. Award DE- SC0021344.

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### Skyrmion lattice formation and destruction mechanisms probed with SANS

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Magnetic skyrmions are 3D chiral structures which have been promoted for their potential application in magnetic data and logic (i.e. spintronic) technologies. The chiral winding bestows a non-trivial topology which provides protection against data corruption in skyrmion spintronic devices. The topological qualities also allow the skyrmion to behave as a quasi-particle which motivates a fundamental interest in skyrmion materials and systems.

In many skyrmion-harboring systems, the skyrmions form hexagonally ordered lattices.[1] While the dynamics of individual skyrmions are likely in the gigahertz range ( $10^{-9}$  s) [See Presentation by N. Tang et al.], recent works have suggested that skyrmion lattice dynamics, including creation, destruction and rotation, may take much longer, occurring over milliseconds to seconds.[2, 3] This discrepancy between the dynamics of single skyrmions and the collective dynamics encodes the underlying quasiparticle interactions.

In this work, we use time-resolved small angle neutron scattering (T-SANS) as a unique tool which is able to resolve the collective ordering of these nanoscale magnetic structures in-situ as the lattice transforms. Measurements were performed by stepping the field into and out of the skyrmion stability envelope and capturing the SANS diffraction pattern as a function of time. The magnitude of the magnetic field step and temperature were used as control variables to investigate their role in determining the formation timescales. A range of B20 skyrmion materials, including MnSi, FeCoSi, and Cu<sub>2</sub>OSeO<sub>3</sub>, were tested, allowing magnetic parameters, such as saturation magnetization, DMI and magnetocrystalline anisotropy, to be investigated. In all of the measurements, the formation rate of skyrmion lattice was confirmed to be slow, taking 10's of milliseconds.

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## The Development of Transverse Neutron Polarimetry at NIST and Its Application in Neutron Scattering of Magnetic Topological Materials

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Topological spin textures in chiral magnets have attracted considerable attention by virtue of their exotic phases and emergent electrodynamics, making them promising candidates for information carriers in spintronic devices. Among them, magnetic skyrmions have been realized across a myriad of lattice forms, playing host to a zoology of defects, energetics, and tunable disorder levels. Investigations using microscopy/holography techniques in thinned and confined geometries have revealed topological transitions by way of emergent (anti)monopole defect proliferation, while polarized x-ray examinations have uncovered twisted surface skyrmions. Unfortunately, visualizations of their formation, topology, and reorientation dynamics in the bulk remain elusive. Transverse neutron scattering polarimetry offers new routes to the direct characterization of bulk skyrmion topologies and spin-dependent momentum correlations of topological phases, providing insights into skyrmion stabilization, transition, ordering, and restructuring processes in the bulk. Here, we discuss the development of transverse polarimetry at the VSANS instrument at the National Institute of Standards and Technology. We explore implementation with a skyrmion sample and neutron scattering tomography technique, and introduce future prospects for integrating structured neutron beams for topological materials' characterization. These developments will establish current prospects for polarized neutron scattering of bulk skyrmion materials, motivating future studies of topological materials through unique neutron scattering techniques.

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## New Incommensurate Magnetic Phases in the Multiferroic Compound $\text{MnCr}_2\text{O}_4$

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Nowadays, chromium-based normal spinel oxides  $\text{ACr}_2\text{O}_4$  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  $\text{MnCr}_2\text{O}_4$ , 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 revealed 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 super-space group formalism, 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.

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**Anisotropic non-collinear spin densities revealed in non-centrosymmetric multiferroics by advanced maximum-entropy reconstruction**

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Polarized neutron diffraction (PND) is a powerful method, which provides direct access to the scattering contribution from the nuclear-magnetic interference and thus reveals the phase difference between the nuclear and magnetic structure. This information allows to construct spin density maps and local susceptibility tensors in order to study the magnetic anisotropy between different crystallographic directions but is generally limited to the case of centrosymmetric structures with collinear magnetic moments. Introducing an advanced approach in the maximum-entropy method for a model-free reconstruction of spin densities, this limitation is overcome.

Single crystal PND was applied to study the magnetic structures in the non-centrosymmetric, unconventional multiferroic  $Ba_2TGe_2O_7$  ( $T = Cu, Co, Mn$ ) compounds. Using the new maximum-entropy approach implemented in a graphical user interface (GUI) based software, a detailed 3D magnetization density distribution in the unit cell was obtained for the first time both in the paramagnetic and the magnetically ordered states. These magnetic ground states vary strongly from an incommensurate cycloidal to a commensurate antiferromagnetic structure dependent on the applied magnetic field and the used transition metal ion  $T$  [1-3].

Compared to the results of regular magnetic structure refinement, the obtained 3D magnetization densities clearly visualize the crystal field effects on the different electron configurations of the transition metal ions  $T$ , imposed by their tetrahedral oxygen environment. Additionally, they allow to precisely study the magnetic anisotropy and ordered moments. Our results demonstrate the reliability of this new approach and software, which is now ready to be used as an efficient and straight forward standard analysis tool in single crystal PND.

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**Neutron polarization analysis of the anisotropic spin wave excitations in multiferroic BiFeO<sub>3</sub>**

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Polarized inelastic neutron scattering experiments have been performed to elucidate the anisotropic behavior of the low energy spin wave excitations in a multiferroic BiFeO<sub>3</sub> [1], which shows a cycloidal spin structure below 640 K. With the neutron polarization analysis for single magnetic domain crystals, magnetic excitation modes in and out of the cycloidal plane below 6 meV were separated successfully. The magnetic excitation spectra were analyzed using the linear spin wave theory. The low-energy magnon density of states consist of several magnon modes, including the two anisotropic modes, F and Y modes, distributed in and out of the cycloidal plane, respectively, which were previously observed using optical spectroscopies. Furthermore, there are other magnon modes that are not active in optical measurements. A model spin Hamiltonian, which reproduces the spin-wave frequencies observed using optical spectroscopies, explains the overall neutron scattering spectra reasonably well.

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**Magnetic chirality induced by chemical substitution in a chiral magnet**

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Exotic physical phenomena are bound to happen in chiral magnets, since broken space inversion, mirror symmetry and time reversal symmetry often accompany new physical phenomena. For example, the Dzyaloshinskii Moriya (*DM*) interactions, allowed by the lattice chirality, could bring about a twist between the magnetic moments and lead to various novel chiral magnetic structures (e. g., magnetic chiral solution and Skyrmion lattice). So far, very few chiral magnets have been discovered. Recently, we successfully synthesized single crystals of  $\text{Ni}_{3-x}\text{M}_x\text{TeO}_6$  ( $M = \text{Mn}$  or  $\text{Co}$ ) which are new chiral magnet candidates. The doped  $\text{Ni}_{3-x}\text{M}_x\text{TeO}_6$  crystals crystallize in a chiral polar space group  $R\bar{3}$  with  $M$  atoms occupy the Ni site. Strong *DM* interactions exist in  $\text{Ni}_{3-x}\text{M}_x\text{TeO}_6$  and induce chiral helimagnetic structures. Polarized neutron diffraction experiments on  $\text{Ni}_{3-x}\text{M}_x\text{TeO}_6$  revealed strong magnetic chirality, suggesting that one type of chiral domain dominates in our crystals. In this work, we will discuss the novel magnetic structures, bulk magnetic susceptibility and magnetic chirality of  $\text{Ni}_{3-x}\text{M}_x\text{TeO}_6$ .

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## Field and polarization dependence of magnons in collinear $\text{CuFeO}_2$

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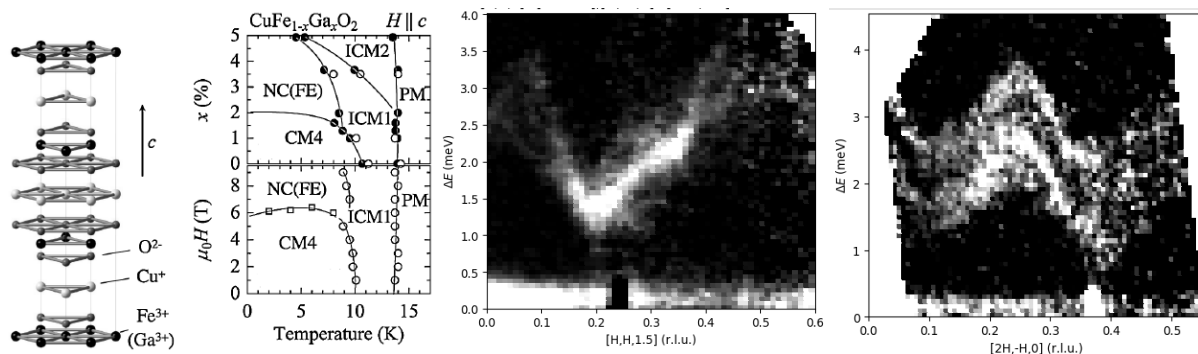
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Electromagnons are magnons that couple to frequency-dependent electric fields via a spin-induced electric polarization [1]. Electromagnons strongly couple to phonons with the same frequency and wavevector.  $\text{CuFeO}_2$  is a critical model system for fundamental understanding of the electromagnon-phonon coupling in a frustrated system due to its rich phase diagram. At ambient pressure, it notably supports a collinear 4-sublattice state ( $4\text{SL}-\uparrow\uparrow\downarrow\downarrow$ ), [2] which exists at low temperature and field up to 6 T. It is suggested that  $\text{CuFeO}_2$  is the only known material to support an electromagnon in its collinear phase. There is currently no good explanation for the disappearance of the electromagnon in the multiferroic noncollinear state above 6 T.

To understand the presence of the electromagnon in the collinear state and its absence in the cycloidal state, we have carried out high-resolution inelastic neutron scattering measurements at the HYSPEC spectrometer with polarization analysis and high magnetic fields up to 5 T. Our experimental results are combined with calculations of the magnon modes based on a microscopic model that couples the polarization to a time-dependent electric field. Understanding the behavior of the electromagnons in this material will more generally advance our knowledge about the coupling between electric fields and spins in multiferroic materials.



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**Wide Angle Polarization Analysis and first results with PASTIS-3 for IN20**

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XYZ polarization analysis for inelastic neutron scattering is a powerful method for the separation of magnetic, nuclear coherent and incoherent scattering. However, in the thermal neutron range, these experiments have typically been carried out using the conventional triple-axis technique with a single analyzer and detector, where polarized cross sections are measured point by point. We will here present the results of the third generation PASTIS device for XYZ wide-angle polarization analysis [1]. The PASTIS-3 device uses two independent polarized <sup>3</sup>He neutron spin filters for polarizing and analyzing the neutron spins. The incident neutron beam polarization can be inverted by reversing the spin state of the polarizing entrance cell and the <sup>3</sup>He analyzer cell provides a continuous 102-degree coverage of scattering angle. To obtain a high spatial homogeneity of the magnetic field in any field direction, a new coil design has been developed using sets of tilted coils. The setup has been tested on the thermal triple-axis instrument IN20 together with the multi-angle analyzer Flatcone. Finally, we will discuss the future possibilities for wide-angle polarization analysis on direct-geometry TOF-spectrometers such as PANTHER at the ILL.

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**Design of the PoLAR Cold Neutron Spectrometer at the NCNR**

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The NCNR is currently designing a new multi-axis cold neutron crystal spectrometer, PoLAR, to replace the SPINS cold triple axis on the NG-5 beamline. The new primary spectrometer will consist of a doubly elliptic supermirror guide and double focusing monochromator that have been optimized via Monte-Carlo to maximize the flux at the sample position. An integral part of the design is the inclusion of a V-cavity polarizer within this incident beam. Analysis of the guide's focusing optics has revealed that, with proper optimization, a V-cavity polarizer is exceptionally well suited to the guides elliptic geometry. Details of the guide, monochromator and V-cavity optimization will be presented. As well, the NCNR performed a 5-year publication study of the usage of polarized neutrons on cold spectrometers worldwide. A synopsis of these results will be presented.

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## New options on the polarized neutron single crystal diffractometer POLI at MLZ

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Polarized neutron diffraction (PND) is a powerful tool for studying condensed matter physics and to probe the spin and orbital properties of unpaired electrons. It allows to unambiguously determine complex magnetic correlations and small ordered moments, separate magnetic and nuclear contributions, and study spin-orbital entangled states by mapping out the magnetization density at the unit cell level. The single crystal diffractometer POLI, built on the hot source of the MLZ, is particularly dedicated to these polarized neutron measurements and can additionally host even bulky sample environments [1]. Currently, three standard setups are implemented on POLI: 1) zero-field spherical neutron polarimetry (SNP) using third generation CRYOPAD; 2) PND in magnetic field by the so-called Flipping-Ratio (FR) method; 3) non-polarized diffraction under various special conditions. Here, we report on our recent improvements and extensions in the instrumental performance and capabilities.

A new actively shielded asymmetric split-coil superconducting magnet with a maximal field of 8T has been procured and implemented on POLI. It is especially designed to facilitate high-field FR measurements and features low stray fields, large vertical and horizontal access and a wide sample space suitable for e.g., piezo goniometers and pressure cells. Combined with a newly built compact-size solid-state supermirror bender polarizer, a high neutron polarization above 99% could be confirmed for the magnet's complete field range [2].

Additionally, a new state-of-the-art in-situ SEOP polarizer and analyzer, maintaining a high and stable neutron polarization efficiency and transmission over a long period of time, have been built and will be available at POLI by the end of 2022 [3]. As a magnetic shield is added to the SEOP polarizer, they can be used for both FR and SNP setup options at POLI, increasing the experimental efficiency greatly. Also, the transfer of the BIDIM26 area detector (26x26 cm<sup>2</sup>) [4] from LLB to POLI is currently in progress and in the long-term plan, an upgrade to a larger area detector is foreseen.

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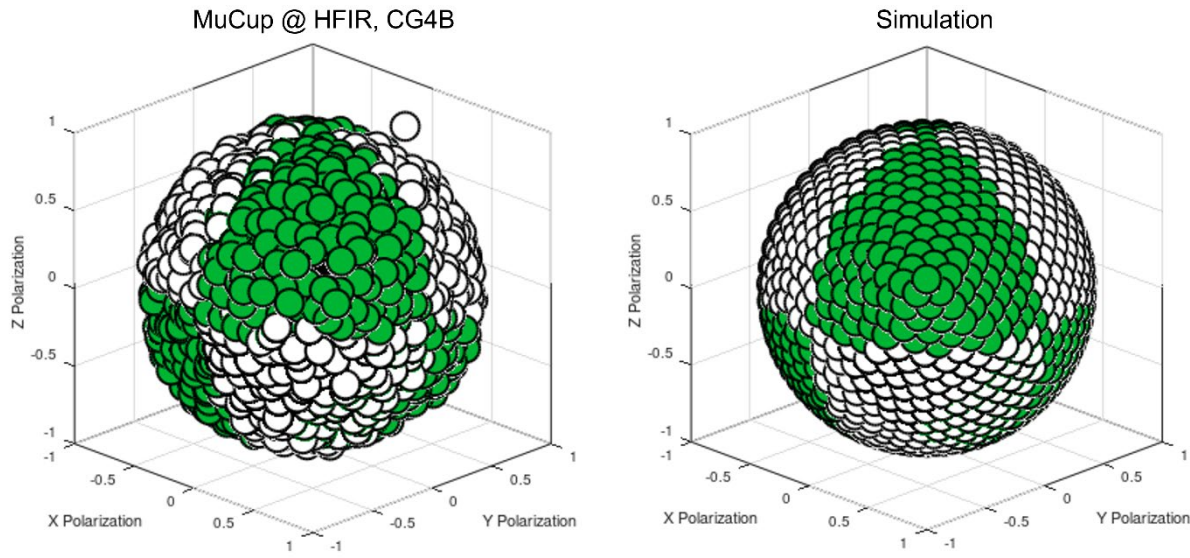
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## Latest Development in Spherical Neutron Polarimetry at ORNL

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In this talk we will describe the latest developments in Spherical Neutron Polarimetry at Oak Ridge National Laboratory. We will cover both hardware developments as well as software techniques, data reduction, and user-interface.



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## Poster Session

Sponsored by Advanced Research Systems

Wednesday, July 27<sup>th</sup> 2022

5:30 – 7:00 pm

- P1. Magnetic structure and interlayer coupling of  $[\text{Fe}_3\text{Si}/\text{FeSi}_2]_{20}$  superlattice**  
Takayasu HANASHIMA (NSTC)
- P2. Single Crystal Silicon Windows in Neutron Scattering Instruments**  
Qiang YE (NCNR)
- P3. Polarised neutrons for European Spallation Source (ESS) instruments**  
Annika STELLHORN (ESS, LUND University)
- P4. A first polarized neutron diffraction experiment test at a time-of-flight single crystal neutron diffractometer SENJU at J-PARC.**  
Shingo TAKAHASHI (Ibaraki University)
- P5. Self-compensated Neutron Super Mirror Magnetic Yoke to Reduce Stray Field**  
Earl BABCOCK (JCNS)
- P6. Upgrade and commissioning of guide test station with polarization analysis at HANARO**  
Ki-Yeon KIM (KAERI)
- P7. POLREF: Time of flight Polarised Reflectometer for Magnetism in thin Films**  
Andrew CARUANA (STFC)
- P8. Development of polarized neutron at the China Spallation Neutron Source**  
Tianhao WANG (CSNS)
- P9. Upgrade of the neutron spin echo spectrometer at the NIST Center for Neutron Research**  
Antonio FARAONE (NCNR)
- P10. Status of the NCNR Spin Filter Program**  
Shannon WATSON (NCNR)
- P11. Development of sample cells for the investigation of solid/liquid interfaces**  
Hannah BURRALL (Uppsala University)

**P12. Development on the spin analyzed QENS capability on DCS at NCNR**

Wangchun CHEN (NCNR)

**P13. Compensation optics for phase shifts of pumping light by mirror reflections in spin-exchange optical pumping**

Takashi INO (KEK)

**P14. Development of neutron resonance spin-echo spectroscopy using ellipsoidal focusing mirrors at MLF, J-PARC**

Fumiaki FUNAMA (ORNL)

**P15. Overview of the Polarized  $^3\text{He}$  Program at the Oak Ridge National Laboratory**

Chenyang JIANG (ORNL)



## Magnetic structure and interlayer coupling of [Fe<sub>3</sub>Si/FeSi<sub>2</sub>]<sub>20</sub> superlattice

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Ken-ichiro SAKAI<sup>3</sup>, Hiroyuki DEGUCHI<sup>4</sup>, Yoshiaki HARA<sup>5</sup>, Satoshi TAKEICHI<sup>6</sup>, and  
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The interlayer couplings between magnetic layers are the most dominant factors that determine the performance of spin-valve devices and depend on the electronic state of the spacer. However, the interlayer couplings in artificial lattices with semiconductor spacers are still not well understood. Fe<sub>3</sub>Si/FeSi<sub>2</sub>/Fe<sub>3</sub>Si artificial lattice consists of magnetic layers (Fe<sub>3</sub>Si) and non-magnetic semiconductor spacers (FeSi<sub>2</sub>). It has recently attracted attention in spintronics application fields because of its numerous merits. Iron and silicon are rich resources with little country risk due to the export control policies of resource-rich countries and the rapid increase in global demand. They are also an inexpensive, sustainable, and environmentally safe resource. In this presentation, we report on the temperature and field dependence of the magnetic structure and interlayer coupling of the [Fe<sub>3</sub>Si/FeSi<sub>2</sub>]<sub>20</sub> superlattice. Polarized neutron reflectivity measurements (PNR) were performed in the temperature between 4 K and room temperature under in-plane magnetic field conditions (1 T and 5 mT) using the polarized neutron reflectometer SHARAKU (BL17) at MLF J-PARC in Japan.

Under 5 mT, the moment of the magnetic layer Fe<sub>3</sub>Si forms an antiferromagnetic structure through the non-magnetic spacer layer FeSi<sub>2</sub>. The total energy of interlayer coupled superlattice system with an applied field  $H$  is written as

$$E = -M_s \cdot t_{FM} \cdot H \cdot \sum_{i=1}^N \cos(\gamma_i) - J_1 \cdot \sum_{i=1}^{N-1} \{\cos(\gamma_i - \gamma_{i+1})\} - J_2 \cdot \sum_{i=1}^{N-1} \{\cos(\gamma_i - \gamma_{i+1})\}^2$$

where  $J_1$  and  $J_2$  are the bilinear and biquadratic constants, and  $N (=20)$  is the number of superlattice repetition, and  $\gamma_i$  ( $i = 1, 2, \dots, N$ ) is the tilt angle of the moment relative to field. From the above equations and magnetic structure, we obtained the temperature variation of  $J_1$  and  $J_2$ . Furthermore, the electronic state of the nonmagnetic spacer layer of the [Fe<sub>3</sub>Si/FeSi<sub>2</sub>]<sub>20</sub> superlattice was evaluated using the interference model [1] proposed by Bruno.

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## Single Crystal Silicon Windows in Neutron Scattering Instruments

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Neutron scattering signal to noise ratio has always been the battlefield in SANS experiments. Using single crystal silicon windows can significantly reduce the neutron scattering background thus increasing the signal to noise ratio to great extent. We have designed and made different shapes/kinds of single crystal silicon windows in different sample environment equipments, including closed cycle refrigerators, dilution refrigerators, superconducting magnets, etc. Neutron scattering background signals are also compared between silicon tails in different shapes, quartz and aluminum of different thicknesses.

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## Polarised neutrons for European Spallation Source (ESS) instruments

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Polarised neutron instrumentation is now fully incorporated into the ESS baseline work plan [1]. Of the currently approved 15 instruments [2], 7 of 8 “first-instruments”, which will begin hot-commissioning upon beam-on-target, will provide polarization option to users. In total 12 instruments will provide polarised neutrons, many from day-1 in the user program. They include: imaging instrument ODIN, diffractometers DREAM, MAGiC, and HEIMDAL, spectrometers BIFROST, CSPEC, T-REX and MIRACLES, SANS instruments LoKI and SKADI, and reflectometer ESTIA and FREIA.

The equipment will come from in-kind partners, externally funded projects, collaborations and in-house development. Depending on the instrument configuration, there will be combinations of different types of polariser, analyser and spin-flipper to get the optimal performance and cost-effectiveness. Some of the major techniques employed will be MEOP and SEOP based polarised <sup>3</sup>He neutron spin filters, polarising supermirrors, and radio-frequency gradient-field spin flippers. We also aim to adopt innovative designs where applicable.

Even at an early stage of ESS operation, the neutron flux is expected to be on par with the flux on some polarised neutron instruments at major facilities. To capitalise on the flux gain, and also to ensure equipment incorporation without undue disruption to instrument construction and the user program, the work plan is being carried out in parallel, with the aim of delivering polarised neutrons for first-science experiments as instruments are entering operation.

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**A first polarized neutron diffraction experiment test at a time-of-flight single crystal neutron diffractometer SENJU at J-PARC.**

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SENJU is a time-of-flight single crystal neutron diffractometer which was designed for precise crystal and magnetic structure analysis at the Materials and Life science experimental Facility (MLF) in Japan Proton Accelerator Research Complex (J-PARC). In the near future, we would like to conduct polarized neutron diffraction experiments at SENJU at which a polarized neutron beam has not been available. We have been developing <sup>3</sup>He spin filters based on spin-exchange optical pumping (SEOP) method at J-PARC MLF [1], and applied it to SANS (TAIKAN), reflectometer (SHARAKU), Spin-echo (VIN-ROSE) and imaging instrument (RADEN) of J-PARC MLF [2-5].

In this experiment, we have installed the ex-situ <sup>3</sup>He spin filter into SENJU as a polarizer, and performed a polarized neutron diffraction experiment of a Heusler single crystal Cu<sub>2</sub>MnAl. An incident neutron spin polarity was alternated by flipping the <sup>3</sup>He polarization by a NMR equipped into the <sup>3</sup>He spin filter [6]. The neutrons polarized by passing through the <sup>3</sup>He spin filter flew to the sample through a magnetic guide field. A 0.3 T magnetic field was applied to the sample so as to be magnetically saturated. An intensity of the Bragg peak (111) of Cu<sub>2</sub>MnAl changed drastically depending on the neutron spin polarities.

In this paper, the detailed experimental setup and experimental results are described and analytical performance of the SENJU with the <sup>3</sup>He spin filter is discussed.

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## Self-compensated Neutron Super Mirror Magnetic Yoke to Reduce Stray Field

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We describe a super mirror (SM) magnetic yoke using permanent magnets designed to greatly reduce stray magnetic fields by using self compensation. This yoke is a minor modification to the typical existing magnetic yokes used for polarized SM arrays, often consisting of rows of very strong permanent magnets, such as NbFeB, arranged on either side between a cavity made of a pair of thick ( $> 1$  cm) soft iron plates. Such configurations can produce high fields (on the order of 500 G) over the large volume of the SM array, however they also create an external dipole field. One can passively shield such devices with additional magnetic layers or shells of  $\mu$ -metal, soft iron, or even steel, but this adds extra weight, complexity and size while not completely trapping the stray magnetic flux. Therefore, we developed and produced a modification to the existing magnetic yoke to compensate the stray fields at long range. This is done by adding a balanced amount of magnets with opposite magnetization to the original yoke, thus effectively canceling the stray field at distances of relevance to neutron instrumentation. The final device is similar to a simplified cladded magnet structure, and can be produced essentially as a bolt-on addition to existing polarized SM array magnetic yokes. This modification, in addition to eliminating the stray dipole fields at long range, actually increases the magnetic field inside the active area of the yoke.

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## Upgrade and commissioning of guide test station with polarization analysis at HANARO

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Guide-test station (G-TS) instrument at CG1 beamline in cold neutron guide hall at HANARO has been dedicated to test the unpolarized neutron supermirrors produced in-house. In order to make it feasible to measure polarizing supermirrors and magnetic thin films, we adopted polarizing neutron optics such as polarizer, neutron spin flippers, spin analyzer, guide field. HOPG (002) monochromator, made of seven pieces of slabs (40mm'20mm'2mm), deflect out neutrons with wavelength of 4.34 Å by a take-off angle of 80° from neutron guide with a cross-section of 20 mm wide'150 mm high. Monochromatic neutron wavelength is confirmed via time-of-flight technique and neutron flux is measured to be 1.12E6 n/sec/cm<sup>2</sup> at sample position at the wide open slit condition in case of vertically focusing monochromator. Double reflection polarizer/wavelength filter device, switchable between polarized and unpolarized beam channels, is adopted from Dr. Thomas Krist, Nano Optics Berlin GmbH, Germany. Compared to He-3 polarizer or Heusler crystals, neutron beam with high polarization as well as high transmission can be available. Spin-up neutrons are produced from double reflection polarizer when neutron beam is incident on mirrors within angular bandpass of 0.2 degree around 1 degree. In addition, this solid state device is maintenance-free in that it filters out second harmonic neutrons and makes widely used N<sub>2</sub>-cooled Be filter unnecessary. Lastly, background noise is low because it is located right after monochromator inside heavy concrete shielding blocks and most of unwanted neutrons are unable to come out of the beam shutter. Spin analyzer is made of a single blade of m=3 Fe/Si supermirrors coated on both side of Si wafer. This analyzer was also fabricated by NOB GmbH. Spin down neutron is transmitted while, spin-up neutrons are totally reflected if incidence angle is in between their critical angles. To flip the neutron spin polarization by 180°, radio frequency gradient field spin flippers (SF) were in-house fabricated. Two SFs are located upstream and downstream beam with respect to sample position. Ac current via RCL series resonating circuit is applied to rf coil, producing horizontal ac field. Vertical dc magnetic field strength could be adjustable by a hybrid architecture combining iron plate and dc electromagnet. Neutron spin can be flipped by 180° when Larmor frequency associated with precession motion around dc vertical field is set to be equal to the ac resonating frequency near the center of rf-coil. It turns out that 1<sup>st</sup> SF has 115.5kHz, V<sub>pp</sub>=3.5 V, dc field =3.9mT, dc current= 3.5A and 2<sup>nd</sup> SF has 140.0kHz, V<sub>pp</sub>=3.5 V, dc field =4.8mT, dc current= 3.0A, respectively. Finally, polarized neutron beam with overall spin flipping ratio (~90) and polarization (~97%) using a combination of polarizer and spin flipper and spin analyzer can be available at the G-TS instrument.

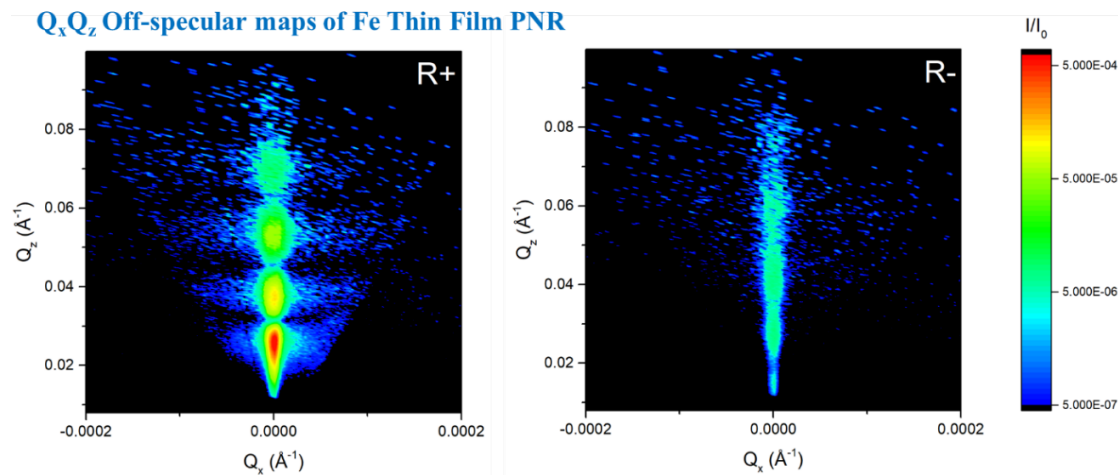
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## POLREF: Time of flight Polarised Reflectometer for Magnetism in thin Films

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Polarized Neutron Reflectometry (PNR) measures surfaces, buried interfaces and layers, yielding information about layer thicknesses, densities, surface/interface roughness and interdiffusion. Uniquely it can provide the magnetic equivalents of these quantities, including the total in-plane magnetisation [1,2]. A large variety of thin-film phenomena can be investigated using the POLREF beamline, including topological insulators, proximity-induced and fundamental magnetism, superconductivity, and spintronic devices. Furthermore, POLREF can perform off-specular PNR and specular Polarization Analysis (PA) measurements. In principle, if the problem can be made flat and is in the right length scales ( $\sim 1$  nm – 200 nm) then it can be measured by PNR. The POLREF time of flight PNR beamline is located in the second target station at the ISIS Neutron and Muon source [3,4]. With a polarised wavelength band of 2-15Å ( $P_{\text{EFF}} \sim 98\%$ ), low instrument backgrounds of  $I/I_0 < 10^{-7}$  and a resolution of  $dQ/Q$  better than 1%,  $Q_{\text{MAX}} = 0.25\text{-}0.3 \text{ \AA}^{-1}$  is routinely accessible for small (10x10 mm) samples within reasonable count times. The POLREF beamline has gone through several recent upgrades. Here, we will present the current capabilities of the POLREF beamline, including science highlights and how to get access to the ISIS neutron facility and POLREF beamline.



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## Development of polarized neutron at the China Spallation Neutron Source

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We present the current status of the polarized neutron techniques development at the China Spallation Neutron Source (CSNS). After three years of initial research and development, the CSNS continues its effort on developing polarized neutron capability in parallel to the beamline commission. An in-house maintained Spin-Exchange Optical Pumping (SEOP) polarized <sup>3</sup>He system has been commissioned, along with its <sup>3</sup>He cell filling station. Two in-situ operating SEOP <sup>3</sup>He neutron spin filtering systems are also developed and commissioned at the beamlines at CSNS. With the established capability, the CSNS polarized neutron test is now coordinating customized polarized neutron instrument development for several beamlines at the CSNS. Specific design was made for the VSANS, reflectometer, spectrometer and imaging beamline.

Advanced neutron polarization manipulation and experiment method are also developed in parallel to enhance the future polarized neutron application capability at the CSNS.

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## Upgrade of the neutron spin echo spectrometer at the NIST Center for Neutron Research

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Neutron Spin Echo (NSE) spectroscopy measures the dynamics of materials on longest time scales among neutron spectroscopic techniques. Currently instruments in the US routinely reach Fourier times of 100 ns. However, recent advances in the optimization of the precession field significantly increase the field integral homogeneity and therefore the maximum Fourier time, as already implemented on IN-15 at Institut Laue-Langevin and J-NSE-Phoenix at Heinz Maier- Leibnitz Zentrum. The University of Delaware, in collaboration with the National Institute of Standards and Technology Center for Neutron Research (NCNR), has received funding from the National Science Foundation through the Mid-scale Research Infrastructure- 1 program to acquire, assemble and commission a new NSE spectrometer employing optimally designed superconducting precession coils developed for the J-NSE-Phoenix, increasing the maximum Fourier time 2.5x. The installation of the new instrument is planned for 2023 during an outage of the NCNR to install a new D cold source, which will provide about a factor 2 increase in the neutron flux at long wavelength regions. Taking advantage of the new design, the increased flux provided by the new cold source, and a number of instrument elements optimized for long wavelength operation, a Fourier time of 300 ns should be achieved routinely, with the possibility of reaching 700 ns for strongly scattering samples. As the planned upgrade extends the longest accessible time, the upgraded instrument will expand the opportunities for the studies various materials systems especially in soft matter fields.

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S. Pasini, O. Holderer, T. Koziellewski, D. Richter, M. Monkenbusch, *Review of Scientific Instruments* **90**, 043107 (2019).

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### Status of the NCNR Spin Filter Program

**Shannon M. WATSON**<sup>1</sup>, Hannah BURRALL<sup>2,3</sup>, Wangchun CHEN<sup>1</sup>, Ross ERWIN<sup>1</sup>, Thomas GENTILE<sup>1</sup>

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As <sup>3</sup>He neutron spin filters (NSFs) continue to be used as an instrumental tool for the polarized neutron scattering community at the NCNR, development for current and new instruments has resulted in improvements in polarized neutronic performance, magnetostatic cavity improvements to increase achievable Q ranges, cell lifetimes, neutron spin transport, and minimization of <sup>3</sup>He polarization loss occurred during the adiabatic fast passage (AFP) NMR based <sup>3</sup>He polarization inversion. Instrument specific advancements include the improvement of performance on the Multi-Angle Crystal Spectrometer (MACS), development of a new large Q shielded solenoid and a compact low field (up to ~0.2 T) assembly for the Very Small Angle Neutron Scattering (VSANS) instrument and increased applied sample field on the Thermal Axis Spectrometer (TAS) instrument.

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## Development of sample cells for the investigation of solid/liquid interfaces

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The new design of sample cells for the investigation of solid/liquid interfaces by neutron reflection is presented. The design has evolved from earlier work [1] to allow smaller sample volumes and faster flow rates. Use of standardized components and a modular design allows a wide range of experiments that include grazing incidence scattering and conventional small-angle scattering using alternative neutron transparent back pieces and gaskets. The design is easily adapted for experiments with polarized neutron beams such as those with magnetic reference layers by replacing the usual stainless-steel hardware with brass or nylon. Various flow arrangements to fill and replenish the liquid in the cell as well as continuous stirring are also described.

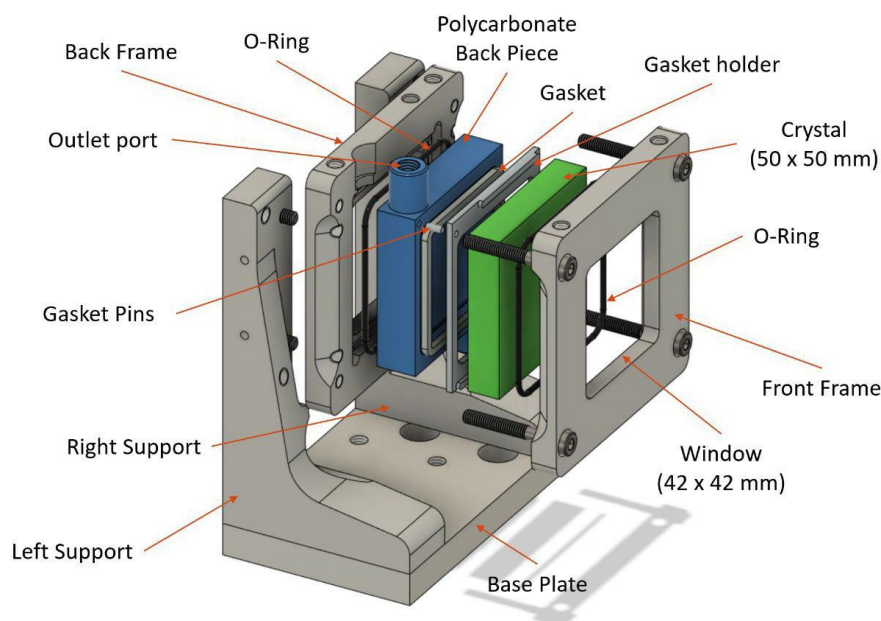


FIG. 1. Diagram of new cell design showing assembly of various components.

[1] A. R. Rennie, M. S. Hellsing, E. Lindholm, and A. Olsson, *Review of Scientific Instruments* **86**, 016115 (2015).

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**Development on the spin analyzed QENS capability on DCS at NCNR**

**Wangchun CHEN<sup>1</sup>, Antonio FARAONE<sup>1</sup>, Shannon M. WATSON<sup>1</sup>, NAGAO<sup>1,2</sup>, Nicholas BUTCH<sup>1</sup>, Craig BROWN<sup>1</sup>**

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Neutron polarization analysis on QENS instruments allows for separation of the coherent and spin-incoherent scattering and QENS studies of both the collective and single-particle dynamics. QENS instruments typically require a large array of neutron detectors for coverage of a wide range of momentum transfers and good energy resolutions ( $<100 \mu\text{eV}$ ). This requires a simultaneous coverage of large scattering angles of the spin analyzer and has then made neutron polarization analysis on QENS instruments challenging. Here we report recent development of a wide-angle polarization analysis capability on the Disk-Chopper Spectrometer (DCS) at the National Institute of Standards and Technology Center for Neutron Research (NCNR). The new polarized beam capability is planned to use a  $^3\text{He}$  spin filter to polarize the incident beam and a “horseshoe”-shaped  $^3\text{He}$  wide-angle spin filter [1] to spin analyze the scattered neutron polarization. Flipping of the neutron polarization is accomplished by inverting the  $^3\text{He}$  polarization of the incident spin filter using the adiabatic fast passage nuclear magnetic resonance technique. We present the status of the QENS capability with wide-angle polarization analysis on DCS and the results of the proof-of-principle experiment of spin-analyzed QENS measurements of partially deuterated ( $\text{CH}_3\text{OD}$ , D 99.5 % purity) methanol [2].

[1] W.C. Chen *et al.*, J. Phys.: Conference Series, **746**, 012016 (2016).

[2] W.C. Chen *et al.*, Physica B, **564**, 166-171 (2019).

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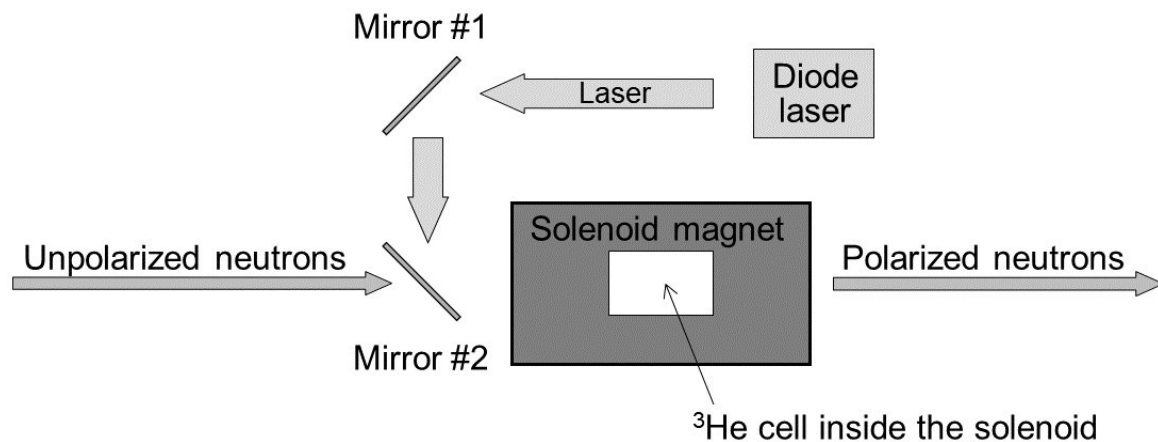
## Compensation optics for phase shifts of pumping light by mirror reflections in spin-exchange optical pumping

Takashi INO<sup>1</sup>

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In spin-exchange optical pumping or SEOP, <sup>3</sup>He nuclei are polarized through spin exchange with optically polarized alkali metal atoms. For efficient optical pumping of alkali metal, circular polarization of pumping light is essential, and mirror reflection is usually avoided since it introduces a phase shift between the S and P polarization components and hence spoils circular polarization [1]. Mirrors are, however, occasionally used to reflect the pumping light to illuminate <sup>3</sup>He cells parallel to the static magnetic field. The figure below illustrates such an *in-situ* polarized <sup>3</sup>He neutron spin filter (NSF) for the incident neutron beam polarization in POLANO, a polarized neutron spectrometer at the J-PARC spallation neutron source [2]. The pumping laser is reflected twice by dielectric mirrors for two reasons. One is simply that the space for the NSF is limited, and the other is to shine the laser along the neutron beam.

We discuss phase shifts by mirror reflection and propose simple compensation optics for them. Retardation was measured for different dielectric mirrors as well as for a gold-plated mirror. Applying our compensation optics before entering any mirror, perfect or near-perfect circular polarization was produced after the reflection.



Schematic of an *in-situ* polarized <sup>3</sup>He neutron spin filter in POLANO, an inelastic spectrometer at J-PARC [2]. The mirrors are dielectric multilayer coatings on silicon wafers.

[1] Joseph H. Apfel, *Applied Optics* **21**, 733 (1982).

[2] T. Ino *et al.*, *J. Phys.: Conf. Ser.* **862**, 012011 (2017).

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## Development of neutron resonance spin-echo spectroscopy using ellipsoidal focusing mirrors at MLF, J-PARC

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<sup>5</sup>Department of Nuclear Engineering, Kyoto University, Kyoto, Japan

Neutron resonance spin echo (NRSE) spectroscopy is a type of neutron spin echo spectroscopy which uses resonance spin flippers (RSFs) [1]. NRSE spectrometers with focusing mirrors enable experiments with a high energy resolution and signal-to-noise ratio simultaneously [2]. We are developing an NRSE spectrometer using ellipsoidal focusing mirrors at Materials and Life Science Experimental Facility (MLF), Japan Proton Accelerator Research Complex (J-PARC) [3, 4, 5].

We have successfully identified time-of-flight MIEZE (TOF-MIEZE) signals for elastically scattered neutrons at the sample under a focusing geometry [6]. This is the first experimental result which shows the feasibility of the NRSE spectroscopy using ellipsoidal focusing mirrors before and after the sample position. Furthermore, we have proposed a double-focusing geometry in which two identical ellipsoidal mirrors are arranged in series [7]. This new geometry enables us to correct the path length differences between RSFs for large divergent beams using a complete ellipsoidal focusing mirror. A numerical calculation shows that a Fourier time of 1  $\mu$ s is achievable using this geometry.

[1] R. Gähler, et al., *Z. Phys. B*, **65**, 269 (1987).

[2] M. Bleuel, et al., in: F. Mezei, et al., (Eds.), *Neutron Spin Echo Spectroscopy*, Springer, Future Developments in Resonance Spin Echo, 176 (2002).

[3] M. Hino, et al., *J. Nucl. Sci. Technol.*, **54**, 1223 (2017).

[4] H. Endo, et al., *Physica B*, **564**, 91 (2019).

[5] T. Hosobata, et al., *JPS Conf. Proc.*, **22**, 011010 (2018).

[6] F. Funama, et al., *JPS Conf. Proc.*, **33**, 011088 (2021).

[7] F. Funama, et al., *Nucl. Instrum. Methods Phys. Res. A*, **1010**, 165480 (2021).

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## Overview of the Polarized $^3\text{He}$ Program at the Oak Ridge National Laboratory

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<sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN 37931, USA

Polarized neutron scattering is an indispensable technique in modern neutron scattering, which takes advantage of the unique property of the neutron spin and its interaction with matter. To date, every major neutron scattering facility in the world is committed to providing polarized neutron capability to general users. Nuclear spin-polarized  $^3\text{He}$  gas has large spin dependent neutron absorption cross sections, and polarized  $^3\text{He}$  based neutron spin filters have been widely used to polarize or analyze neutron beams worldwide. Compared to other commonly used neutron polarizing techniques like Heusler crystals and polarizing supermirrors, polarized  $^3\text{He}$  has several unique features: First, it can work over a wide neutron wavelength/energy range. Second, it can accept large divergent neutron beams while not changing the beam divergence. Third, it can be used as a high-efficiency neutron spin flipper by flipping the  $^3\text{He}$  polarization through nuclear magnetic resonance (NMR). Because of these advantages, over the last decade the Oak Ridge National Laboratory (ORNL) has invested many resources in the development of polarized  $^3\text{He}$  systems based on spin-exchange optical pumping (SEOP). In particular, great efforts have been made in developing in situ polarized  $^3\text{He}$  systems, with which the  $^3\text{He}$  polarization will be kept stable throughout the whole experiment on the beamline where it is deployed. Different sized in situ systems have been built to suit the needs of each individual neutron instrument that has requested polarized  $^3\text{He}$ . We will show the design, construction and performance of these systems.

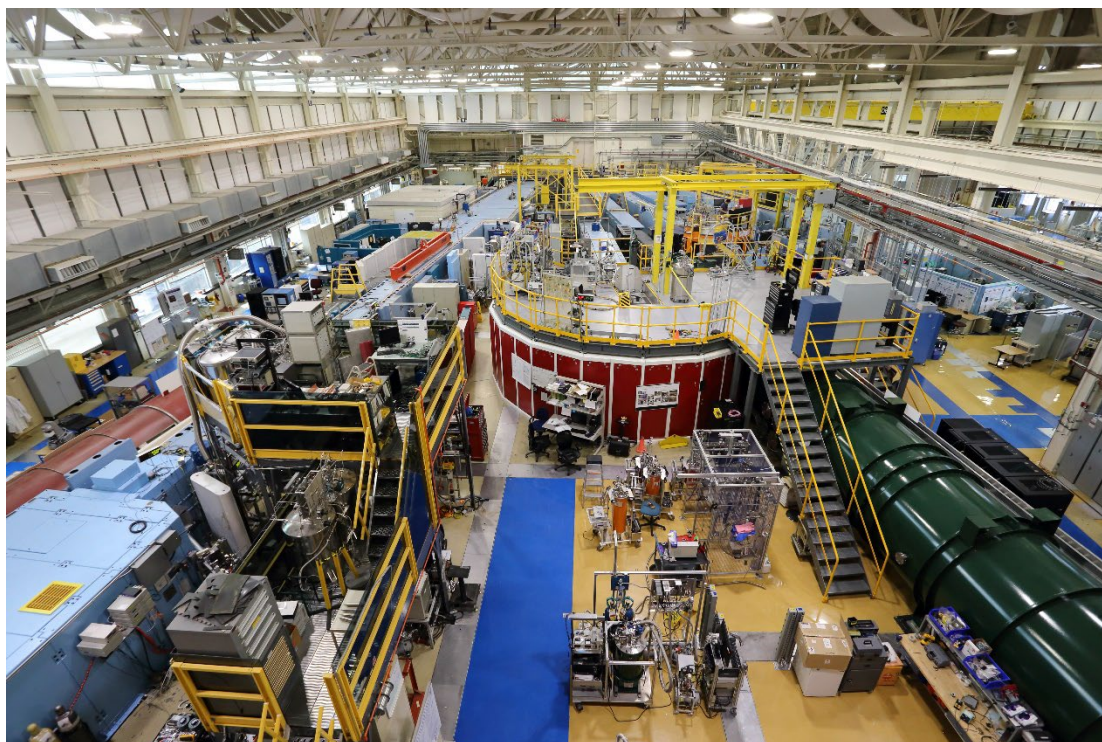
E-mail of the corresponding author: [jiangc@ornl.gov](mailto:jiangc@ornl.gov)

## NCNR Tour

Registered PNCMI attendees are invited to tour the research facilities of the NIST Center for Neutron Research (NCNR) on **July 29<sup>th</sup>, 2022**. The tour will last roughly 4 hours, and transportation by bus will be provided from the Graduate Annapolis hotel. Alternatively, you may travel to NIST by car. In that case, however, you will be required to show your vehicle registration or rental agreement at the NIST Visitor Center.

If you are interested in the tour, be sure to check the appropriate box when registering for the Conference. **No on-site registration can be accepted.** Once you register, a link will be sent for you to complete a required Visitor Registration form. An accepted government-issued ID will be required to gain access to NIST.

More information on the NIST Center for Neutron Research is available on the NCNR website.



*The cold neutron guide hall at the NCNR: visible in the foreground is the sample environment staging area, with the Disk Chopper Spectrometer (DCS) immediately behind it. The new Very Small Angle Neutron Scattering (vSANS) instrument is being assembled to the right in front of the High Flux Backscattering (HFBS) instrument. To the left of the mezzanine the Neutron Physics research station is visible, as well as the SANS (NG7) guide and the Neutron Interferometry cave. Taken in 2019. Credit: Yiming Qiu*



## Conference Dinner

We are pleased to announce that the PNCMI 2022 conference dinner on **Thursday, July 28<sup>th</sup>**, will be a crab cake dinner (a Maryland tradition) at Buddy's Crabs & Ribs in downtown Annapolis. Prior to dinner, all registered conference attendees are invited to explore Downtown Annapolis, Maryland. The Things To Do page highlights some of the more popular sights around Annapolis.



The crab dinner is included with conference registration. Dinner at Buddy's will be served from 6:00 to 8:00 pm as a buffet with a variety of offerings. (Note: non-seafood options are available via the buffet.) Attendees will be provided 1 drink ticket.

## Places to Eat

As a coastal city, Annapolis is traditionally known for its fresh seafood and Maryland Blue Crab. Annapolis also offers a culinary variety of other options. A brief listing of some of the cafes and restaurants near the conference location is provided below. More can be found on the PNCMI 2022 website or by web search.

### In the Hotel

**Trophy Room**: Coastal plates and throwback cocktails. Kitchen & Bar hours available on website

401-263-7777 ext. 3225

**Poindexter Coffee**: Coffee, lunch, and all-day breakfast. Open Daily, 6:30 AM – 12 PM

479-442-5555 ext. 3400

### Within Walking Distance

**Lemongrass**

167 West St – 3 min. walking  
Thai  
410-280-0086

**Tsunami**

51 West St – 4 min. walking  
Sushi Bar/Japanese Cuisine  
410-990-9868

**Luna Blu Ristorante Italiano**

36 West St – 4 min. walking  
Italian  
410-267-9950

**Metropolitan Kitchen & Lounge**

169 West St – 3 min. walking  
American  
410-280-5160

**49 West Coffeehouse & Winebar**

49 West St – 4 min. walking  
Quaint, great desserts  
410-626-9796

**Rams Head Tavern**

33 West St – 5 min. walking  
American, Craft Brewery  
410-268-4545

**Stan & Joe's Saloon**

37 West St – 4 min. walking  
Irish/ American  
410-263-1993

**Level**

69 West St – 3 min. walking  
Italian  
410-268-0003

**Cafe Normandie**

185 Main St – 9 min. walking  
French  
410-263-3382

**Joss Cafe & Sushi Bar**

195 Main St – 9 min. walking  
Japanese, Sushi  
410-263-4688

## Things to Do

### Maryland State House

A short walk east of the conference hotel. See the Maryland State House website for more information about this historic landmark.



### United States Naval Academy

Take a guided tour of the academy and learn about the traditions that guide the education and training of future officers.



### Visitors

<https://www.usnabsd.com/for-visitors/>

Please note the requirements for entry and have proper ID.

### Annapolis Towne Centre

A blend of culture and commerce where you can shop, dine, and more. Less than 4 miles from downtown, visit the Towne Centre website to explore local offerings.



### City Dock

City Dock connects Annapolis to the Chesapeake Bay. Walk down by the water and discover a collection of local boutiques, gift shops, art galleries, pubs, restaurants and historic inns.



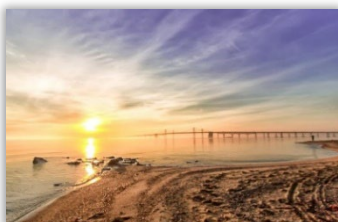
### Annapolis Maritime Museum

Explore the maritime heritage and ecology of the Chesapeake Bay. Museum admission is FREE. Click here to explore the museum's events and exhibits.



### Sandy Point State Park

Just a 15-minute drive across the Severn River, Sandy Point State Park is known for its scenic views of the Chesapeake Bay. Explore activities ranging from boat rentals to picnicking and more on the park's website.



### Explore Baltimore

Baltimore is the largest city in Maryland and has much to offer. The Inner Harbor area features museums, restaurants, concert venues, coffee houses, and more.



### Explore DC

Visit the monuments, memorials, and Smithsonian museums around the National Mall, take a tour of the U.S. Capitol Building, or explore the National Zoo. There is much to see, do, and eat in the capital.



## Sponsors

We'd like to extend our gratitude to the following sponsors for making the 14<sup>th</sup> Polarized Neutron for Condensed Matter Investigations (PNCMI) conference possible.



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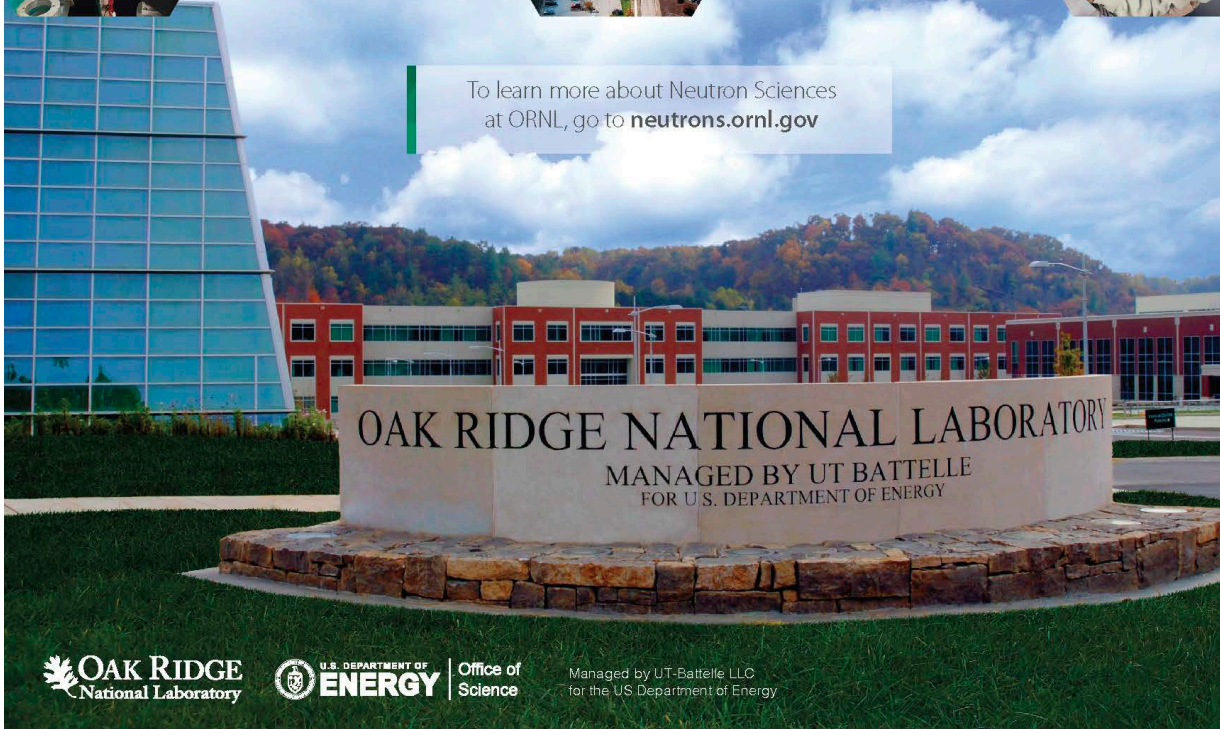
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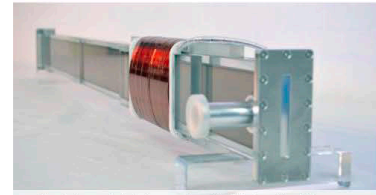
To learn more about Neutron Sciences at ORNL, go to [neutrons.ornl.gov](http://neutrons.ornl.gov)



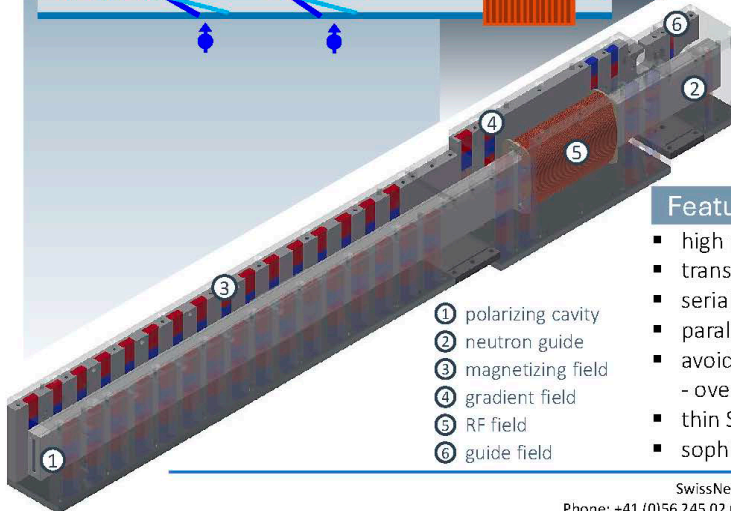
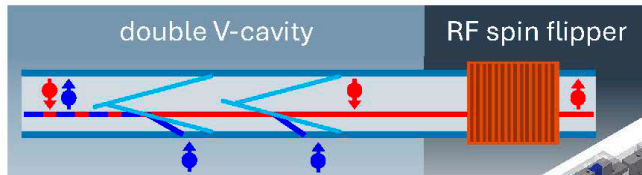
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# Spin Selector for Neutrons



Guide with V-cavity & RF spin flipper



- ① polarizing cavity
- ② neutron guide
- ③ magnetizing field
- ④ gradient field
- ⑤ RF field
- ⑥ guide field

## Features of RF spin flipper

- wavelength range: typically 2 – 20 Å
- no material in the beam
- gradient magnetic field
- RF field:  $B_{RF} \cong 100 - 150$  kHz
- electronics provided

## Features of polarizing cavities

- high polarization:  $P \cong 99\%$
- transmission:  $T = \Phi_{polarized,out} / \Phi_{unpolarized,in} \cong 35\%$
- serial (double or triple V) for high polarization
- parallel (multi-channel) arrangements
- avoid streaming of “up” neutrons:
  - overlaps at tip
  - intrusion at sides
- thin Si-wafer ( $t = 0.3$  mm) for high transmission
- sophisticated simulation tools available (McStas)

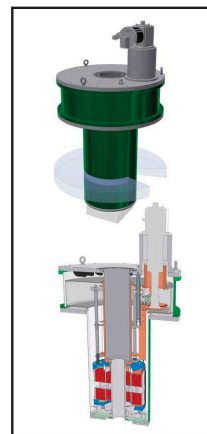
SwissNeutronics AG | Bruehlstrasse 28 | CH-5313 Klingnau | Switzerland  
 Phone: +41 (0)56 245 02 02 | E-mail: tech@swissneutronics.ch | www.swissneutronics.ch

# HIGH FIELD MAGNETS FOR NEUTRON SCATTERING



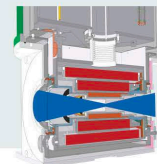
## 9 T pillar separated magnet

- » Integral closed-cycle VTI (Ø50 mm)
- » Removable He-3 insert
- » Cryogen-free cooling
- » 280 mK sample temperature
- » Automated z-axis movement and sample rotation
- » 165° continuous window (3mm Aluminium in path)



## 10 T ring-separated magnet

- » Ultra-slim outer vessel
- » 80 mm warm bore
- » Designed for DR insertion
- » 300° scattering angle
- » Tilttable to 10°



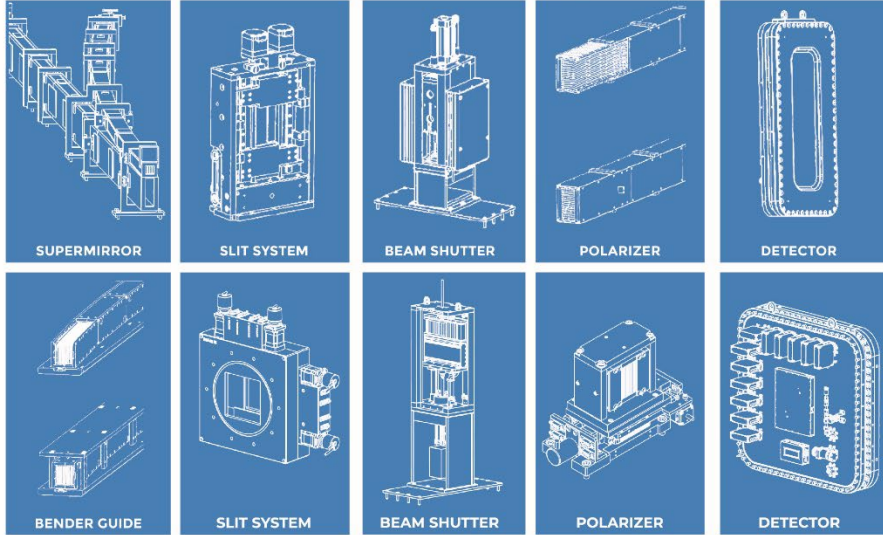
www.cryogenic.co.uk



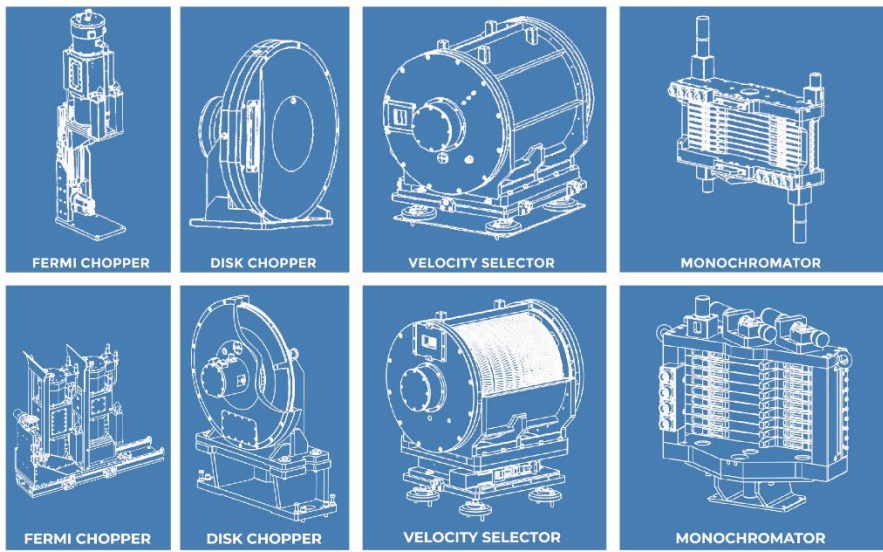
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