AONSA

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4th Asia-Oceania Conference on Neutron Scattering

BOOK OF ABSTRACT

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The 4th Asia-Oceania Conference on Neutron Scattering (AOCNS)

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Book of Abstract

Table of Contents

AONSA The 4th Asia-Oceania Conference on Neutron Scattering

AONSA Prize Ceremony

Abstract ID: 74

AONSA Prize Ceremony

Small Science at Large Facilities

Presenter: Yasuhiko Fujii (Retired, Emeritus Professor of the University of Tokyo, Japan)

Keywords: small science, large facilities, neutron scattering, synchrotron x-ray scattering

It's my great honor and pleasure to be awarded this year's AONSA Prize 2023. The citation is written as "For his outstanding achievements in the structural and dynamical study of phase transitions of condensed matter by neutron scattering, promotion of the neutron science in Japan as well as the national user program for neutron scattering facilities, and dedicated contributions for the promotion of neutron science in the Asia-Oceania region."

My talk will touch on these points concisely and then emphasize complementary use of synchrotron x-rays with neutrons for deeper understanding of the phase transition mechanism.

Neutron scattering used to be only one such "small science at large facilities" as an experiment can be conducted by a small number of researchers or even alone but it requires large facilities of research reactor or accelerator. It's in contrast to "large science at large facilities" represented by a high-energy physics research organized by several hundreds of worldwide researchers to explore unknown elementary particle at a large-scale accelerator facility. In the mid 1970's, synchrotron x-ray scattering appeared as another "small science at large facilities" with very similar style for managing facility operation and users program to neutron's case. Inversely speaking, the "large facilities for small science" will form platform of both communities with the same destiny to be shared as "More Is Different" (P.W. Anderson, Science 177, 393 (1972)).

In the mid 1990's when Prof. John White served as Chair of Commission on Neutron Scattering of IUCr (International Union of Crystallography), he began to talk enthusiastically about any possible organization of neutron scattering community in our Asia-Pacific region (tentatively called at that time). Such his global view of our community widely influenced several countries forming neutron scattering society and planning new neutron sources in the 2000's. The culmination of such a trend resulted in the formal establishment of our AONSA in 2008, which John served as the first Vice President and next the second President of AONSA. Unfortunately all of us missed him regrettably who passed away on Aug. 16, 2023.

In the Asia-Oceania Region, there are several organizations to be related to our AONSA such as AsCA (Asia Crystallographic Association), AOFSRR (Asia-Oceania Forum for Synchrotron Radiation Research), AAPPS (Association of Asia-Pacific Physical Societies) etc. hopefully moving together.

I would like to greatly appreciate a large number of collaborators working together scientifically and/or administratively in almost half-century of my academic career.

The 4th Asia-Oceania Conference on Neutron Scattering

Plenary Presentations (PL)

Abstract ID: 170

PL1

Multiple-Wavevector Magnetic Order

Presenter: Taka-hisa ARIMA (RIKEN Center for Emergent Matter Science, Japan)

Keywords: Multiple-Q order, magnetic skyrmion, magnetic meron, magnetic hedgehog

In contrast to simple (anti-)ferromagnetic systems, a magnetic material with long-wavelength magnetic order is generally sensitive to external stimuli. If such a magnetic material crystalizes in the cubic or uniaxial symmetry, the magnetic modulation vector Q is not uniquely determined. In some cases, Q changes from place to place, resulting in a multi-domain state. In other cases, multiple Q's coexist at the same place.

Atypical multiple-Q state termed magnetic skyrmion lattice was first reported by Muehlbauer and coworkers in 2009. Other examples include the meron/antimeron lattice and hedgehog/antihedgehog lattice. These multiple-Q states can also be regarded as a crystal of particle-like magnetic objects. The objects may also form a glass, liquid, or gas state. Observation of such states is however a big challenge.

I will discuss neutron studies on such multiple-Q magnetic order.

Abstract ID: 19

PL2

The Development of Neutron Techniques at Extreme Conditions and the High-Pressure Neutron Diffractometer at China Spallation Neutron Source (CSNS)

Presenter: Yusheng Zhao[1,2] ([1]Southern University of Science and Technology; [2]Eastern Institute for Advanced Stud)

Keywords: Neutron Diffraction, Neutron Imaging, Extreme Conditions, High Pressure

The development of neutron techniques under extreme conditions is invaluable to condensed matter physics, crystal chemistry, materials science, and earth and planetary sciences. *In-situ* neutron diffraction experiments at high-pressures (P) provide unique opportunities to investigate materials under these harsh conditions. Some extremely difficult studies, e.g., Debye–Waller factor as a function of pressure and temperature, can only be derived using *in-situ* high-P neutron diffraction techniques, which realize its full potential in a broad spectrum of scientific problems. Puzzles in earth science such as the global carbon cycle and the role of hydrous minerals for water exchange between lithosphere and biosphere can be directly addressed. The pressure and temperature effects on hydrogen bonding in ice, hydrates, and hydrocarbon phases can only be refined using high-resolution neutron diffraction. The uniqueness of neutron diffraction in resolving pair-distribution-functions can advance the study of liquid, melts, and amorphous phases under high-P conditions. Moreover, by introducing *in-situ* shear and/or differential stress, the yield strength and texture development of metals and minerals accompanied with phase transitions at high-P conditions can be studied. In this talk, I will first review the development of the high-P neutron experimental techniques in the last 50 years and then introduce the high-P neutron facility newly established at CSNS.

As one of the cornerstone research platforms within the Shenzhen Material Genome Large-Scale Facilities project, the high-pressure neutron diffractometer has been designated as Beamline BL-15 at CSNS and is currently under construction by the Southern University of Science and Technology (SUSTech) and CSNS. The beamline is expected to be commissioned in early 2024, with neutron diffraction and imaging as its primary techniques in conjunction with various sample environments under extreme conditions. Its main design parameters are as follows: 1) the d-spacing range (90° detector in the single frame mode): 0.5 – 5 Å; 2) the resolution: $\Delta d/d \leq 0.6\%$ (90° detector); and 3) the neutron flux at the sample position: $> 5 \times 10^6$ n/s/cm² @ 100 kW. The extreme sample environments include: 1) high-pressure (P) and temperature (T) [P (max) = 20 GPa, T (max) = 1300 K); 2) low-T and high magnetic field [B (max) = 9 T, T (min) = 4 K]; and 3) high-P percolation (pore pressure ≤ 150 MPa, confining pressure ≤ 200 MPa, deviatoric stress ≤ 300 MPa, and sample

temperature: 270 K ≤ T ≤ 370 K). The high penetrating power of neutrons presents great advantages in designing pressure cells with various kinds of high strength metals, alloys, and ceramics. A suite of pressure devices, such as true triaxial multi-anvil press, piston cylinder, P-E cell, gas/liquid high-P cell, portable cubic press, and ZAP cell, etc., will be used to provide extreme P-T conditions and the flexibility of switching experimental systems between the portable and transferable devices. The high-P facility is augmented by simultaneous multi-mode *in-situ* measurements for physical parameters such as mechanic, thermal, acoustic, optical, and electrical properties under extreme conditions.

High-P neutron facility at CSNS will provide scientists with a new venue to carry out frontier interdisciplinary research under comprehensive extreme sample environments of high pressure, high/low temperature, and/or high magnetic field. Similar techniques have been successfully used to study the equations of state, structural phase transitions, and thermomechanical properties of metals, ceramics, and minerals. We have previously conducted researches using neutron diffraction technique on the formation/decomposition kinetics of methane, CO_2 and hydrogen hydrate clathrates, and hydrogen/CO_2 adsorption of inclusion compounds such as metal–organic frameworks (MOFs). High-P neutron facility at CSNS is expected to have a positive impact on the basic science research in physics, chemistry, materials science, energy science, and earth and planetary sciences, and therefore create ample opportunities for new discoveries in science and technology.

Abstract ID: 97

PL3

Neutron scattering in the era of new challenges: quantum science and Van der Waals magnets

Presenter: Je Geun PARK (Seoul National University, Korea)

Keywords: Neutron scattering in the era of new challenges: quantum science and Van der Waals magnets

Neutron scattering has long been a tool of choice when it comes to studying the structure and dynamics of materials, not to mention the famous quotation, “Where atoms are and what atoms do”.

However, these advantages we have enjoyed collectively have been eroded over the years as new tools have been continuously developed and challenged the dominance of neutron scattering. In my humble view, the latest and most profound challenges do not come from other emerging experiment techniques, but from enormous scientific challenges we might otherwise miss. You may or may not agree with me, but I would say that these new scientific challenges are quantum science and van der Waals magnets, including many other two-dimensional (2D) materials.

In this talk, I will take up the task of the latter. As you all know, two-dimensional (2D) magnetism has long been a fertile playground where we have developed fundamental concepts, going far beyond the usual realm of magnetism. These contributions are numerous and far-reaching: the Ising model, the Mermin-Wagner theorem, and the BKT transition, to name only a few.

However, these instrumental developments have been mainly confined to theoretical discussion and few experimental investigations. The scientific scene underwent a complete revolution, with van der Waals magnets discovered in 2016 when people, including my group, realized the first monolayer magnetic systems using van der Waals (vdW) magnets.

These new materials have shown several salient features not seen in other three-dimensional magnets. For example, many vdW magnets invariably exhibit a strong spin-lattice coupling. Other unusual features include the photonic process unseen before, like unusual Floquet states and evidence of a quantum entangled exciton state. I will take you through my experience of how I have been using neutron scattering for my research with these new vdW magnets.

Abstract ID: 20

PL4

RIKEN Accelerator-driven compact neutron systems, and their capabilities

Presenter: Yoshie OTAKE (RIKEN Center for Advanced Photonics, Japan)

Keywords: Compact neutron systems, non-destructive test, infrastructure

RIKEN Accelerator-driven compact neutron source, RANS, has been operated since 2013[1]. There are two major goals of RANS research and development. One is to establish and realization of CANS (Compact Accelerator-driven Neutron Source) models that can be easily operated, non-destructively measured, and quantitatively evaluated, as a floor-standing type for industrial use as non-destructive analysis equipment. Another goal is to invent a novel transportable compact neutron system for the preventive maintenance of large-scale construction such as a bridge and highway. As of fall of 2023, two accelerator-based compact neutron source systems, RANS (7 MeV Proton, Be target) and RANS-II (2.49 MeV proton, Li target), as well as RANS-μ (252Cf) which have started real bridge measurements, are in constant operation. In addition, RANS-III, a transportable compact neutron system for non-destructive inspection of bridge decks, is being developed for on-board use. There are more than six kinds of instruments, and neutron measurements are available with RANS and RANS-II. The transmission imaging [2], neutron diffractometer towards stress measurement [3], small angle scattering instruments with thermal and/or cold moderators at RANS, fast neutron scattering time-of-flight imaging [4,5], neutron activation analysis with RANS and RANS-II, and neutron-induced prompt gamma-ray analysis with RANS, RANS-II, and RANS-μare available. The visualization of water retention leading to the deterioration of grading inside floor slabs and the deterioration of suspension bridge cable anchorage has been developed into a quantitative assessment in RANS-II with the advancement of measurement technology. RANS-μ is a non-destructive, quantitative evaluation of salinity inside concrete bridges to a depth of 7 cm, and has already been used to measure salinity in more than two outdoor bridges. The linear accelerator-based pulsed neutron source is 5 m long and 2 m wide, as demonstrated in RANS-II, and the system is capable of stable daily operation. The compact pulsed neutron system is a very good, easy-to- use, and convenient system for materials development and characterization, which is difficult with smaller stationary neutron sources, such as neutron diffraction, small-angle neutron scattering, and fast neutron scattering imaging. The RANS project is challenging the deployment of the technology for non-destructive detection inside concrete structures into space, as it will enable water exploration and, elemental exploration on the Moon and Jupiter.

Reference:

[1] Y. Otake, “A Compact Proton Linac Neutron Source at RIKEN”, “Applications of Laser-Driven Particle Acceleration”eds. Paul Bolton, et al. (2018) Chapter 19 pp.291-314 CRC Press

[2] Y. Yoshimura, et al.,“Neutron transmission imaging of water penetration of fly ash concrete exposed in marine and inland environments” AILCD International Conference “Beyond Growth- Bridging Wakamatsu + Tobata”, pp.233-236 (2019).

[3] Iwamoto, C. , et al., “Improvement of Neutron Diffraction at Compact Accelerator-driven Neutron Source RANS Using Peak Profile Deconvolution and Delayed Neutron Reduction for Stress Measurements”, ISIJ Int. 62, No. 5, pp.1013—1022, (2022).

[4] Y. Ikeda, et al. “Non-destructive measurement for water and voids in concrete with compact neutron source”, Plasma and Fusion Research Vol.13 pp.2406005-1-5 (2018)

[5] K. Fujita, et al., “Non-destructive test system for defect in floor slab with scattered neutrons”, Proceedings of The 22nd Symposium on Decks of Highway bridges, (2020)pp.47-52

Abstract ID: 30

PL5

Illuminating the structure of polymer brushes with neutron reflectometry

Presenter: Erica Wanless (University of Newcastle (Australia))

Keyword: polymer brush, neutron reflectometry

Polymer brush coatings are routinely used to change the interfacial behaviour of solids for targeting a wide range of applications. Many physicochemical techniques can reveal fundamental characteristics of the brush such as thickness (ellipsometry), wettability (contact angle) or stiffness (quartz crystal microbalance with dissipation monitoring). However, it is only neutron reflectometry that can reveal the internal brush nanostructure; the polymer volume fraction profile. Thus neutron reflectometry is critical to increasing our understanding of brush structure in different environments such as pH (for polyelectrolyte brushes [1]) or temperature variations (for thermoresponsive brushes [2,3]).

Recently we have focused considerable attention on improving the modelling of the diffuse polymer brush volume fraction (VF) profiles. Subtle features in the brush depth profile have traditionally challenged the interpretation of the acquired relatively featureless reflectivity profiles. In particular, uncertainty surrounding multimodality of polymer VF profiles. Confidence in fitting has been increased by using a Bayesian statistical approach.[4] and co-refinement of directly comparable ellisopmetric data [5].

Using these approaches, subtle conformational changes in thermoresponsive polymer brush depth profiles have been revealed: these brushes undergo a well- to poorly- solvated phase transition over a given temperature range. Examples will be discussed from our recent studies of poly (N-isopropylacrylamide) and poly (oligo(ethylene glycol) methyl ether methacrylate) brushes. These exemplar systems readily reveal specific ion effects (character that is a function of ion identity rather than solely attributed to ionic strength) when exposed to electrolytes from across the Hofmeister series [3,6]. Furthermore, nonmonotonic VF profiles have revealed (a) monomer enrichment near the substrate arising during copolymer brush synthesis [7], or (b) ion binding to the brush [8].

Recent work has also deployed neutron reflectometry to probe brushes in nonaqueous solvents [9]. Finally, as confined biomacromolecules lubricate natural environments, such as knee joints, our efforts to use neutron reflectometry to probe confined polymer brushes will be discussed [10].

References:

[1] T. J. Murdoch et al., Macromolecules 49, 9605 (2016). DOI: 10.1021/acs.macromol.6b01897

[2] T.J. Murdoch et al., J. Colloid Interface Sci., 526, 429 (2018). DOI: 10.1016/j.jcis.2018.04.086

[3] T.J. Murdoch et al., Macromolecules, 49, 6050 (2016). DOI:10.1021/acs.macromol.6b01001

[4] Gresham et al., J. Appl. Crystallogr. 54, 739 (2021). DOI: 10.1107/s160057672100251x

[5] H. Robertson et al., SoftwareX 20 101225 (2022). DOI: 10.1016/j.softx.2022.101225

[6] T.J. Murdoch et al., Polymer, 138, 229 (2018). DOI: 10.1016/j.polymer.2018.01.053

[7] E.C. Johnson et al, Langmuir, 36, 12460 (2020). DOI: 10.1021/acs.langmuir.0c01502

[8] H. Robertson et al., J. Colloid Interface. Sci., 634, 983 (2023). DOI: 10.1016/j.jcis.2022.12.114

[9] H. Robertson et al., Poly. Chem., 14, 1526 (2023). DOI: 10.1039/d2py01487d

[10] I.J. Gresham et al., Macromolecules 54, 2541 (2021). DOI: 10.1021/acs.macromol.0c02775

Abstract ID: 43

PL6

Engineering Four Kinds of Stresses in Materials

Presenter: Yandong Wang (University of Science and Technology Beijing, China)

Keywords: Neutron diffraction, Multiscale stress, Deformation, Engineering materials

Multiscale stresses in engineering components were generally generated during various types of industrial processes, while their accurate evaluations and effective controls govern advanced manufacturing. Three kinds of stresses in polycrystalline engineering materials were defined over a history of almost century according to their length scales ranging from millimeters for balancing macro-portions (Type I), to micrometers for accommodating grains/phases (Type II), and to atomic-size due to the existence of point/linear defects (Type III). With the rapid progress in Time- of-Flight (TOF) neutron diffraction and synchrotron-based X-ray techniques, a revisit to previous terminology of Type III stress could trigger a re-evaluation of separated ones emerging with further definition of Type III stress on the sub-micrometer scale related to various configurations of linear defects and Type IV stress on the atomic scale related to the point defects. This talk will introduce recent progresses in advanced methods for characterizing four kinds of stresses. The implications of *in-situ* diffraction experiments for establishing micromechanical models will be presented with the aim to advise the advanced manufacturing. Our recent work on the studies of micromechanical behaviors in superalloys and high entropy alloys will be also given, with a focus on some important experimental findings on microscopic mechanisms related to the localized fatigue deformation and confined phase transformation.

The 4th Asia-Oceania Conference on Neutron Scattering

Facility Report (FL)

Abstract ID: 235

FL1

Current Status and Prospects of China Spallation Neutron Source

Presenter: Sheng WANG (IHEP, Beijing)

Keywords: China Spallation Neutron Source, CSNS-II, Neutron Scattering

The China Spallation Neutron Source (CSNS) comprises an 80-MeV LINAC, a 1.6 GeV proton rapid cycling synchrotron, a tungsten target station, and the experimental hall for 22 neutron instrumentations. Over 1000 research proposals have been carried out since the user program opened in August 2018. More than 300 articles covering a large number of fields such as battery, alloy, magnetism, catalyst and polymer, published in Science, Nature, PRL, JACS, Nature Communication and Advance Material etc. CSNS achieved the designed power of 100 kW in 2020, and has been running with the beam power of 140 kW since 2022.

We have operated two diffractometers (GPPD and MPI), one SANS and one reflectometer (MR). Besides, two instruments (EMD and ANIS) started trial operation, three instruments (VSANS, ERNI and HD) are under commissioning and other two instruments are under construction.

To improve the facility performance and meet the user requirements, the upgrade project (CSNS-II) will be launched soon. The proton beam power will be upgraded to 500 kW, and 9 Neutron instruments, Muon and Proton beamlines will be constructed.

Abstract ID: 79

FL2

Neutron Science at JRR-3 - Overview, Recent Outcomes and Future Prospects

Presenter: Kenji Nakajima (Materials Sciences Research Center)

Keywords: JRR-3, Facility Report, Instruments, Reactor, Neutron Source

JRR-3 is the multipurpose research reactor. After the major upgrading, which was finished in 1990, the reactor is running at thermal power of 20 MW. At 7 horizontal beam tubes in the reactor hall and at 2 thermal guide tubes and 3 cold guide tubes in the guide hall, 28 neutron instruments are installed, which are operated by Japan Atomic Energy Agency, Universities including University of Tokyo, Tohoku University, Ibaraki University, Kyoto University and QST. JRR-3 was shut down for after Great East Japan earthquake in 2011 due to the reinforcement work to fit the new regulation, and user program was resumed in 2021. In spite of 10 years interruption of the user operation, now our neutron science at JRR-3 is producing fruitful results in the wide range of field from basic science to industrial applications. In this talk, overview, current status and future prospects of neutron science done at JRR-3 will be given.

QST: National Institutes for Quantum Science and Technology

Abstract ID: 237

FL3

Update from the Australian Centre for Neutron Scattering, ANSTO

Presenter: Jamie Schulz (ANSTO, Australia)

The Australian Centre for Neutron Scattering (ACNS) utilises neutrons from Australia's multi-purpose research reactor, OPAL, to solve complex research and industrial problems for Australian and international users via merit-based access and user-pays programs. The neutron beam facilities of OPAL consist of neutron beam tubes that penetrate the reflector vessel, a cold neutron source, beam shutters and neutron guides. A suite of 15 neutron beams instruments utilise both the thermal and cold neutron beams for both atomic and molecular structure determination and dynamics measurements, residual stress measurement and neutron imaging. An update will be given on the OPAL reactor and its neutron beam facilities, recent upgrades, user program, and future plans.

Abstract ID: 192

FL4

Current Status of HANARO Neutron Beam Facility

Presenter: Young-Soo Han (Korea Atomic Energy Research Institute)

Keywords: HANARO, Regulation, Neutron, Secondary Battery

HANARO is the only large multipurpose reactor in Korea. It has been operated for 28 years since its initial criticality in February of 1995 and the cold neutron source was installed in 2009. Currently, 5 thermal neutron instruments and 8 cold neutron instruments are operational. Until 2013, the operation of HANARO was successful, with the reactor running for an average of more than 160 days per year. As a result, the number of annual users of neutron beam facilities reached 687 in 2013.

HANARO faced the first serious challenge in 2014 when the nation's nuclear regulator, the Nuclear Safety and Security Commission (NSSC), ordered KAERI to reinforce the outer walls of the reactor building in preparation for severe seismic events. The construction took more than 3 years, during which the fledging user community had to find out ways to access foreign neutron science facilities.

Although the reactor is now officially back online since December 2017, the facility is now facing another unprecedented challenge in the form of a unique regulation. Since July 2018, NSSC requires research reactor operators to report virtually all unplanned shutdown events to the Commission before approved to restart. As a result, from mid-2014 to 2020, HANARO had operated only for less than two months. Although there is still the regulation that hinder normal operations, 71 days had been operated in 2021, 88 days in 2022, and 69 days have been operated so far in 2023. Fortunately, discussions have begun to change the regulations in NSSC. Currently, the proportion of industrial users among all users exceeds 15%, and users who study the secondary battery field are making good research results.

The 4th Asia-Oceania Conference on Neutron Scattering

Scientific Parallel Session M1. Condensed Matter Physics

The 4th Asia-Oceania Conference on Neutron Scattering

M1. Keynote Talks

Abstract ID: 65

M1-KT1

Manipulation of Spin-Triplet Superconductivity in the $YBa_2Cu_3O_7/La_{0.67}Sr_{0.33}MnO_3$ superlattice system

Presenter: Hsiung CHOU (Department of Physics, National Sun Yat-sen University, Kaohsiung, 80424, Taiwan; NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA; Department of Applied Physics, National University of Kaohsiung, Kaohsiung, Taiwan)

Keywords: superconductivity

Spin-triplet superconductivity behaves differently from singlet superconductivity, for it can be stabilized under the present of a magnetic field. This unique property has significant application in cutting-edge research on the development of spintronics, quantum computing, and the search for Majorana Fermions. In the parallel spin state (S_z=±1), the triplet pairs can survive and transport inside a ferromagnetic layer as a non-dissipation spin-polarized current. Keizer et al. (2006) and Sanchez et al. (2022) realized this concept in superconductor/ferromagnet planar junction where superconducting current conduction through the ferromagnetic layer was observed when the superconducting electrodes were separated by 430 nm and 1000 nm, respectively. Due to the emerging of triplet superconducting pairs at YBCO/LSMO interfaces, our group observed an extraordinary collective behavior with the enhancement of superconducting critical current under a magnetic field. However, not every SC/FM interface serves as the nurturing ground for generating spin-triplet superconductivity, highlighting the inherent instability of SC/FM interfaces and the urgent need for developing a pathway to customize interface conditions to produce triple superconducting pairs. In this presentation, I will illustrate a method that utilizes the interface Cu moment as an interfacial layer and control its direction by applying an external magnetic field. By controlling the direction of Cu moment at interfaces, we are able to control the generation of the triplet pairs in the parallel state. Additionally, neutron reflectivity measurements can probe the magnetic profile of superlattice films which is important for studying the basic characteristics of triple pairs.

Abstract ID: 59

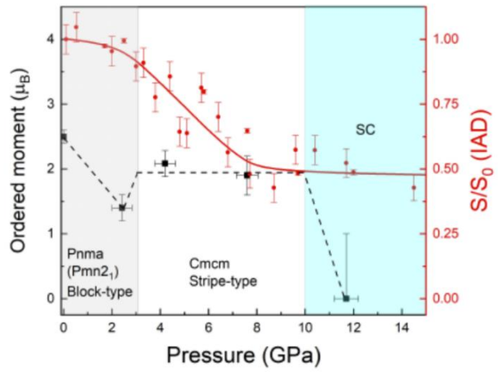
M1-KT2

Quantum materials under extreme conditions: a neutron scattering investigation

Presenter: P. Foury-Leylekian (Laboratoire de Physique des Solides, Université Paris Saclay, CNRS, Orsay, France)

Keywords: Mott insulator, superconductors, multiferroics, pressure, magnetic field

Mott insulators are among the most fascinating of all quantum materials. Due to strong electronic correlations, exotic electronic states such as superconductivity, AFM or even multiferroicity can emerge under the effect of chemical doping, magnetic field, temperature or pressure. Neutron scattering is an invaluable tool for investigating in detail these systems and the microscopic mechanisms that stabilize them. I will present neutron scattering results under extreme conditions of pressure, magnetic field and temperature in several families of compounds currently being studied. These include the multiferroics with strong magnetoelectric coupling RMn_2O_5 and Fe spin ladders $BaFe_2X_3$ (X = Se, S) superconductors under pressure.



Pressure dependence of ordered moment per Fe from Powder Neutron Diffraction at 3K and local moment from the IAD (red points, right scale) deduced from XES at 300 K. The red solid and black dash lines are the guides for eyes.

Abstract ID: 26

M1-KT3

Possible Dirac quantum spin liquid in a kagome antiferromagnet

Presenter: Shiliang LI (Institute of Physics, Chinese Academy of Sciences, China)

Keywords: quantum spin liquids

Quantum spin liquids (QSLs) have been theoretically shown to exist in the two-dimensional kagome lattice with Heisenberg antiferromagnetic interactions. While many kagome materials have shown interesting properties that may come from the fractionalized excitations in QSLs, the existence of intrinsic magnetic impurities makes it hard to further nail down the nature of the ground states. Recently, a new kagome compound $YCu_3(OH)_6Br_2[Br_{1-x}(OH)_x]$ has been successfully synthesized and is free of magnetic impurities. Here I will report our inelastic neutron scattering results on $YCu_3(OD)_6Br_2[Br_{0.33}(OD)_{0.67}]$, which show cone-like low-energy spin excitations. Our results give evidence that this system may host a Dirac QSL.

Abstract ID: 40

M1-KT4

Localized magnetic excitations in classical spin glasses

Presenter: Maiko KOFU (J-PARC Center, JAEA, Japan)

Keywords: spin glass, magnetic excitation

Spin glasses (SGs) are ubiquitous in magnetic materials having competing interactions and randomness. Time, temperature and magnetic-field dependent magnetic relaxation describe the characteristics of SGs and have been studied experimentally and theoretically. On the other hand, excitation features in a SG state remain elusive. To explore an elementary excitation inherent to the SG state, inelastic neutron scattering (INS) experiments have been performed for three systems with significantly different spin glass transition temperatures (T_f = 0.4-32 K), a magnetic ionic liquid (C_4mim$FeCl_4$) [1], iron aluminosilicate glass (FeO-Al_2O_3-SiO_2), and $Cu_{1-x}Mn_x$ dilute alloys, using AMATERAS and DNA spectrometers at J-PARC. The former two materials are amorphous and the latter is crystalline, where their SG state is well separated from magnetically ordered phases.

Interestingly, a similar feature has been observed in all three systems, although the energy scale of magnetic scattering is rather different. Below T_f, the INS spectrum displays a broad peak at low energy with a high energy tail, and its intensity is scaled by the Bose population factor. The excitation intensity changes with momentum transfer, reflecting short-range magnetic correlations, but the spectral shape of the excitations does not. Therefore, the excitations are nondispersive localized mode. Above T_f, the spectrum significantly changes with temperature, indicating the emergence of magnetic relaxation process. The low-energy magnetic excitation in the SG state is highly reminiscent of “boson peak”, local vibrational modes commonly observed in structural glasses. The observed magnetic excitations can be termed magnetic boson peak. The broad spectrum is attributed to a multitude of metastable states in SGs. Each state is imposed to have a short-range correlation with a different size and spin configuration and the corresponding excitation could be described as Bose-scaled local modes, like enclosed magnons. Our study demonstrates that the magnetic boson peak presents regardless of whether the material is crystalline or amorphous. We believe that the Bose-scaled broad excitation peak is a general characteristic of classical systems with quenched disorder.

Reference:

[1] M. Kofu et al., Sci. Rep. 11, 12098 (2021).

The 4th Asia-Oceania Conference on Neutron Scattering

M1. Invited Talks

Abstract ID: 143

M1-IT1

Stability and Scaling Behaviour of Magnetic Skyrmions in Cu_2OSeO_3

Presenter: Clemens ULRICH(University of New South Wale)

Keywords: SANS, skyrmions, topological spin systems, magnetic neutron scattering

A skyrmion is a topological stable particle-like object comparable to spin vortex at the nanometre scale. It consists of an about 50 nm large spin rotation which order in a 2 dimensional, typically hexagonal superstructure perpendicular to an applied external magnetic field. Its dynamics has links to flux line vortices as in high temperature superconductors. Cu_2OSeO_3 is a unique case of a multiferroic materials where the skyrmion dynamics could be controlled through the application of an external electric field. The direct control of the skyrmion dynamics through a non-dissipative method would offer technological benefits. Important for technological applications would be a stability range of the skyrmion phase up to room temperature. While room temperature skyrmion materials exist, Cu_2OSeO_3 orders magnetically below 60 K. Our combined small angle neutron scattering and SQUID magnetization measurements did provide direct evidence that the stability range of the skyrmion phase can be extended in Te-doped Cu_2OSeO_3.[1] Besides the information about the skyrmion range in the H-T phase diagram, neutron scattering provides also the full information about the orientation and skyrmion distances in the skyrmion lattice. The data provide new aspects about the scaling behavior of the skyrmion and helical distances. This offers new valuable information on the parameters in the spin Hamiltonian, which are responsible for the formation of the fascination quantum protected objects.

References:

1 arXiv:2303.02653

Abstract ID: 122

M1-IT2

Multi-*q* spin texture in the hexagonal quantum magnet $Yb_3Ru_4Al_{12}$

Presenter: Taku Sato (IMRAM, Tohoku University)

Keywords: Neutron Small Angle Scattering, Quantum Magnets, Skyrmion

Topological spin textures in magnetic materials have been intensively studied for more than a decade, since the celebrated discovery of magnetic skyrmion texture in the itinerant chiral magnet MnSi.[1] Skyrmionic or other topological spin textures were originally related to the antisymmetric Dzyloshinskii-Moriya interactions, activated by the spatial inversion-symmetry breaking. Much recently, skyrmion lattice formation has been reported in centrosymmetric magnets, widening the class of materials realizing topological spin texture. In the present work, we studied centrosymmetric hexagonal quantum magnet $Yb_3Ru_4Al_{12}$, where the magnetic ion Yb^{3+} forms pseudo spin s = 1/2 due to the crystalline electric field effect.[2] In the small angle neutron scattering (SANS) pattern obtained at the base temperature T = 0.3 K under zero field, we clearly found 12 spots, indicative of either multi-domain and/or multi-q magnetic order. By performing detailed field-history experiment under in-plane magnetic field, we found that the base-temperature zero-field magnetic structure is of double-q nature; the pattern indeed consists of reflections from three domain of the double-q order. The double-*q* structure transforms into an intriguing triple-q structure at finite in-plane magnetic field, before ending up with the trivial fully polarized state. Formation of double-q structure under zero field at the base temperature is a prominent characteristic of this compound and should be attributed to its quantum nature.

References:

1 S. Muhlbauer et al., Science 323, 915 (2009).

2 S. Nakamura et al., Phys. Rev. B 91, 214426 (2015)

Abstract ID: 128

M1-IT3

Symmetric and antisymmetric interactions in multiferroic manganites

Presenter: Igor Zobokalo (Petersburg Nuclear Physics Institute)

Keywords: polarized neutron scattering, multiferroics, magnetic properties

Magnetic interactions in the orthorhombic rare earth manganese oxides RMnO$_3$ and RMn$_2$O$_5$ have attracted much interest with respect to the electrical systems of these families. Electric polarization in both RMnO$_3$ and RMn$_2$O$_5$ arises due to the ordering of magnetic manganese ions and is of the same order of magnitude, which allows one to suppose that the mechanisms responsible for this phenomenon are similar. However, if in RMnO$_3$ Mn^{3+} ions, located in an octahedral surroundings of oxygen, form a single manganese magnetic system, then in RMn$_2$O$_5$ there are two manganese systems formed by Mn^{3+} ions located near the base of the oxygen pyramid, while Mn^{4+} ions surrounded by oxygen octahedra. One consequence of this difference is the difference in the proposed microscopic mechanisms of multiferroicity in RMnO$_3$ and RMn$_2$O$_5$. As a magnetic mechanism that ensures the occurrence of ferroelectric polarization in orthorhombic manganites RMnO$_3$, atomic displacements due to minimization of the Dzyaloshinskii -Moriya (DM) interaction energy i.e. antisymmetric striction — are considered [1]. For the explanation of magnetoelectric interactions in RMn$_2$O$_5$, the model of symmetric exchange striction is more often used [2], which is associated with an almost collinear magnetic order. In both cases, these theoretical approaches consider the manganese magnetic structure only.

In order to clarify experimentally the applicability of one or another model for describing the mechanisms of multiferroicity in these compounds, single crystals of RMn$_2$O$_5$ (R = Eu, Tb, Nd) [3 - 6], RMnO$_3$ (R = Dy, Ho) [7, 8] were studied using polarized neutron diffraction. The results obtained for all measured RMn$_2$O$_5$ crystals (R = Eu, Tb, Nd) [3 - 6] indicate the presence of a chiral contribution to magnetic scattering in these systems. Thus, measurements of the intensity of scattered neutrons for two directions of polarization of neutrons incident on the crystal, made on TbMn$_2$O$_5$, show the presence of chiral scattering in three magnetically ordered phases [4]. Chiral scattering was also observed for the compounds EuMn$_2$O$_5$ [3], NdMn$_2$O$_5$ [5], and Nd$_{0.8}$Tb$_{0.2}$Mn$_2$O$_5$ [6]. Moreover, this type of scattering was absent at those temperatures where there is no ferroelectric polarization. The connection between the antisymmetric DM interaction and electricity is also evidenced by the fact that in the course of research it was possible to change the population of chiral domains by applying an external electric field [4–6].

In the DyMnO$_3$, electrical polarization occurs at the temperature of the transition to the cycloidal chiral structure and smoothly increases with a further decrease of temperature. However, when Dy^{3+} was ordered into a structure with a propagation vector different from that one of the Mn3+ magnetic system, a decrease in electric polarization was observed [9]. At the same time, for

compounds with partial replacement of Dy by Ho, such an effect was not observed [10]. Our studies allow one to make the assumption that the increase in polarization in $DyMnO_3$ is due to the influence of rare earth magnetic systems. Its ordering at such high temperatures is induced by magnetic order on manganese with a corresponding propagation vector. This situation contributes to the (symmetric) exchange-striction mechanism of generation of electric polarization. Due to spontaneous ordering of a rare-earth system with a different wave vector, this mechanism is switched off. Measurements on the substituted manganite $Dy_{0.8}Ho_{0.2}MnO_3$ show that in this compound spontaneous ordering of the rare-earth subsystem occurs with the same wave vector as that of the manganese subsystem. Thus, the coherent spatial propagation of two magnetic systems leads to increased polarization. Our series of studies of $RMnO_3$ and RMn_2O_5 allows us to draw reasonable conclusions that these compounds involve both magnetic mechanisms of ferroelectric polarization generation: both symmetric and antisymmetric striction.

References:

[1] I.A. Sergienko and E. Dagotto, Phys. Rev. B 73, 094434 (2006).

[2] P.G. Radaelli and L.C. Chapon, J.Phys.: Condens. Matter 20, 434213 (2008).

[3] Zobkalo I.A., Polyakov V.A., Smirnov O.P., Gavrilov S.V., Plakhty V.P., Golosovsky I.V., Sharigin
S.V., Solid State Physics, 38(4), 725, 1996.

[4] I.A. Zobkalo, S.V. Gavrilov, A. Sazonov and V. Hutanu, J. Phys.: Condens. Matter 30, 205804 (2018).

[5] I. A. Zobkalo, A. N. Matveeva, A. Sazonov, S. N. Barilo, S. V. Shiryaev, B. Pedersen, and V. Hutanu, Phys. Rev. B 101, 064425 (2020).

[6] I. Zobkalo, S. Gavrilov, A. Matveeva, A. Sazonov, S. Barilo, S. Shiryaev and V.Hutanu, IEEE Transactions on Magnetics 58, 1 (2022)

[7] A.N. Matveeva, I.A. Zobkalo, M. Meven, A.L. Freidman, S.V. Semenov, K. Yu. Terentjev, N.S. Pavlovskiy, M.I. Kolkov, K.A. Shaykhutdinov and V. Hutanu, J. Magn. Magn. Mat. 569, 170415 (2023).

[8] A.N. Matveeva, I.A. Zobkalo, A. Sazonov, A.L. Freidman, S.V. Semenov, M.I. Kolkov, K. Yu. K.
Terentjev, N.S. Pavlovskiy, K.A. Shaykhutdinov and V. Hutanu, Physica B 658, 414821 (2023).

[9] O. Prokhnenko, R. Feyerherm, E. Dudzik, S. Landsgesell, N. Aliouane, L. C. Chapon, and D. N. Argyriou, Phys. Rev. Lett. 98, 057206 (2007).

[10] N. Zhang, S. Dong, Z. Fu, Z. Yan, F. Chang & J. Liu, Sci. Rep. 4, 6506 (2014)

Abstract ID: 215

M1-IT4

Neutron scattering studies of magnetic topological Kagome metals

Presenter: Yixi Su (Forschungszentrum Jülich, Germany)

Keywords: quantum materials, magnetism, single-crystal neutron diffraction

Magnetic topological kagome metals, in which topologically non-trivial band structures, magnetism and electronic correlation effects can often be intertwined, have recently emerged as an exciting platform to explore exotic states and novel functionalities. In this talk, I will mainly present our recent single-crystal neutron diffraction studies of complex magnetic orders in several archetypical magnetic kagome metals, including the realization of flat-band engineered spin density wave in the magnetic Weyl semimetal Mn_3Sn,[1] as well as the observations of various field-induced magnetic phases that give rise to the emergent topological Hall effect in the magnetic kagome metal RMn_6Sn_6.[2]

We thank Xiao Wang, Fengfeng Zhu, Yishui Zhou as well as many other co-workers and collaborators for their contributions.

References:

1 X. Wang, et al., arXiv: 2306.04312 (2023).

2 Y. Zhou, et al. (unpublished).

Abstract ID: 140

M1-IT5

Coherent magnetic excitations in a topological Kondo semimetal

Presenter: Michael Smidman (Zhejiang University)

Keywords: Inelastic neutron scattering, heavy fermions, Kondo lattice

CeNiSn is an unusual example of a Kondo semimetal, for which transport measurements evidence the opening of a gap in the electronic structure due to Kondo hybridization between the Ce-4*f* and conduction electrons at low temperatures, yet a fully-fledged Kondo insulating state fails to develop. More recently, CeNiSn has also been proposed to be a topological Kondo insulator, where the nonsymmorphic symmetry leads to unusual topologically protected surface states. Previous inelastic neutron scattering measurements using triple-axis spectrometers showed evidence for magnetic excitations with a spin-gap at certain momentum transfers. We have recently performed inelastic neutron scattering measurements on single crystals of CeNiSn using a cold-neutron time-of-flight spectrometer, allowing for a wider range of energy and momentum transfers to be measured. We reveal the presence of dispersive coherent magnetic excitations in CeNiSn at low temperatures, with a gap at all momentum transfers. Comparisons to electronic structure calculations suggest that these dispersive excitations correspond to transitions of strongly renormalized heavy bands, which have a non-trivial topology.

Abstract ID: 103

M1-IT6

Spin correlations in van der Waals ferromagnet VI_3

Presenter: Jun Zhao (Fudan University)

Keywords: Neutron scattering; van der Waals ferromagnet; magnetic order; magnetic excitation

Vanadium Triiodide (VI_3), a van der Waals ferromagnetic material, exhibits magnetic properties that are not fully understood. In this study, we present neutron diffraction measurements in VI_3 that revealed a ferromagnetic order with the moment direction tilted away from the *c*-axis at 4 K. A spin reorientation accompanied by a structure distortion within the honeycomb plane is observed, before the magnetic order completely disappears above T_C = 50 K. Our refinements suggest the presence of a considerable orbital moment antiparallel to the spin moment in this system. Through inelastic neutron scattering, we uncover distinct magnetic excitations that cannot be readily explained by conventional magnetic interactions. We will discuss the implications of these unconventional magnetic interactions on VI_3's intriguing magnetic properties, including its pronounced anomalous thermal Hall effects and tunable magnetism.

Abstract ID: 12

M1-IT7

Polarized Neutron Diffraction: A Key Tool to Probe Spin Density and Local Anisotropy in Magnetic Materials

Presenter: Arsen Goukassov (Leon Brillouin Laboratory, CEA-CNRS, France)

Keywords: polarized neutrons diffraction

Polarized neutron diffraction (PND) is a powerful method for characterizing the local magnetic anisotropy. This technique is based on the susceptibility approach, where measured flipping ratios are used to fit the local magnetic susceptibility tensors for each magnetic site, which allows quantifying the magnetic anisotropy at the atomic level.[1] It became a reference in mapping the magnetic anisotropy at the atomic scale in molecular based magnets.[2] Recently, this approach has been extended to study the magnetic anisotropy in powders,[3] which opens large possibilities in the studies of highly interesting powder materials, like frustrated magnets,[4] multiferroics, single molecule magnets [5] or nanoscale systems.[6] In the talk, we review the recent studies using PND to analyze the local magnetic anisotropy in various magnetic material. On an example of single-molecule magnet with Co (II) complex we show that the crystallites in a high magnetic field start orienting their easy axes along the field, (Fig.1b),[3] thus creating a “magnetically induced preferred orientation”. We show that this effect improves the precision in the determination of the local anisotropy parameters in complex compounds. Newly developed "CrysPy" library applied for the PND data analysis will be also presented.[7]

References:

1. A. Gukasov and P.J. Brown, Journal of Physics: Condensed Matter, 2002, 14, 8831-39.

2. D. Luneau and B. Gillon. Magnetochemistry 2021, 7, 158

3. I. A. Kibalin and A. Gukasov. Phys. Rev. Res. 2019 1, 033100.

4. I. A. Kibalin et al. Phys. Rev. Res., 2020 2 033509.

5. S. Gupta et al., JACS Au 2023, 3, 429−440

6. I. Golosovsky at al. Small Methods 2023, 2201725

7. CrysPy library web page: https://www.cryspy.fr/

Abstract ID: 104

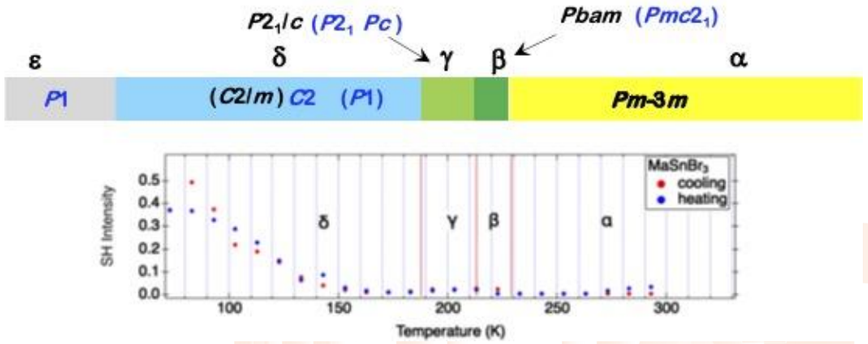
M1-IT8

Phase Transitions of the Lead-Free Methylammonium Tin Halide Perovskites $MASnX_3$ (X = I, Br)

Presenter: Miwako Takahashi (University of Tsukuba)

Keywords: Methylammonium Tin Halide Perovskites, Phase transitions, Neutron scattering, Second harmonic generation

Methylammonium Tin Halide Perovskites $CH_3NH_3SnX_3$ ($MASnX_3$, X = I, Br) are candidates of lead-free light-absorbing materials for photovoltaic devices. They undergo successive phase transitions caused by tilting or distorting of the SnX_6 octahedra and orientational ordering of the organic *MA* cation. The structures of low temperature phases are still controversial due to the difficulty of accurate determination for the orientation of organic cation. To determine the structures at low temperature phases and elucidate the ordering mechanism of the organic cation through the phase transitions, we have performed neutron diffraction measurements using single-crystal diffractometer SENJU (BL18) and powder diffractometer SuperHRPD (BL08) installed at MLF, J-PARC. The temperature dependance of diffraction patterns showed clear structural change between three phases for X = I, and between five phases for X=Br. The results of the structural analysis revealed several candidates of the space groups for the low temperature phases. To complete the determination of the structure of these phases, second harmonic generation (SHG) measurements were performed. For X = I, no SH intensities were observed throughout all the phases, indicating the structures are centrosymmetric. On the other hand, SH signal was found to grow below 150 K for X = Br, showing the lost of centrosymmetry occurred in the low temperature phases. It is considered that the orientational ordering of the organic *MA* cation causes to lose the centrosymmetry. Combining the results of neutron and SHG measurements, the space groups were determined for β and γ phases of X = I and for β to δ phases of X = Br.



Phase diagram with candidates of space groups obtained by neutron diffraction, and temperature dependence of SH intensity of $MASnBr_3$. From the increase of SH intensity below 150K, space groups are determined to be centrosymmetric *Pbam* and $P2_1/c$ for β and γ phases respectively, and non-centrosymmetric C2 for delta phase.

Abstract ID: 71

M1-IT9

Chiral Spin Liquid Ground State in $YBaCo_3FeO_7$

Presenter: Werner Schweika (European Spallation Source, Forschungszentrum Julich)

Keywords: Highly frustrated magnetism

A chiral spin liquid state is discovered in the highly frustrated, layered kagome system $YBaCo_3FeO_7$ by polarized diffuse neutron scattering.[1] From the antisymmetric part of scattering, related to vector chirality, we determine the chiral correlation function by Fourier analysis. The chiral short-range order indicates the emergence of chiral lumps. It can be described by cycloidal waves, which originate from the trigonal sites and extend into the kagome layers. The observed vector chirality agrees with the underlying antisymmetric Dzyaloshinskii-Moriya exchanges arising from broken spatial parity. This chiral spin liquid state is stable down to lowest temperatures despite of strong antiferromagnetic spin exchange. The observation of a possible short-range ordered ground state raises a fundamental challenge. However, based on the fundamental theory of classical magnetic order, we show that such a ground state may arise from the antisymmetric exchange acting as a frustrating gauge background stabilizing local spin lumps. The scenario may appear in many highly frustrated magnetic systems in non-centrosymmetric compounds and has similarities to the avoided phase transition in coupled gauge- and matter-fields for sub-nuclear particles.

References:

[1] W. Schweika et.al., Chiral Spin Liquid Ground State in $YBaCo_3FeO_7$, Phys. Rev. X 12, 021029 (2022).

Abstract ID: 109

M1-IT10

Geometric approaches to spiral spin liquids

Presenter: Shang Gao (University of Science and Technology of China)

Keywords: neutron scattering, spiral spin liquid, geometry

Spiral spin liquids are correlated paramagnetic states with sub-dimensional degeneracy in the ground state manifolds. Recent studies establish spiral spin liquids as candidate hosts for exotic correlations like fraction quadrupoles and magnetic skyrmions, yet their experimental realization in real materials is still limited. Here we propose two geometric approaches to spiral spin liquids, including the effective lattice approach and the line-graph approach. Both approaches are verified through neutron scattering experiments performed on model compounds.

Abstract ID: 33

M1-IT11

Explorations of Kitaev Quantum Magnets

Presenters: Jinsheng Wen (Nanjing University)

Keywords: quantum spin liquids, frustration, alpha-$RuCl_3$, Kitaev model

The Kitaev model is an exactly solvable quantum-spin-liquid model defined on a honeycomb lattice with S = 1/2. The key element underlying this model is the bond-anisotropic Kitaev interaction. However, in a spin-only system, it is unrealistic to have such anisotropic interactions. In this talk, I will show that the Kitaev interaction can be realized in a Mott insulator α-$RuCl_3$, which has an effective spin of 1/2 by entangling the spin and orbital degrees of freedom. I will also show that by applying an in-plane magnetic field, the zigzag magnetic order ground state in α-$RuCl_3$ can be completely suppressed, and a quantum-spin-liquid state can be achieved. More recently, we extend the Kitaev physics to higher-spin system, where we find in a honeycomb-lattice antiferromagnet $Na_3Ni_2BiO_6$ that there is a profound 1/3 magnetization plateau, which is stabilized by the Kitaev interaction. This will also be discussed in the presentation.

Abstract ID: 98

M1-IT12

NEUTRON SCATTERING STUDY ON LOW-TEMPERATURE SPIN DYNAMICS OF MOLECULAR MAGNETS

Presenter: Zhendong Fu (Songshan Lake Materials Laboratory)

Keywords: Inelastic neutron scattering, molecular magnet, spin dynamics

Molecular wheels have attracted much attention for their remarkable spin dynamic properties at the crossover between classical and quantum regimes. A cyclic complex $\{Cr_8Y_8\}$ has been discovered and investigated. Magnetic susceptibility data suggest weak ferromagnetic (FM) coupling between CrIII moments.[1] Thus $\{Cr_8Y_8\}$ represents a rare FM example of molecular chromium rings. We have performed low-temperature heat capacity (HC) and inelastic neutron scattering (INS) measurements to characterize the spin dynamics of $\{Cr_8Y_8\}$.[2] Schottky anomalies are observed in HC data and can be well fitted with the multilevel model, giving important information about the energy gaps between spin levels. The INS results obtained on time-of-flight INS spectrometers show INS peaks corresponding to the transitions within S = 12 ground states and between the S = 12 ground state and the S = 11 excited state. A single-J model with a unique exchange constant J = 0.151 meV can well reproduce the low-lying energy levels and their Zeeman splitting upon applied magnetic fields, indicating that the single-J model can be a good approach for the low-T spin dynamics of $\{Cr_8Y_8\}$. In order to verify the possible zero-field splitting (ZFS) as suggested by the low-T HC data, we have measured the high-frequency electron spin resonance (HF-ESR) spectra of $\{Cr_8Y_8\}$.[3] We have observed a sharp resonance peak due to the transitions between the S = 11 quantum levels and a broadband corresponding to a distribution of resonance peaks due to the ZFS of the S = 12 quantum levels. By analyzing HF-ESR spectra, the expected S = 12 ground state is confirmed and its ZFS parameter D is determined to be −0.069 K. The small ZFS is attributed to the axial magnetic anisotropy and further confirmed by a field-induced single-molecule magnet behavior by an AC susceptibility measurement down to 50 mK.

Abstract ID: 126

M1-IT13

Quantum Magnetism in Rare-earth Perovskites

Presenter: Liusuo Wu (Southern University of Science and Technology, China)

Keywords: Rare earth perovskite, Quantum magnets

The rare-earth perovskite has been widely used as a substrate for the growth of epitaxial ferroelectric and multiferroic thin films, while its detailed magnetic properties at low-temperature were rarely reported. For rare earth ions, the presence of strong spin–orbit coupling combined with crystal field splitting usually produce a doublet ground state with very strong single ion anisotropy. Naively, one would expect that such doublets should behave as classical (Ising) spins. However, our work of the rare-earth perovskite $YbAlO_3$ provides a natural realization of the Heisenberg spin 1/2 single-chain Hamiltonian, with the observation of critical Tomonaga–Luttinger liquid behaviors and spinon confinement–deconfinement. These results demonstrate that f-electron-based magnets can provide realizations of various aspects of low dimensional quantum physics, and suggest that other members of the rare earth perovskite family are also worth exploring.

Abstract ID: 111

M1-IT14

Features of the neutron resonance spin-echo spectrometer at J-PARC MLF and its application to spin dynamics

Presenter: Tatsuro Oda (ISSP, The University of Tokyo)

Keywords: Neutron spin echo, MIEZE, quasi elastic neutron scattering, spin fluctuation

At the beam line BL06 of J-PARC MLF, two resonance type neutron spin-echo spectrometers, named MIEZE and NRSE, have been installed jointly by High Energy Accelerator Research Organization (KEK) and Kyoto University.[1] During the commissioning, we demonstrated features of the modulation of intensity with zero-effort (MIEZE) type spin-echo spectroscopy in combination with the time of flight (TOF) method. Specifically, the derivative of phase with respect to TOF can be a useful indicator for instrumental tuning [2] and phase correction.[3]

The MIEZE-type spin echo spectroscopy can provide a suitable time-space range for investigating phase formation and stabilization of topological order, which has recently attracted much attention. The MIEZE instrument has also the advantage that it can be easily applied to magnetic samples subjected to a high magnetic field. We will present the features of the MIEZE instrument and experimental results to observe the spin fluctuations in long-range magnetic orders with relaxation times ranging from picoseconds to nanoseconds.[4, 5]

References:

1. https://mlfinfo.jp/en/bl06/

2. T. Oda, M. Hino, H. Endo, H. Seto, Y. Kawabata, Phys. Rev. Appl. **14**, 054032 (2020)

3. T. Oda, H. Endo, H. Ohshita, T. Seya, Y. Yasu, T. Nakajima, M. Hino, Y. Kawabata, Nucl. Instrum. Methods A **1012**, 165616-165616 (2021)

4. T. Nakajima, T. Oda, M. Hino, H. Endo, K. Ohishi, K. Kakurai, A. Kikkawa, Y. Taguchi, Y. Tokura, T. Arima., Phys. Rev. Res. **2**, 043393 (2020).

5. S. Aji, T. Oda, Y. Fujishiro, N. Kanazawa, H. Saito, H. Endo, M. Hino, S. Itoh, T. Arima, Y. Tokura, T. Nakajima, Phys. Rev. B **108**, 054445 (2023)

Abstract ID: 133

M1-IT15

Ising spins in a metallic antiferromagnetic chain

Presenter: Xiyang Li (The University of British Columbia)

Keywords: metallic chain, Ising spins, inelastic neutron scattering, spinon, soliton

To date, research has primarily focused on insulating spin chain systems, which exhibit a plethora of novel quantum phenomena.[1] Here, we investigate a new metallic compound Ti_4MnBi_2 [2] using neutron scattering, DMRG, and first-principles density-functional theory.[3] Utilizing the AMATERAS@J-PARC and DNA@J-PARC instruments, we observed distinctive signals in Ti_4MnBi_2 single-crystal: a gapped magnetic excitation continuum exclusively dispersing along the chain around the Brillouin-zone center down to 0.3K, and a temperature-induced gapless excitation continuum, suggesting elementary excitations as fractional spin S = 1/2 spinons and solitons. Combined with magnetization measurements, we demonstrated spinon gap opening due to Ising-like interactions. The fundamental physics can be elucidated through a frustrated J1-J2 model related up-up-down-down spin chains. Our results shed light on the study of novel quantum spin dynamics in metallic spin chains.

References:

1. Quantum physics in one dimension, T. Giamarchi (Oxford University Press Inc., New York 2004).

2. A. Pandey, P. Miao, M. Klemm, H. He, H. Wang, X. Qian, J. W. Lynn, and M. C. Aronson*, “Correlations and incipient antiferromagnetic order within the linear Mn chains of metallic Ti4MnBi2”, Phys. Rev. B 102, 014406, (2020).

3. X. Y. Li†, K. Foyevtsova, A. Nocera, M. Oudah, D. Reig-i-Plessis, S. Priyadarshi, Y. P. Cai, K. M. Kojima, N. Murai, M. Kofu, K. Nakajima, M. Matsuura, H. Tamatsukuri, S. X. Chi, A. M. Hallas, A. M. Tsvelik, I. Zaliznyak, G. Sawatzky, M. C. Aronson*, “A dimer Ising-like antiferromagnetic chain”, (In preparation).

The 4th Asia-Oceania Conference on Neutron Scattering

M1. Contributed Talks

Abstract ID: 124

M1-CT1

Four-phonon induced anomalous thermal conductivity of GeTe

Presenter: Jiawang Hong (Beijing Institute of Technology)

Keywords: inelastic neutron scattering, thermal conductivity, four phonon scattering, first-principles

Four-phonon interaction plays an important role in the temperature dependent thermal conductivity of strong anharmonic materials. Here, the anharmonic phonon properties of a promising thermoelectric material candidate, α-GeTe, are investigated by the inelastic neutron scattering measurement and temperature dependent molecular dynamic simulation. The strong four-phonon interaction is observed at high temperature, which causes the deviation of the temperature dependent thermal conductivity from $\kappa L \sim T^{-1}$ rule. This work provides microscopic insight to the thermal transport of α-GeTe and demonstrates the important role of four-phonon interaction in solids at high temperature.

Abstract ID: 72

M1-CT2

Complex lattice dynamics and giant phonon anharmonicity in superionic argyrodites

Presenter: Qingyong Ren (Institute of High Energy, Chinese Academy of Sciences)

Keywords: Phonon anharmonicity, Superionic, Thermoelectric, Lattice thermal conductivity

The superionic state is a novel state of matter between the ordered crystalline and disordered liquid or molten states. Due to their good electrical properties and ultra-low lattice thermal conductivity, superionic materials are an excellent class of thermoelectric materials and have great application prospects in energy conversion [1]. Studying the underlying mechanism of its ultra-low lattice thermal conductivity is an important frontier topic in condensed matter physics and materials science. Currently, researchers have proposed many different explanations, but there is a lack of exact experimental support. On the other hand, due to their strong ion transport properties, superionic materials have also attracted much attention in energy storage as excellent solid electrolytes [2]. Nonetheless, a deep understanding of the lattice dynamics across the superionic phase transition remains elusive.

In this work, we systematically studied the microstructure, ion diffusion, and lattice dynamics of Ag8SnSe6, an argyrodite-type compound, through single crystal growth, synchrotron X-ray and neutron scattering techniques as well as machine-learned molecular dynamics simulations [3]. We identify a critical interplay of the vibrational dynamics of mobile Ag and a host framework that controls the overdamping of low-energy Ag-dominated phonons into a quasi-elastic response, enabling superionicity. Concomitantly, the persistence of long-wavelength transverse acoustic phonons across the superionic transition challenges a proposed ‘liquid-like thermal conduction’ picture. Rather, a striking thermal broadening of low-energy phonons, starting even below 50 K, reveals extreme phonon anharmonicity and weak bonding as underlying features of the potential energy surface responsible for the ultralow thermal conductivity and fast diffusion. Our results provide fundamental insights into the complex atomic dynamics in superionic materials for energy conversion and storage.

References:

[1] H. Liu, X. Shi, F. Xu, L. Zhang, W. Zhang, L. Chen, Q. Li, C. Uher, T. Day and G. J. Snyder, Nat. Mater. 11, 422 (2012).
[2] N. Kamaya, K. Homma, Y. Yamakawa, M. Hirayama, R. Kanno, M. Yonemura, T. Kamiyama, Y. Kato, S. Hama, K. Kawamoto and A. Mitsui, Nat. Mater. 10, 682 (2011).
[3] Q. Ren, M. K. Gupta, M. Jin, J. Ding, J. Wu, Z. Chen, S. Lin, O. Fabelo, J. A. Rodríguez-Velamazán, M. Kofu, K. Nakajima, M. Wolf, F. Zhu, J. Wang, Z. Cheng, G. Wang, X. Tong, Y. Pei, O. Delaire and J. Ma, Nat. Mater. 22, 999 (2023).

Abstract ID: 156

M1-CT3

Complex magnetic structures in EuPtAs

Presenter: Wu Xie (China Spallation Neutron Source CSNS)

Keywords: Noncentrosymmetric, Topological spin texture, Dzyaloshinskii–Moriya interaction

Topological spin textures (TSTs) such as magnetic skyrmion are interesting microscopic magnetic structure with both novel properties and great potential for applications [1]. While first popular in some transition-metal compounds such as MnSi [1,2], the search of TSTs in rare-earth compounds has become a hot topic in recent years. Firstly, a chiral cubic compound EuPtSi was found to host a complex field-temperature phase diagram in which a magnetic skyrmion phase [3] with different characteristics to that of MnSi was reported. Later on, a series of rare-earth based compounds have been reported to host TSTs with different mechanisms and characteristics, including GdPdSi and Gd3Ru4Al12 [4], CeAlGe [5], NdAlSi [6], etc.

We have recently characterized the physical properties and phase diagrams of EuPtAs with the NC polar structure, which is isostructural to CeAlGe [7,8]. Using the x-ray resonant magnetic scattering technique, we have studied the magnetic structures in different phases. Our results suggest that EuPtAs exhibits incommensurate magnetic structure below TN followed by a lock-in transition at TM. Together with the neutron diffraction measurements, our studies indicate noncollinear magnetic structures in EuPtAs at zero field, while the evidences for potential TST under magnetic fields have also been observed.

Reference:

[1] Nagaosa et al., Nat. Nanotechnol. 8, 899 (2013).
[2] S. Mühlbauer et al., Science 323, 915 (2009).
[3] C. Tabata, et al., J. Phys. Soc. Jpn. 88, 013702 (2019).
[4] T. Kurumaji, et al., Science 365, 914 (2019); Nat. Commun. 10, 5831 (2019).
[5] P. Puphal et al., Phys. Rev. Lett. 124, 017202 (2020).
[6] J. Gaudet et al. Nat. Mater. 10. 1038 (2021).
[7] G. Wenski et al., Z. Anorg. Allg. Chem 543, 49 (1986).
[8] W. Xie et al., Phys. Rev. B 104, 174425 (2021).

Abstract ID: 44

M1-CT4

$FeGe_{1-x}Sb_x$: a series of novel kagome metals with noncollinear antiferromagnetism

Presenter: Peng Cheng (Renmin University of China)

Keywords: Kagome metal, magnetic order, neutron diffraction, charge density wave

Kagome metal is an important material platform to explore correlated quantum states intertwined with topological band structures. Motivated by the recent discovery of charge density wave in a kagome lattice antiferromagnet FeGe [1], we investigate the impact of Sb doping on the structural, charge and magnetic order of FeGe. The charge density wave is rapidly suppressed by Sb doping (~1.5%) and the antiferromagnetic ordering temperature gradually shifts to 280 K for $FeGe_{0.7}Sb_{0.3}$. For $FeGe_{1-x}Sb_x$ with x > 0.1, new crystal structures with slightly distorted Fe kagome lattice are formed. Interestingly, using the XingZhi triple-axis spectrometer at China advanced research reactor (CARR), we have discovered that noncollinear antiferromagnetic (AFM) structures widely exists below TN in these kagome metals. These noncollinear magnetic orders could possibly be unconventional and resulted from the onsite repulsion and fillings conditions of kagome flat band, as predicted by a recent theoretical work.[2] Besides, noncollinear AFM order is important in realizing anomalous Hall effect and has been rarely observed in kagome metals besides Mn_3Sn material family. Therefore, our findings may stimulate numerous research interests in new kagome metals FeGe1−xSbx.

Reference:

[1] X. K. Teng et al., Nature 609, 490 (2022)
[2] Y.-P. Lin et al., arXiv:2307.11810 (2023)

Abstract ID: 31

M1-CT5

Studying magnetic-depth profile of FeRh films by polarized neutron reflectometry

Presenter: Sungkyun Park (Pusan National University, Busan, Korea)

Keywords: Antiferromagnetic, Polarized Neutron Reflectometry

FeRh exhibits a first-order metamagnetic phase transition from antiferromagnetic (AFM) to ferromagnetic (FM) around 370 K. Additionally, it undergoes a volume expansion of approximately 1% and a variation in electrical resistivity due to the increasing density of states at the Fermi level. Therefore, utilizing the near room-temperature phase transition characteristics in modern spintronic applications gets more attention due to advantageous AFM characteristics. To adapt device architecture, the interface characteristics of FeRh film are essential. Previously, it has been known that the pristine FeRh films exhibit residual ferromagnetism in the AFM state (i.e., below transition temperature). Therefore, it is disadvantageous to obtain magnetically clean interfaces owing to the formation of residual ferromagnetism at the interfaces.

In this presentation, we examined the temperature- and depth-dependent magnetic properties of DC-sputtered FeRh films to enhance our understanding of the residual ferromagnetism in the AFM state. Detailed polarized neutron reflectometry, X-ray diffraction, and cross-sectional microscope analysis were performed to examine the magnetic, structural, and chemical properties of FeRh film. As a result, we found non-uniform magnetic properties at the interfaces. Furthermore, each interface has magnetic characteristics that differ due to the different origin, such as interdiffusion and lattice mismatch.

This work is partly supported by NRF(RS-2023-00281671, RS-2023-00221154, 2023R1A2C1005252, and 2022M3H4A1A04085306) and KAERI.

Abstract ID: 82

M1-CT6

Probing the noncollinear interlayer coupling in NiFe/NiO/NiFe trilayers using polarized neutron reflectivity

Presenter: Xiaozhi Zhan (Institute of High Energy Physics)

Keywords: interlayer coupling, antiferromagnetic insulator, polarized neutron reflectivity, Monte Carlo simulations

The interlayer exchange coupling (IEC) in magnetic multilayers has attracted considerable attention since the discovery of giant magnetoresistance effect in ferromagnet (FM)/spacer/FM systems,[1] which sparked the development of spintronics.[2] The spacer could be nonmagnetic or antiferromagnetic. The latter suggests that the antiferromagnetic spin structure can play a crucial role in modifying interlayer coupling.[3] Moreover, antiferromagnets (AFMs) have emerged as key materials in spintronic devices due to their unique features compared to ferromagnets.[4] The propagation of spin currents through AFMs has a significant impact on spin transport properties and provides opportunities for the manipulation of SOT.[5] Therefore, investigating the role of AFMs in IEC of magnetic films is of great importance to advance the field of AFM spintronics.

Different types of AFM metal have been used as spacers, resulting in the observation of 90-degree IEC between FM layers.[6, 7] This phenomenon can be well explained within the proximity model, which assumes significant thickness fluctuation in the AFM spacer.[8] Furthermore, noncollinear coupling can also be observed in systems with an AFM insulator (AFMI), such as Fe_3O_4/NiO/Fe_3O_4,[9] NiFe/NiO/Co,[10] Fe/NiO/Fe,[11] Co/NiO/Fe [12]. A. Brambilla et al. argued that the proximity model cannot reproduce the magnetization behaviors in FM/AFMI/FM system, where a significant contribution of interface direct exchange couplings is expected 11. Due to the difficulty in directly characterizing the AFM spin structures, there are still controversies in understanding the mechanism of noncollinear IEC across AFMI layer. 9-10,12

We investigated the interlayer coupling and magnetization reversal behaviors in NiFe/NiO/NiFe trilayers using polarized neutron reflectivity and Monte Carlo (MC) simulations. Our results reveal that the shape of NiFe loops transitions from square to tilted as the NiO thicknesses decrease, indicating changes in the direction of NiFe layer's easy axis. This phenomenon can be attributed to variations occurring at NiO/NiFe interfaces for different NiO layer thicknesses. With thin NiO layer, interdiffusion at the NiO/NiFe interfaces leads to frustrated coupling, resulting in a noncollinear interlayer coupling. This observation is supported by MC simulations. Conversely, hardly any coupling frustration is observed for the sample with a thick NiO layer. Our findings propose a novel way to tailor the interlayer coupling through interface engineering.

References:
[1] Grunberg P., Schreiber R., Pang Y., Brodsky M. B. and Sowers H. 1986 Phys. Rev. Lett. 57, 2442-2445.
[2] Baibich M. N., Broto J. M., Fert A., Vandau F. N., Petroff F., Eitenne P., Creuzet G., Friederich A. and Chazelas J. 1988 Phys. Rev. Lett. 61, 2472-2475.
[3] Liu Z. Y. and Adenwalla S. 2003 Phys. Rev. Lett. 91.
[4] Jungwirth T., Marti X., Wadley P. and Wunderlich J. 2016 Nat Nanotechnol 11, 231-241.
[5] Zhu R., Shang T., Hu S., Zhang Y. Y., Qiu X. P., Cheng W. J., Jiang D. M. and Zhan Q. F. 2020 J. Magn. Magn. Mater. 512, 167042.
[6] Filipkowski M. E., Krebs J. J., Prinz G. A. and Gutierrez C. J. 1995 Phys. Rev. Lett. 75, 1847-1850.
[7] Adenwalla S., Felcher G. P., Fullerton E. E. and Bader S. D. 1996 Phys. Rev. B 53, 2474-2480.
[8] Slonczewski J. C. 1995 J. Magn. Magn. Mater. 150, 13-24.
[9] van der Heijden P. A. A., Swuste C. H. W., de Jonge W. J. M., Gaines J. M., van Eemeren J. T. W. M. and Schep K. M. 1999 Phys. Rev. Lett. 82, 1020-1023.
[10] Camarero J., Pennec Y., Vogel J., Bonfim M., Pizzini S., Ernult F., Fettar F., Garcia F., Lancon F., Billard L., Dieny B., Tagliaferri A. and Brookes N. B. 2003 Phys. Rev. Lett. 91, 027201.
[11] Brambilla A., Biagioni P., Portalupi M., Zani M., Finazzi M., Duo L., Vavassori P., Bertacco R. and Ciccacci F. 2005 Phys. Rev. B 72, 174402
[12] Wu J., Choi J., Scholl A., Doran A., Arenholz E., Wu Y. Z., Won C., Hwang C. Y. and Qiu Z. Q. 2009 Phys. Rev. B 80, 012409.

Abstract ID: 73

M1-CT7

Field induced phase transitions in $NiNb_2O_6$ single crystal

Presenter: Arpita Rana (Banaras Hindu university Varanasi)

Keywords: field induced phase transition, Ising spin chain

We present the structural, magnetic and thermodynamic properties of High-quality $NiNb_2O_6$ single crystals that are grown by self-growth technique. The room temperature X-ray powder diffraction refinement of crushed single crystals confirms the columbite structure which consists of a zigzag Ising spin chain of magnetic Ni ions along the c axis. $NiNb_2O_6$ shows an antiferromagnetic order below 5.7 K. Furthermore, field-induced phases are observed along the axis. The H-T phase diagram is made from the magnetic susceptibility χ and specific heat capacity. The analysis of C_P reveals the presence of short-range magnetic correlation above T_N.

Abstract ID: 112

M1-CT8

Neutron diffraction studies of a spin supersolid candidate with giant magnetocaloric effect

Presenter: Wentao Jin (School of Physics, Beihang University, Beijing 100191, China)

Keywords: single-crystal neutron diffraction, spin supersolidity, magnetocaloric effect

Supersolidity constitutes an exotic quantum state of matter with intertwined solid and superfluid orders. Although proposed for long in theory, such a state remains elusive in condensed matter. Here we discover a giant magnetocaloric effect that reflects a magnetic analogue of the supersolid in the triangular-lattice antiferromagnet $Na_2BaCo(PO_4)_2$. The demagnetization cooling process has revealed two prominent valley-like regimes, with the lowest accessible temperature attaining below 100 mK from the initial temperature of 2 K and under a field change of 2.5 T. Not only the experimentally determined series of critical fields but also the demagnetization cooling profile show excellent agreement with the theoretical simulations based on the easy-axis triangular lattice Heisenberg model. We further locate the proposed spin supersolid phases through neutron diffraction measurements, which reveal the coexistence of three-sublattice solid ordering and interlayer incommensurability indicative of the spin superfluid ordering. Our results indicate a strong entropic effect of the spin supersolid phase and related quantum phase transitions, paving thus a viable way for its applications in sub-Kelvin refrigeration.

Abstract ID: 203

M1-CT9

Single-crystal neutron diffraction of frustrated quasi-two-dimensional magnets

Presenter: Hao Deng (Shanghai Tech University)

Keywords: frustrated, Single-crystal diffraction

Frustrated magnetic structures are configurations in which localized magnetic spins interact through competing exchange interactions, leading to a macroscopic degeneracy and giving rise to exotic phenomena. Frustrated magnetism offers excellent opportunities for discovering new states and properties of matter, making it a highly active research field. Neutron scattering is one of the most powerful tools for studying magnetic structures and dynamics because it enables the measurement of energy and momentum of incoming and outgoing neutrons. In this report, several examples of applications in resolving frustrated systems will be presented, including the discovery of the Kagome Spin Ice state in quasi-two-dimensional lattices using single-crystal neutron diffraction [1], the ability to control the length scale of spin correlations by tuning external magnetic fields [2], and the revelation of the absolute direction of the Dzyaloshinskii-Moriya interaction (DMI) in weak ferromagnets [3].

Reference:

1. K. Zhao#, H. Deng#, H. Chen#, K. A. Ross, V. Petříček, G. Günther, M. Russina, V. Hutanu, P. Gegenwart “Realization of the kagome spin ice state in a frustrated intermetallic compound”, Science, 367 (6483), 1218-1223 (2020)

2. Y. Li, S. Bachus, H. Deng, W. Schmidt, H. Thoma, V. Hutanu, Y. Tokiwa, A. A Tsirlin, P. Gegenwart, “Partial Up-Up-Down Order with the Continuously Distributed Order Parameter in the Triangular Antiferromagnet TmMgGaO4” Physical Review X, 10 (1), 011007 (2020)

3. H. Thoma, V. Hutanu, H. Deng, V. E. Dmitrienko, P. J. Brown, A. Gukassov, G. Roth, and M. Angst*, “Revealing the absolute direction of the Dzyaloshinskii-Moriya interaction in prototypical weak ferromagnets by polarized neutrons”, Physical Review X, 11, (1), 011060(2021)

Abstract ID: 50

M1-CT10

Coexisting magnons and fractionalized spin excitations in partially magnetized quantum spin liquid candidate $NaYbSe_2$

Presenter: Zhen Tao (Beijing Normal University)

Keywords: Quantum spin liquid, spin excitation, inelastic neutron scattering

Quantum spin liquids (QSLs) are exotic, highly-entangled quantum states with fractionalized elementary excitations, in which localized spins remain disordered but long-range correlated even at absolute zero temperature due to strong quantum fluctuations, forming liquid-like states. $NaYbSe_2$ single crystal, which resembles a perfect triangular-lattice antiferromagnet without intrinsic disorder, has been suggested to be a QSL candidate. Previous neutron scattering experiments on $NaYbSe_2$ supported the ground state of NaYbSe2 is a QSL with a spinon Fermi surface [1]. Moreover, the H-T phase diagram is highly anisotropic and includes different quantum phases expected for a triangular-lattice antiferromagnet, which classifies $NaYbSe_2$ as a unique model system [2]. We use inelastic neutron scattering to study the magnetic excitation of $NaYbSe_2$ under multiple magnetic fields. The spectrum reveals a clear X-shaped excitation boundary occurs at the Γ point. As the magnetic field increases to 8.8 T, a spin wave peak appears at the Γ point and almost reaches the same energy scale as the spinon continuum. Overall, our results systematically provide spin excitation spectrum for different quantum phases and present the coexistence of magnons and fractionalized spin excitations in partially magnetized quantum spin liquid candidate $NaYbSe_2$.

Reference:

[1] P.-L. Dai et al., Spinon Fermi Surface Spin Liquid in a Triangular Lattice Antiferromagnet NaYbSe2, Phys. Rev. X 11, 021044 (2021).

[2] K. M. Ranjith et al., Anisotropic field-induced ordering in the triangular-lattice quantum spin liquid NaYbSe2, Phys. Rev. B 100, 224417(R) (2019).

Abstract ID: 16

M1-CT11

Neutron Diffraction of Quasi-two-dimensional Honeycomb and Triangular Lattice Frustrated Magnets

Presenter: Alexander Kurbakov (Petersburg Nuclear Physics Institute, NRC Kurchatov Institute, Gatchina, Russia)

Keywords: Quasi-two-dimensional magnetism, frustrated magnets, honeycomb and triangular sublattice

This work is devoted to one of the most relevant areas in modern condensed matter physics: the study of the magnetism of layered oxides with exchange or geometric frustrations characteristic of honeycomb ($A_3M_2SbO_6$, $A_2M_2TeO_6$) and trigonal ($MSnTeO_6$, A_2MTeO_6, A_2MXO_4) superstructure of magnetic ions. The structure and static and dynamic magnetic properties were studied comprehensively both experimentally (neutron powder diffraction, magnetization, specific heat, dielectric permittivity, and ESR techniques) and theoretically by means of ab initio DFT calculations within the spin-polarized generalized gradient approximation. Long-range magnetic ordering and short-range spin correlations were studied by unpolarized and polarized neutron scattering. Symmetry and subsequent full-profile analysis of neutron data revealed the model of the ground state spin structures. It is established that the type of spin ordering in layered magnets with a honeycomb lattice is extremely sensitive to the initial atomic composition. Zigzag-type spin structures were proposed for $Li_3Ni_2SbO_6$ and $Na_3Co_2SbO_6$, but with significant differences in the zigzag type. The ground state of the magnetic subsystem in $Na_3Co_2SbO_6$ is described by a superposition of two propagation vectors k and corresponds to a complex non-collinear magnetic structure. The spin structure of $Li_3Co_2SbO_6$ is not zigzag-type and can be represented as FM honeycomb layers AFM coupled to each other. The magnetic ground state of MnSnTeO6 has a complex nature, is formed as a result of frustrations and is described by a set of cycloids (k = (0, 0, 0.183). Magnetic structure in Na_2MnTeO_6 is commensurate 120º spin helix with k = (1/3, 1/3, 1/3) in variance with planar spin structure in structurally equivalent Li_2MnTeO_6 with k = (1/3, 1/3, 0). Thus, a comparative study of Na_2MnTeO_6 and Li_2MnTeO_6 has revealed an important aspect of the effect of interlayer coupling on magnetism in layered quasi-two-dimensional magnets.

Abstract ID: 214

M1-CT12

Anisotropic exchange coupling, ground state, and magnetic field effect of Kitaev compound YbOCl

Presenter: Zheng ZHANG (Institute of Physics, Chinese Academy of Sciences)

Keywords: Rare-earth chalcohalide, Kitaev model, anisotropic exchange coupling, ground state, magnetic field effect

Rare-earth chalcohalide *RE*Ch*X* (*RE* = rare earth; Ch = O, S, Se, Te; *X* = F, Cl, Br, I) is a newly reported family of Kitaev compound. The family offers a platform where a strong spin-orbit coupling meets a van der Waals layered and undistorted honeycomb and triangular spin lattices, which outputs highly anisotropic exchange couplings required by the Kitaev model. YbOCl is the first single crystal of the family we grew, with a size up to ~15 mm. We have performed magnetization and high magnetic field electron spin resonance measurements from 2 to 300 K. We develop the mean-field scenario for the anisotropic spin system, with which we are able to well describe the experiments and reliably determine the fundamental parameters. Through comprehensive thermodynamic and neutron scattering measurements down to 50 mK, we have identified a 120°-ordered antiferromagnetic phase below 1.3 K. With the experiments under magnetic fields, we are able to establish a magnetic field-temperature phase diagram around the spin ground state. The most unusual finding is that a relatively small magnetic field (~ 0.1 - 2 T) significantly enhances quantum spin fluctuations in the ground state. The observation is consistent with the dominant Kitaev interaction and points to a spin-liquid-like behavior. The present study offers new insights into the highly anisotropic spin systems and opens alternative avenues for exploring Kitaev spin physics.

Abstract ID: 205

M1-CT13

Phase transitions and unusual excitations in selected strongly-correlated *f* electron compounds

Presenter: Benqiong LIU (Chinese Academy of Environmental Planning)

Strongly-correlated *f* electron compounds represent an ideal testing ground for the study of novel ground states such as unconventional superconductivity, magnetic ordering, Fermi-liquid. These systems also show multiple degrees of freedom like spin, orbit, and lattice; where phonons, low-lying magnetic or crystal electric field (CEF) excitations share close energies. In this presentation, we will briefly introduce our recent study of phase transitions and unusual excitations in selected strongly-correlated f electron materials, e.g., magnetic phase transition in $CeSb_2$ [1] $CeAuGa_3$ [2] and U_3O_8 [3] at low temperature, phase transition confirmed in $CeAl_2$ under high pressure, [4] and two distinct magneto-elastic hybrid excitations observed in $CeAuAl_3$ (a CEF-phonon bound state, and anticrossing of the low-energy CEF with acoustic phonons at zero magnetic field).[5, 6]

References:

[1] B. Liu*, L. Wang, I. Radelytskyi, et al., J. Phys.: Condens. Matter 32, 405605 (2020)

[2] B. Lv, B. Liu*, Nucl. Anal. 1, 100002 (2022)

[3] B. Lv, Y. Xia, S. Hu, B. Liu*, Phys. Scr. 98, 075921 (2023)

[4] Y. Cheng, R. He, Y. Xia, T. Han, L. Fang*, S. Huang, B. Liu§, Phys. Rev. B 105, 064102 (2022)

[5] B. Liu*, P. Čermák, C. Franz, et al., Phys. Rev. B 98, 174306 (2018)

[6] P. Čermák, A. Schneidewind, B. Liu, et al., PNAS 116, 6695-6700 (2019)

Abstract ID: 202

M1-CT14

Magnetic structure and spin wave measurement on rare-earth orthochromite $TbCrO_3$

Presenter: Kaitong SUN (University of Macau)

Keywords: magnetic structure, spin wave measurement, rare-earth orthochromite

Rare-earth orthochromites exhibit intriguing physical properties, making them captivating subjects for advanced functional materials and spintronic devices. In this study, we employed neutron powder diffraction (NPD) and inelastic neutron scattering (INS) techniques to explore the magnetic structure as well as the spin wave dispersion in rare-earth orthochromite material $TbCrO_3$. Our research aims to solve the magnetic structure dominated from Cr^{3+} ions and unravel the spin correlation function between Cr^{3+} - Cr^{3+} ions.

We conducted our research using state-of-the-art neutron instruments at two world-class facilities: neutron powder diffraction experiments at GPPD, CSNS, and inelastic neutron scattering studies at 4SEASONS, J-PARC. Through neutron powder diffraction, we determined that orthorhombic $TbCrO_3$ exhibits a G-type antiferromagnetic ordering along the c-axis. Additionally, the inelastic neutron scattering study allowed us to simulate the spin wave dispersion along the full Brillouin zone using linear spin wave theory. This simulation enabled us to derive the antiferromagnetic Heisenberg Hamiltonian, extracting vital magnetic exchange parameters J1 and J2 for nearest and next-nearest neighbors, Dzyaloshinskii–Moriya interactions, and single-ion anisotropy.

The insights gained from this study provide valuable information for understanding the magnetic behavior in rare-earth orthochromites. The knowledge gained from this research contributes to the advancement of both fundamental and applied research in the field of strongly correlated electron systems and lays the foundation for future studies exploring the rich magnetic phenomena in rare-earth orthochromites.

The 4th Asia-Oceania Conference on Neutron Scattering

Scientific Parallel Session M2. Materials Science and Chemistry

M2. Keynote Talks

Abstract ID: 47

M2-KT1

Structural studies of solid-state ionic conductors at the limits of diffraction and beyond

Presenter: Chris Ling (The University of Sydney, Australia)

Keywords: ionic conductors, QENS, diffraction, dynamics

The structures of solid-state ionic conductors are a compromise between long-range (and hence long-term) lattice stability and short-range coordinative flexibility. To rationally design improved versions for applications such as fuel cells and batteries, we need to understand how this compromise is reached. Diffraction methods alone are inadequate – whether using X-rays or neutrons, *ex-situ* or *operando*, conventional crystallography or total scattering analysis – because of their dynamic nature. The time-averaged structure is not the whole story. In this talk I will show how we use experimental X-ray and neutron spectroscopy, and computational structure and dynamics calculations, to supplement diffraction when studying solid-state oxide, proton and lithium ionic conductors. We can then validate the insights gained by making targeted chemical modifications and testing their effects on structure and functional physical properties.

Abstract ID: 52

M2-KT2

Microscopic and mesoscopic understanding of magnetization reversal phenomenon by neutron diffraction and neutron depolarization

Presenter: Amit KUMAR (Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India)

Keywords: magnetization reversal, neutron diffraction, neutron depolarization

The phenomenon of magnetization reversal or negative magnetization (NM) in magnetically ordered systems, where it does not arise due to diamagnetism, is defined as a crossover of dc magnetization from a positive value to a negative value below the magnetic ordering temperature. We have extensively investigated the technologically important magnetization reversal phenomenon in spinels, garnets, perovskites, molecular magnets, and intermetallic compounds, and revealed a microscopic (atomic level) as well as mesoscopic (magnetic domain length scale) understanding of the phenomenon using neutron scattering [1-6]. We have written a very first and comprehensive review [3] on the subject covering all physics-related aspects of the phenomenon and its implications in magnetic memory, magneto-caloric and spin resolving devices. The understanding of magnetization reversal has been further strengthened by revealing a direct correlation between the phenomenon and other important physical properties, such as exchange bias (EB) reversal, crystal structure modulations, and magneto-electric effect by employing neutron scattering [7-16].

In my talk, some of our recent results will be presented. Special attention will be focused on importance of neutron diffraction and neutron depolarization techniques in realizing atomic level understanding of negative magnetization. We have obtained a physics understanding of the NM and EB phenomena and their correlations in the negative magnetization materials belonging to perovskites and intermetallic compounds. Particularly, anomalous behavior of EB has been correlated to the temperature/magnetic-field induced spin reorientation phenomenon. Implications of the results on electrical properties will also be discussed to highlight the intercorrelated structural, magnetic, and electrical properties of these materials.

Reference:

[1] A. Kumar et al., Phys. Rev. Lett. 101, 207206 (2008).

[2] S. M. Yusuf, A. Kumar et al., Appl. Phys. Lett. 95, 182506 (2009).

[3] A. Kumar et al., Physics Reports 556, 1- 34 (2015).

[4] A. Kumar et al., Phys. Rev. B 96, 014427 (2017).

[5] A. Kumar et al., J. Appl. Phys. 121, 223903 (2017).

[6] A. Kumar et al., Physica B 551, 104 (2018).

[7] M. Ghanathe, A. Kumar et al., J. Appl. Phys. 125, 093903 (2019).

[8] MY Yang, S Seong, E Lee, M Ghanathe, A. Kumar et al., Appl. Phys. Lett. 116, 252401 (2020).

[9] Deepak, A. Kumar et al., J. Appl. Physics 127, 213903 (2020).

[10] M. Ghanathe, A. Kumar et al. J. Magn. Magn. Mater. 523, 167632 (2021).

[11] Deepak, A. Kumar et al., Phys. Rev. Mater. 5, 124402 (2021).

[12] Deepak, A. Kumar et al., Phys. Rev. Mater. 6, 074405 (2022).

[13] M. Ghanathe, A K Bera, A. Kumar et al., ACS Appl. Electron. Mater. 4, 394 (2022).

[14] M. Ghanathe, A. Kumar et al., J. Magn. Magn. Mater. 561, 169689 (2022).

[15] Deepak, A. Kumar et al., J. Phys.: Condens. Matter 35 065802 (2023).

[16] P. S. Patnaik, A. Kumar et al., Phys. Rev. B 108, 014438 (2023

Abstract ID: 92

M2-KT3

The preparation and irradiation effect of advanced materials for spallation/fusion materials

Presenter: Wen YIN (Institute of High Energy Physics, Chinese Academy of Sciences, China)

Keywords: spallation/fusion materials, irradiation effect, hetero-interfaces, helium bubbles

The structural materials used in fusion and target materials in spallation neutron sources need to endure much higher temperatures, higher neutron doses and extremely corrosive environment. Meanwhile, abundant helium atoms are generated by high-energy nuclear reaction. Hence, the development of advanced radiation tolerance and corrosion resistant materials is important. For the development of advanced radiation tolerance, one of the most promising strategies is to improve the sink strength of material by inducing hetero-interfaces (such as nanocomposites) and/or to seek a material with higher sink strength (such as metallic glasses). Here, the helium irradiation effect of multilayered nanocomposites with different interfaces structure and metallic glasses is investigated. The result shows that the nanocomposites are stable under ~ 1 DPA (Displacement Per Atoms). After helium irradiation, the helium enriched sublayers are formed at BCC/FCC interface in W/Ni nanocomposites, but not found in BCC/BCC interface (W/Ta nanocomposites). Compared with traditional metals, the metallic glasses with abundant free volume possess better radiation tolerance. But the helium bubbles are also formed at 10000 appm/dpa. Meanwhile, the soften of the metallic glasses are present at low irradiation dose. It is interesting that the combination of amorphous structure and hetero-interfaces (a CAC-type nanocomposite) present excellent swelling resistance under irradiation.

In order to improve the corrosion resistant of tungsten (target material), a Tantalum (Ta) coated tungsten (W) targets were prepared by hot isostatic pressure (HIP) diffusion welding. Here, the preparation technology, mechanical properties and diffusion behavior at W-Ta interface are investigated. The results show that, obvious diffusion layer was found at W-Ta interface during diffusion welding of W and Ta. And the thickness of the diffusion layer increases as the HIP temperature increase. More, the W–Ta layers were well bonded with the tensile strength of ~70 MPa.

Abstract ID: 142

M2-KT4

Hydride ion conducting materials

Presenter: Genki Kobayashi（RIKEN,Japan）

Keywords: hydride ion conductor, solid electrolyte, solid-state ionics

Hydride ions (H^-) are attractive mobile ions in terms of fast ion conduction in solids because of their inherent characteristics of monovalent, moderate size, and high polarizability. In addition, its strong reducing ability (–2.23 V vs. SHE) is potentially effective for high reactivity in energy (material) conversion and energy density in batteries. In 2016, we reported the first solid electrolyte, a series of La-Sr-Li oxyhydrides with the K_2NiF_4-type structure [1], with pure H– conductivity and have since developed H^- conducting materials, including solid electrolytes and electrodes. Recently, we found H^- conductors that exhibit high conductivity above 10 mS/cm [2-4], which is the standard for practical performance.

In this talk, I present the progress of our material development and the prospects for device applications.

Reference:

[1] G. Kobayashi et al., Science, 351, 1314 (2016).

[2] F. Takeiri, A. Watanabe, G. Kobayashi et al., Nat. Mater., 21, 325 (2022).

[3] K. Okamoto, G. Kobayashi et al., Adv. Sci., 10, 2203541 (2023).

[4] K. Okamoto, G. Kobayashi et al., J. Mater. Chem. A, 10, 23023 (2022).

The 4th Asia-Oceania Conference on Neutron Scattering

M2. Invited Talks

Abstract ID: 177

M2-IT1

Magnetic structure in kagomé magnets and Invar phenomenon

Presenter: Xianran Xing (Institute of Solid State Chemistry, University of Science and Technology Beijing, Beijing, 100083, China)

Keywords: Kagomé magnets, Invar phenomenon

The Invar anomaly is a century-old enigma arising from isotropic spin-lattice coupling in face-centered cubic lattice. In this work, we extend the Invar behavior to kagomé analogue with single magnetic element Fe by utilizing thermodynamic phase stability rather than by altering chemical composition. On transforming from hexagonal to cubic symmetry, the magnetic ordering changes from antiferromagnetic to ferromagnetic. Due to resulting in lifting of the interplanar magnetic frustration, magnetic ordering is enhanced which enables strong temperature-induced longitudinal spin fluctuations, leading to large magnetic compensation for lattice thermal expansion. Outcome from this work demonstrates the interplanar spin-lattice correlation in a cubic symmetry and will be essential to insight into the nature of Invar anomaly.

References:

[1] P. Mohn, A century of zero expansion. Nature, 400, 18-19 (1999).

[2] Q. Li, K. Lin, Z. Liu, L. Hu, Y. Cao, J. Chen, and X. Xing, Chem. Rev., 122, 8438 (2022).

[3] Y. Cao, S. Khmelevskyi, Q. Li, K. Lin, X. Xing, Phys. Rev. Lett., 127, 055501 (2021).

Abstract ID: 175

M2-IT2

Magnetic structures of two-dimensional (2D) van der Waals (vdW) antiferromagnetic(AFM) magnets

Presenter: Jinbo Yang (Peking University)

Keywords: Magnetic structure, neutron diffraction, spin-lattice interaction

Two-dimensional (2D) van der Waals (vdW) antiferromagnetic(AFM) magnets with novel magnetism and good stability provide an ideal platform for conducting fundamental research and developing spintronic devices. In recent work, the AFM structures of $CrPS_4$ and *MOX* (*M* = Cr, Dy; *X* = F, Cl, Br) were determined using neutron diffraction. The spin-lattice coupling effects were investigated using magnetic torque, structural and magnetic measurements under high pressure, first-principles calculations, etc. $CrPS_4$ possesses an A-type AFM ground state with a propagation vector k = (0, 0, 1/2), whose magnetic moment lies in the ac plane with a small deviation of 8.94° from the c axis. The weak interlayer coupling between neighboring monolayers and low magnetic anisotropy energy shows a relatively small spin-flop field and low canted-antiferromagnetism-to-ferromagnetism threshold. Applying hydrostatic pressure decreases the spin reorientation and magnetic transition temperature due to the shrinkage of the quasi-one-dimensional CrS_6 chains along the b-axis and the suppressed intralayer ferromagnetic exchange coupling, respectively. In another Cr-based vdW compound, CrOCl, we found the AFM order with a fourfold magnetic superstructure (k = (0, 1/4, 0)) at low temperatures. The ordered magnetic moment is parallel to the c-axis, the magnitude of which is modulated. The AFM to-ferrimagnetic (FiM) metamagnetic transitions (MTs) of few-layer CrOCl are revealed to be triggered by collective magnetic moment flipping rather than the established spin-flop mechanism when external magnetic field (H) enforces a lattice reconstruction interlocked with the five-fold periodicity of the FiM phase. Compared with the above transition-metal-based vdW materials, the 4*f*-electron magnetism of rare-earth vdW materials shows stronger magnetic dipolar interactions and larger magnetic moments. In the DyO*X* (*X* = F, Cl, Br) compounds, the ordered moments are about 10 μB / Dy3+ at low temperatures, almost the same as the saturation moment of a free Dy^{3+}. The DyOF compound crystallizes in $R\bar{3}m$ and becomes antiferromagnetic at TN = 3.7 K with k = (0, 0, 3/2) where the magnetic moments remain *ab* inplane. However, the DyOBr compound crystallizes in *P*4/*nmm* and becomes antiferromagnetic at TN = 9.6 K with k = (0, 0, 0) where the magnetic moments remain in the direction of c axis, which is similar to DyOCl compounds due to the same crystal structure. Furthermore, there are no remarkable changes occur to antiferromagnetic transition temperature in DyO*X* (*X* = F, Cl, Br) compounds when a moderate hydrostatic pressure ($p \leq 1.0$ GPa) is applied, suggesting strong lattice stability in the rare-earth vdW materials. Exploring novel anenter code heretiferromagnetic ground states in the above vdW materials helps study two-dimensional magnetism and further design high-density and stable antiferromagnetic memory devices.

Abstract ID: 77

M2-IT3

Studies of hydrogen bonds in functional molecular crystals by single-crystal neutron diffraction at SENJU

Presenter: Takashi Ohhara (J-PARC Center, Japan Atomic Energy Agency)

Keywords: J-PARC, SENJU, Molecular crystal, Hydrogen bond

Hydrogen bonds in molecular crystals are one of the research areas extensively investigated by the single-crystal neutron diffraction technique. Traditionally, various types of hydrogen bonds in relatively small organic molecules or molecular complexes have been analyzed to investigate the nature of the hydrogen bond itself by single-crystal neutron diffraction. On the other hand, recent improvements in neutron sources and single-crystal neutron diffractometers make single-crystal neutron structural analyses of molecular functional crystals in which hydrogen bonds have crucial rules in their functions possible. Even though such molecular functional crystals tend to be made from relatively large molecules or molecular complexes and have small crystal volumes, state-of-the-art diffractometers can measure single-crystal diffraction data of those crystals within the realistic beam time.

SENJU, a time-of-flight Laue-type single-crystal neutron diffractometer at J-PARC, is one of the world's limited single-crystal neutron diffractometer capable of measuring a sub-millimeter size molecular crystal [1]. In this presentation, the authors will show what kind of structural research of hydrogen bonds in functional molecular crystals, e.g., proton transfers in temperature-induced spin-transfer metal complexes [2] and a salt-cocrystal continuum formation in a photo-functional organic crystal [3], conducted at SENJU.

References:

[1] T. Ohhara, R. Kiyanagi, K. Oikawa, T. Kawasaki, I. Tamura, A. Nakao, T. Hanashima, K. Munakata, T. Moyoshi, T. Kuroda, H. Kimura, T. Sakakura, C-. H. Lee, M. Takahashi, K. Ohshima, T. Kiyotani, Y. Noda, M. Arai, (2016). J. Appl. Cryst., 49, 120.

[2] T. Nakanishi, Y. Hori, Y. Shigeta, H. Sato, S-. Q. Wu, R. Kiyanagi, K. Munakata, T. Ohhara, O. Sato, (2023). Phys. Chem. Chem. Phys., 25, 19394.

[3] Y. Yano, T. Ono, T. Ohhara, Y. Hisaeda, (2021). Chem. Eur. J., 27, 17802.

Abstract ID: 204

M2-IT4

Overview and recent development of PLANET: high-pressure neutron diffractometer at MLF, J-PARC

Presenter: Asami Sano-Furukawa (JAEA)

Keywords: High pressure, High temperature

PLANET is a dedicated beamline for high-pressure at MLF J-PARC, which realizes neutron diffraction experiments under extreme conditions. The beamline is equipped with precise optics, including incident slits and radial collimators, to obtain high-quality data from a small sample in a high-pressure device. Various high-pressure sample environments are available depending on the purpose of the research. The 6-axis multi-anvil press allows routine high-temperature experiments under pressures up to 10 GPa. The pressure range has been extended to over 20 GPa by applying a Kawai-type cell to study iron hydrides, which are particularly important in geophysics. With its newly designed anvil, the Paris-Edinburgh press has extended the pressure range greatly to 40 GPa. The MITO system, which can freely change load at low temperatures, has been particularly effective in studying ice and has contributed to discovering new phases. In this talk, recent technical developments at PLANET and highlight results from user applications will be presented.

Abstract ID: 101

M2-IT5

Neutron scattering study on the phonon spectra of the low thermal conductivity systems

Presenter: Jie Ma (Shanghai Jiao Tong University)

Keywords: Neutron scattering, Thermoelectricity, Low thermal conductivity, Anharmonicity

Due to the promising energy conversion and storage properties, the thermoelectric material has attracted a lot of attention in both scientific research and industrial production. Recently, the "Phonon-Glass Electron-Crystal" approach has been suggested and different methods have been applied to obtain the low lattice thermal conductivity, such as electron-phonon interaction, anharmonicity, phonon folding, etc. The Ag_9GaSe_6-family is a perfect thermoelectric system as an alloy with wooden-like thermal conductivity. However, more details are still missed owing to limited experimental and theoretical studies of atomic dynamics. Here, we performed experiments on recently reported argyrodite-type Ag_8SnSe_6 single crystal with state-of-the-art synchrotron X-ray diffraction, single-crystal neutron diffraction, single-crystal/powder inelastic neutron scattering and quasi-elastic neutron scattering techniques, complemented with large-scale first-principle modeling using machine-learned molecular dynamics. The momentum and energy resolved scattering measurements and simulations enable us to comprehensively map the microscopic correlations of atoms responsible for bulk transport properties. It reveals that the superior thermal transport properties originate from the extremely soft chemical bonds and colossal anharmonic potential energy landscape. Unveiling the essential roles of atomic dynamics should be crucial for further improving the performance of existing materials or designing future materials.

Abstract ID: 160

M2-IT6

Neutron measurement and analysis with machine learning

Presenter: Kanta Ono（Osaka University）

Keywords: Data analysis, Machine learning

Advanced characterization using quantum beams is used in many natural science fields, from condensed matter physics to life sciences, and has become an indispensable tool in scientific research. However, there are problems in measurement and analysis using quantum beams, such as the effective use of limited beamtime in neutron facilities. Solving these problems is necessary for further progress in scientific research. We are promoting efficient, automated, and autonomous neutron measurement and analysis using data science to solve these problems. These research fields are called measurement informatics and are being developed through advances in data science, as well as recent advances in computational resources, and are expected to:

1. enable the optimization and improvement of the efficiency of neutron measurement and analysis.

2. enable observation of previously unobservable phenomena through data sciences.

The research and development of measurement informatics related to quantum beams will make it possible to realize advanced measurements by data science without significant hardware upgrades. The key to the next generation of quantum beam measurement will be using data science to achieve advanced measurements. Autonomous measurement and data analysis will be essential for the next generation of quantum beam measurement.

We will introduce the following topics by integrating X-ray measurement, analysis, and data science.

1) Automatic design of an optimal experiment [1].

2) When should experiments stop [2]?

3) Speed up neutron measurements with data science [3]?

4) Automating data analysis: crystallography and spectroscopy [4,5,6].

5) Decision-making in data analysis [7].

6) Cartography of inorganic materials using crystal structure [8].

References:

[1] Ueno, T., Hino, H., Hashimoto, A., Takeichi, Y., Sawada, M. & Ono, K. (2018). npj Computational Materials 4, 4.

[2] Ueno, T., Ishibashi, H., Hino, H. & Ono, K. (2021). npj Computational Materials 7, 139.

[3] Saito, K., Yano, M., Hino, H., Shoji, T., Asahara, A., Morita, H., Mitsumata, C., Kohlbrecher, J. & Ono, K. (2019). Sci. Rep. 9, 1526.

[4] Suzuki, Y., Hino, H., Kotsugi, M. & Ono, K. (2019). npj Computational Materials 5, 39.

[5] Ozaki, Y., Suzuki, Y., Hawai, T., Saito, K., Onishi, M. & Ono, K. (2020). npj Computational Materials 6, 75.

[6] Suzuki, Y., Hino, H., Hawai, T., Saito, K., Kotsugi, M. & Ono, K. (2020). Sci. Rep. 10, 21790.

[7] Matsumoto, M., Hawai, T. & Ono, K. (2020). Phys. Rev. Applied 13, 064028.

[8] Suzuki, Y., Taniai, T., Saito, K., Ushiku, Y. & Ono, K. (2022). Mach. Learn.: Sci. Technol. 3, 045034.

Abstract ID: 87

M2-IT7

Investigation on the structural properties of cathode materials based on neutron scattering methods

Presenter: Yinguo Xiao (Peking University Shenzhen Graduate School)

Keywords: Cathode materials, Structural properties, Neutron diffraction

Although the research on the cathode materials for lithium-ion batteries has attracted extensive interest, the deep understanding on their structural properties and the insight into their structural evolution are still lack. By taking advantages of sensitive, penetrative and nondestructive properties of neutrons, we adopted *ex-situ* and *in-situ* neutron diffraction techniques to explore the structural characteristics of cathode materials, especially the structural evolution of cathodes during cycling in real time. It is revealed that Li/Ni antisite defects formed in layered cathodes and they varied upon charging and discharging. Moreover, the visualization of the lithium-ion migration pathway in cathode indicated that lithium-ions diffused via different hopping paths at different states of charge. Based on the relationship between structural and electrochemical properties of cathode materials, we modified and optimized the performances of cathodes by adopting different synthesis procedures, which are of scientific and practical significance.

Abstract ID: 172

M2-IT8

Neutron study on magnetocaloric and abnormal thermal expansion materials

Presenter: Fengxia Hu（Institute of Physics, Chinese Academy of Sciences）

Keywords: Neutron powder diffraction, Magnetocaloric effect, Abnormal thermal expansion

Solid state refrigeration based on magnetocaloric effect has important potential applications and is one of the research hotspots of material science and condensed matter physics. Recently, we carried out a series of studies on magnetocaloric materials and abnormal thermal expansion by means of neutron powder diffraction (NPD) [1-5]. By taking advantage of distinct resolution ability of neutrons and X-rays to Fe/Co adjacent elements, the site occupancy of Co atoms was firstly determined in $LaFe_{11.6-x}Co_xSi_{1.4}$, a family known for magnetocaloric effect, by joint refinements of NPD and XRD. On the basis, ab initio calculations were performed on the atomically resolved electronic band structure, which explained the emergence of Invar effect and enhanced excellent mechanical property [1]. A new cycloidal spiral antiferromagnetic (AFM) structure (CyS-AFMb), distinct from the AFM configuration of undoped MnNiGe, was found in magnetocaloric material Mn0.87Fe0.13NiGe with Fe doping [2]. *In-situ* NPD under hydrostatic pressure and magnetic field combined with first principles calculations revealed the spin configuration, instabilities and relevant mechanism, and giant baromagnetic effect was demonstrated. By utilizing cone-spiral magnetic structure and relevant lattice distortion identified by NPD, giant negative thermal expansion (NTE) was observed in Fe-doped MnNiGe compounds, which provides a new strategy for exploring novel NTE materials [5].

References:

[1] H. B. Shen, F. X. Hu, L.H.He, Q.Z.Huang, B. G. Shen, et al, Acta Mater. 260 (2023) 119312.

[2] F. R. Shen, F. X. Hu, L.H.He, Q.Z.Huang, B. G. Shen, et al, J. Am. Chem. Soc. 143, 6798 (2021).

[3] K. M. Qiao, F. X. Hu, B. G. Shen, et al, Nano energy 59, 285 (2019).

[4] J. Z. Hao, F. X. Hu, L.H.He, Q.Z.Huang, B. G. Shen, et al, Chem. Mater. 32, 1807 (2020).

[5] F. R. Shen, F. X. Hu, L.H.He, Q.Z.Huang, B. G. Shen, et al, Mater. Horiz. 7, 804 (2020).

Abstract ID: 70

M2-IT9

Neutron scattering of aqueous electrolyte solutions in the gigapascal pressure range at J-PARC MLF

Presenter: Toshio Yamaguchi (Qinghai Institute of Salt Lakes, CAS)

Keywords: Structure, Electrolyte solutions, High pressure, Ion solvation, Ion association, water structure

Neutron scattering experiments are performed on aqueous solutions of alkali metal chlorides (LiCl, NaCl, KCl, RbCl, and CsCl) and alkaline earth metal chlorides ($MgCl_2$, $CaCl_2$, and $SrCl_2$) at temperatures of 298 to 523 K and pressures of 0.1 MPa to 4 GPa. Neutron scattering data are analyzed by empirical potential structure refinement modeling. Pressure and temperature effects on ion solvation and association and solvent structure are discussed.

Abstract ID: 173

M2-IT10

Neutron scattering study of barocaloric materials

Presenter: Bing Li (Institute of Metal Research CAS)

Keywords: Barocaloric effect, Refrigeration, Heat storage, Quasi-elastic neutron scattering

Barocaloric materials are systems that exhibit significant thermal effects at phase transitions induced by hydrostatic pressure. They can be used for the solid-state refrigeration through a designated cooling cycle. The core physical issue of barocaloric materials is the evolutions of atomic structures and interactions in response to changes of temperature and pressure so that *in-situ* neutron scattering as a function of temperature and pressure is the desirable method for barocaloric materials research. In this presentation, I will report several case studies of colossal barocaloric effects using neutron scattering techniques, in particular quasi-elastic neutron scattering. Pressure-dependent neutron scattering measurements on the prototype neopentyl glycol as well as other novel systems like NH_4SCN and NH_4I reveal that colossal barocaloric effects can be attributed to the interplay between extensive orientational disorder and anharmonic lattice dynamics of materials. Differing from the equilibrium phase transition from plastic to crystal states, the supercooled plastic state is also obtained. At room temperature, the supercooled state is extremely sensitive to pressure such that a few MPa pressure can induce crystallization to the ordered crystal state, eventually leading to a temperature increase by 48 K within 20 s, a significant reduction of visible light transmittance from about 95% to a few percentages, and a remarkable decrease of electrical conductivity by three orders of magnitude. These ultrasensitive baroresponsivities might find their applications in low-grade waste heat recycling, pressure sensors and non-volatile memory devices. It is expected that glassy crystals serve as an emerging platform for exploiting exotic states of matter and the associated fantastic applications.

Abstract ID: 198

M2-IT11

Abatement of air pollution by porous materials

Presenter: Jiangnan Li (University of Manchester)

Keywords: Porous material, Air pollution, deNOx

Anthropogenic nitrogen oxides (NO_x) are major air pollutants causing serious environmental problems and millions of premature deaths1. As the most prevalent form of NO_x, NO_2 contributes to the formation of photochemical smog, the destruction of stratospheric ozone and the global warming2. The development of NO_2 abatement technologies is therefore important, and the state-of-art technique, selective catalytic reduction (SCR) with ammonia, suffers some fatal disadvantages including heavily rely on toxic gas and precious metal catalysts, and incomplete NO_x elimination3. Thus new capture and abatement technologies are urgently required. Complete removal of trace NO_2 from exhaust gas requires the capture system to possess not only long-term stability against highly corrosive and reactive NO_2, but also exceptional selectivity over N_2, moisture, CO_2 and SO_2. Ideally it would also be profitable to convert the captured NO_2 into useful chemicals. Such system enable the integration of nitrogen-based air pollutants into the production of value-added fine chemicals fulfilling the ‘waste-to-chemicals’ target.

Herein we report the development of robust NO2 capture and conversion systems including MFM-300(Al)4, MFM-5205 and Zr-bptc6. MFM-300(Al) is the first reported example that displays fully reversible NO2 adsorption with uptake of 14.1 mmol g-1 at 1 bar and 298 K. The coexistence of helical monomer-dimer chains of NO_2 in MFM-300(Al) provides a foundation for the fundamental understanding of chemical properties of guest molecules within the porous hosts. However, MFM-300(Al) shows only a very low uptake of 1.4 mmol g-1 at low pressure (0.01 bar and 298 K) owing to its inherently moderate binding sites (μ2-OH and aromatic C-H groups) hampering its practical applications. Based on the study of MFM-300 (Al), a robust MOF, MFM-520 was developed from the N-functionalized ligand and $ZnCl_2$ (Fig. 1), which can efficiently confine dimers of NO_2, resulting in a record-breaking adsorption capacity of 4.2 mmol g-1 (0.01 bar and 298 K) with full reversibility and no loss of capacity over 125 cycles. Furthermore, treatment of NO_2@MFM-520 with water in air leads to quantitative conversion of the captured NO_2 into HNO_3, an important feedstock for fertilizer production, and fully regenerates MFM-520, confirming its potential for precious-metal-free deNO_x technologies. The confinement of N_2O_4 inside pores has been established at a molecular level revealing the key role of pore size and geometry in the capture of NO_2. However, the low total uptake of 4.5 mmol g-1 (1.0 bar and 298 K) due to its limited porosity hampers its working capacity. Very recently, a robust Zr-MOF, Zr-bptc was developed by our group from the connection of $\{Zr_6(\mu3\text{-}O)_4(\mu3\text{-}OH)_4(COO)_{12}\}$ clusters and bptc4- ligand. It shows exceptional stability and adsorption of NO_2 at both low (4.9 mmol g-1 at 10 mbar) and high pressures (13.8 mmol g-1 at 1.0 bar). The immobilised NO_2 can be readily transformed to valuable nitro compounds relevant to construction, agrochemical and pharmaceutical industries. The strong binding interactions of NO_2 to the $\{Zr_6(\mu3\text{-}O)_4(\mu3\text{-}OH)_4(COO)_{12}\}$ cluster node have been revealed at molecular level. Our studies on the development of alternative deNO_x technique demonstrates a promising ‘waste-to-chemicals’ process for the recovery and circular utilisation of reactive nitrogen-based wastes.

Abstract ID: 149

M2-IT12

Structural Relaxation in Complex Monatomic or Binary Liquids by Means of Coherent QENS, Mode Distribution Analysis and Van Hove Function Analysis

Presenter: Yukinobu Kawakita (J-PARC Center, Japan Atomic Energy Agency)

Keywords: backscattering spectrometer, ToF, J-PARC

DNA is a time-of-flight backscattering spectrometer installed at the Materials and Life Science Experimental Facility (MLF) in Japan Proton Accelerator Research Complex (J-PARC), Tokai, Japan. Its purpose is revealing pico to nano second dynamics in a wide field of sciences and industrial applications including soft matter, bio-molecules, chemical molecules, battery, catalyst, and magnetism [1,2]. A pulse-shaping chopper equipped at the 7.75 m position from the coupled moderator makes this instrument relatively short in the neutron guide length (42 m from the moderator to the sample position). Its maximum rotation speed of 300 Hz provides us fine energy resolutions up to 1.4 micro second for a sample with dimension of 1 cm wide and 1cm tall. Changing phases of the slit opening of the chopper enables us to select energy bands and even to scan a wide energy transfer range with the highest resolution. Two types of analyzer mirrors of Si 111 and Si 311 cover large momentum transfer ranges of 0.08 to 1.98 Å−1 and 1.79 to 3.39 Å−1, respectively. Frequently used measurement modes are a high-flux mode without rotating the chopper and a high-resolution mode with 225 Hz. Those provides 12 and 3.6 micro eV energy resolutions for a large sample of 1.4 cm wide and 4 cm tall. The back-coat by neutron absorber such as Gd and Gd2O3 for Si analyzer mirrors serves us in realizing extremely high signal-to-noise ratio of 105, which allows us to obtain QENS spectra from a tiny amount of sample or a dilute protein solution. Various conditions of sample environment are available; cryo-furnaces (4 K to 700 K), a 2 K cryostat, a top-loading sample stick for applying electric field, a humidity control system, a cryostat with a samples changer for three samples, an inner atmosphere controller for cryo-furnaces and so on. A high temperature furnace up to 1000 K, 3.5 Tesla cryo-magnet and a sample changer for 20 samples are under commissioning.

Reference:

[1] K. Shibata et al., JPS Conf. Proc. 8, 036022 (2015).

[2] Y. Kawakita et al., EPJ Web of Conference 272 (2022) 02002.

Abstract ID: 41

M2-IT13

Revisit to crystal and magnetic structure of $La(Fe, Si)_{13}$ and $La(Fe, Co, Si)_{13}$ using powder neutron diffraction

Presenter: Jianrong Gao (Northeastern University)

Keywords: Magnetocaloric, Phase transition, Diffraction

$La(Fe, Si)_{13}$ compounds show a large magnetocaloric effect near room temperature. The addition of Co or hydrogen can increase the Curie temperature to room temperature, making this intermetallic material promising for magnetic refrigeration applications. In literature, the large magnetocaloric effect of $La(Fe, Si)_{13}$ has been attributed to a ferromagnetic transition or to a metamagnetic transition. To reconcile this discrepancy, we revisited crystal and magnetic structure of annealed samples of $La(Fe, Si)_{13}$ and $La(Fe, Co, Si)_{13}$ over a broad range of temperature using powder neutron diffraction. The powder X-ray diffraction patterns of the samples were analyzed by means of Rietveld refinement using GSAS software. The refined crystal and magnetic structures at low and high temperatures are in reasonable agreement with previous studies of similar compounds. Beyond this general agreement, our work provided more details about thermally induced changes of crystal and magnetic structures of samples close to respective Curie temperature. The origin of the large magnetocaloric effect in $La(Fe, Si)_{13}$ compounds is discussed in term of the new results.

The work is financially supported by the National Natural Science Foundation of China (grant no. 51831003). The authors are grateful to Oak Ridge National Laboratory for providing neutron beam time at the high-flux isotope reactor.

Abstract ID: 139

M2-IT14

Application of Neutron Beams in Porous Materials' Research

Presenter: Minyoung YOON (Kyungpook National University)

Keywords: Porous materials, Metal-organic frameworks, Coordination polymers, Neutron diffraction, Neutron Scattering

Despite the unique nature of neutron beams, the utilization of neutron beams in the chemistry research field is limited. One of the most critical issues in limiting the use of neutron beams is the presence of hydrogen in chemical materials. However, recent advances in deuterating organic molecules allow using neutron beams for various chemical applications. Crystalline porous materials can provide a unique platform to use neutron beams in chemical research because of their crystalline nature for the structure studies using neutron diffraction and host-guest chemistry to study guest motion and dynamics using neutron (inelastic and quasielastic) scattering. In this work, we will present the use of neutron diffraction to study the location of hydrogen atoms and ions (protons) in crystalline porous materials. MIL-53(Al), a well-known metal-organic framework (MOF), has a breathing behavior, and depending on the loading of D_2 molecules, the MOF adopts unique porous structures. *In-situ* D_2 adsorption neutron diffraction allows the adsorption site of D_2 and the framework structures. In addition, porous CB[6] is the other crystalline porous material with acid molecules in the pores, which shows unusual anisotropic proton conductivity. The quasielastic neutron scattering technique was applied to elucidate its proton conduction behavior. It allowed us to understand more details about the proton motions in the confined space depending on the guest molecules in the pores. Details of these works will be presented.

Abstract ID: 108

M2-IT15

Negative/near zero thermal expansion behavior with wide temperature range in antiperovskite compounds

Presenter: Ying Sun (School of Physics, Beihang University)

Keywords: Zero thermal expansion; Antiperovskite; Neutron diffraction

In recent years, some magnetic metallic compounds have been found to exhibit negative thermal expansion (NTE) or nearly zero thermal expansion (NZTE) behaviors with great application prospects in aerospace, microelectronic devices, precision optical devices and other modern industries. However, it is a big challenge for applications because the responding temperature range for these compounds is not broad enough or far away from room temperature. The application requirement and the bottlenecks encountered during regulation of NTE/NZTE temperature range make it necessary to design the isotropic ZTE materials over a wide temperature range. As the typical NTE material, Mn-based anti-perovskites nitrides Mn3AN, where A is usually a transition metal, possess the colossal magnitude of NTE due to magnetic order-driven volume constriction. In this work, several strategies are put forward to design the wide temperature range of NTE/NZTE behaviors in antiperovskite compounds. For example, we regulated the unique sluggish effect of phase transition by introducing large lattice distortion, which brings about effective relaxation of sharp phase transition and thus broadens the NTE temperature range. In this work, neutron diffraction technique plays an important role in clarifying the behavior of the near zero thermal expansion, which will be discussed in the presentation.

Abstract ID: 138

M2-IT16

Studies on crystal structures and anharmonic thermal vibration of thermoelectric materials $Cu_{2-x}S$

Presenter: Seungyub Song（KEK）

Keywords: Thermoelectric, Neutron powder diffraction

Promising thermoelectric (TE) materials $Cu_{2-x}S$ have a high TE figure of merit ZT because of its extremely low thermal conductivity. For the low thermal conductivity, the large anharmonicity has been pointed out as an origin by several studies. Meanwhile we noticed from previous reports, as Cu-defect occurs the lattice thermal conductivity of $Cu_{2-x}S$ shows abnormal increasing trend. We assumed that this trend is strongly related to anharmonicity.

In this study, we performed neutron diffraction (ND) on $Cu_{2-x}S$ powder sample and conducted Rietveld and Maximum entropy method(MEM). The One-particle potentials (OPPs) for Cu atom was calculated based on MEM results and fitted with theoretical potential function assuming cubic symmetry.

The Rietveld analysis employing a split atom model for Cu at 8c (1/4, 1/4, 1/4) site and 32f (x, x, x; $x \approx 0.33$) site revealed that as Cu defect increases, the occupancy at 32f site decreases. This feature was clearer in the Cu-atom density obtained from MEM.

The fitting results of OPPs showed the anharmonicity-to-harmonicity ratio is maximum at Cu2S and increases as Cu-defect increases implying that the abnormal trend of lattice thermal conductivity is attributed to the anharmonicity.

The 4th Asia-Oceania Conference on Neutron Scattering

M2. Contributed Talks

Abstract ID: 174

M2-CT1

Solvent-free mechanochemical synthesis of organic proton conducting salts incorporating imidazole and dicarboxylic acids

Presenter: Anucha Koedtruad (Spallation Neutron Source Science Center, Dongguan, 523808, China)

Keywords: Organic salts, Proton conducting, Mechanochemistry, Powder neutron diffraction, Solventless synthesis, Deuteration

Anhydrous organic salts incorporating imidazole and dicarboxylic acids can be used as proton conducting electrolytes in fuel cells. Herein, we demonstrated an alternative solvent-free mechanochemical way to synthesize imidazole-succinic acid, $C_3H_4N_2$-$HOOC(CH_2)_2COOH$, and imidazole-glutaric acid, $C_3H_4N_2$-$HOOC(CH_2)_3COOH$, by manual grinding. We investigated phase development upon grinding by powder X-ray diffractometry, solid-state FTIR spectroscopy and differential scanning calorimetry, crystal structures of the obtained materials by powder neutron diffractometry and proton conducting property by AC impedance spectroscopy. We found that this synthesis rout can induce chemical reaction and provides phase-pure materials. The materials crystalize in a triclinic unit cell with space group $P\bar{1}$. The co-former molecules are connected two-dimensionally, forming a layered structure. They show distinct conductivity and activation energy E_a compared to previously reported compounds grown by a conventional crystallization rout via solution. The differences can be related to intrinsic defects and structural disorder introduced by mechanochemical grinding. This work emphasizes potential of the solvent-free mechanochemical synthesis to construct this class of materials and other related ones with tunable conducting property, and potential of the synthesis for preparing fully deuterated salts for specific neutron diffraction study.

Abstract ID: 55

M2-CT2

Solution Structure by X-Ray Neutron Scattering and Its Applications

Presenter: Yongquan Zhou (Qinghai Institute of Salt Lakes, Chinese Academy of Sciences)

Keywords: X-Ray/Neutron scattering, Solution structure, Ionic hydration, Borate solution

Salt lakes contain abundant mineral resources such as sodium (Na), magnesium (Mg), potassium (K), lithium (Li), boron (B), etc. In the past decades, great progress was achieved in salt lake resources separation [1], and researchers found the ion hydration and complex play important roles for the salt lake resource separation. However, Solution structure, and the mechanism study at atomic level isn't an easy work [2].

In the present talk, the methods for solution structure at the atomic level with the neutron scattering (NS), wide angle X-ray scattering (WAXRS) and computer simulations will be summarized. Combining neutron scattering (NS), wide-angle X-ray scattering (WAXS), and molecular dynamics (MD), we quantify ionic hydration degree (hydration ability) systematically for a series of alkali metal (Li^+, Na^+, K^+, Rb^+, Cs^+) and halide ions (F^-, Cl^-, Br^-, I^-) based on static and dynamic hydration numbers. The former is based on the orientational correlation of water molecules bound to an ion derived from the positional information from NS and WAXS. The latter is defined as the mean number of water molecules remaining in the first coordination shell of an ion over a residence time of bound water molecules around the ion from MD. The static and dynamic hydration numbers distinguish hydration from coordination and quantify the ionic hydration degree, which provides a valuable reference for understanding various phenomena in nature [3].

Salt lake borate solutions have some abnormal metastable phenomena, some supersaturated borate solutions cannot be crystallized out by stirring, ultrasonic vibration or adding crystal nucleus. It causes great troubles to boron extraction and lithium battery industry. Based on a better understanding of the structure of borate solutions at molecular level [4,5], we found some solutions for salt lake borate solution crystallization.

References:

[1] Qinghai Institute of Salt Lakes, Chinese Academy of Sciences, Sixty Years of Research on Salt lakes by Chinese Academy of Sciences. 2015, Science Press: Beijing.

[2] Sanders S. 125 Questions: Exploration and Discovery, 2021, Science/AAA Custom Publishing Office: Washington, DC, USA.

[3] Z. Jing, Y. Zhou, T. Yamaguchi, et al. J. Phys. Chem. Lett. 2023, 14 (27), 6270.

[4] Y. Zhou, S. Higa, C. Fang, et al. Phys. Chem. Chem. Phys. 2017, 19(40), 27878.

[5] Y. Zhou, T. Yamaguchi, W. Zhang, et al. Phys. Chem. Chem. Phys. 2020, 22(30), 17160.

Abstract ID: 37

M2-CT3

Macroscopic and microscopic residual stresses in bronze matrix composite surface deposits manufactured via laser melt injection

Presenter: Xingxing Zhang (Institute of High Energy Physics, Chinese Academy of Sciences)

Keywords: Residual stress, Bronze matrix composite, Laser surface processing, Neutron diffraction, Finite element modeling

Nickel-aluminum bronze alloys, renowned for their excellent combination of mechanical properties and corrosion resistance, have found widespread applications across various industries. One key area of interest is enhancing surface wear resistance, as it not only facilitates the utilization of nickel-aluminum bronze alloys in high-value applications but also reduces the need for part replacements and overall costs. Metal matrix composite (MMC) coatings have proven highly effective in significantly improving surface wear resistance [1]. A notable example is the development of a nickel-aluminum bronze matrix composite surface deposit reinforced with spherical fused tungsten carbide (sFTC), comprising WC and W2C. This sFTC/$CuAl_{10}Ni_5Fe_4$ composite has demonstrated the potential to reduce wear by approximately 80% [2, 3].

However, macro and micro residual stresses develop in the MMC coatings, leading to geometric distortion and reducing fatigue strength [4, 5] as well as service life [6]. Therefore, it is crucial to investigate and understand the residual stresses in the MMC coatings. This research employed neutron diffraction to measure the residual stresses in the bronze matrix composite surface deposits manufactured through laser melt injection. A thermo-mechanical finite element model was also developed to complement the experimental measurements. This investigation provides a comprehensive understanding of the residual stress state in the MMC coatings. The findings from this study have significant implications for optimizing the manufacturing process, reducing residual stresses, and ultimately enhancing the performance and extending the service life of the MMC coatings.

References:

[1] Y. Feng, X. Pang, K. Feng, Y. Feng, Z. Li, Journal of Materials Research and Technology 15 (2021) 5597-5607.

[2] H. Freiße, A. Langebeck, H. Köhler, T. Seefeld, Dry Metal Forming Open Access Journal 2 (2016) 001-006.

[3] X.X. Zhang, J.R. Kornmeier, M. Hofmann, A. Langebeck, S. Alameddin, R.P. Alessio, F. Fritzen, J.R. Bunn, S. Cabeza, Strain (2023) e12457.

[4] H. Köhler, K. Partes, J.R. Kornmeier, F. Vollertsen, Physics Procedia 39 (2012) 354-361.

[5] H. Köhler, V. Jayaraman, D. Brosch, F.X. Hutter, T. Seefeld, Physics Procedia 41 (2013) 502-508.

[6] G.A. Webster, A.N. Ezeilo, International Journal of Fatigue 23 (2001) S375-S383.

Abstract ID: 115

M2-CT4

In-situ neutron-diffraction studies of structural-phase transitions in Fe-*x*Ga alloys on High Resolution Fourier Diffractometer

Presenter: Tatiana Vershinina (Joint Institute for Nuclear Research)

Keywords: Fe-Ga alloys, Phase transformation, Neutron diffraction

Ferromagnetic Fe-xGa alloys with increased magnetostriction are being studied by the joint team of JINR (Dubna) - MISIS (Moscow) within the framework of joint projects. The macroscopic properties of alloys are analyzed at MISIS, their atomic and magnetic structures are studied at JINR by using neutron scattering [1]. Neutron experiments are mainly performed at High Resolution Fourier Diffractometer (HRFD) [2] at the IBR-2 pulsed reactor. HRFD is a neutron time-of-flight (TOF) spectrometer with a fast Fourier chopper. Its main purpose is the precision analysis of the crystalline and magnetic structure of polycrystalline samples, but the instrument can also be used to study the structure of single crystals. The key element of HRFD is the fast Fourier chopper, the use of which makes it possible to achieve very high resolution of the diffractometer ($\Delta d/d \approx 0.0015$). Switching to a regular TOF-mode (without Fourier chopper), which makes HRFD as one of the world's best high-intensity diffractometers, is also possible. The use of a high-intensity mode allows *in-situ* (under heating or cooling) studies of crystalline materials with resolution $\Delta d/d \approx 0.015$ and acquisition time of ~ 1 minute for the whole spectrum. Examples of recent studies performed on HRFD are contained in articles [3-5].

The report presents the results of comparative *in-situ* neutron diffraction studies of the evolution of the phase composition of Fe-*x*Ga alloys, carried out during heating and subsequent cooling. In addition, the nuances of using of complementary methods in investigation of Fe-*x*Ga alloys will be discussed. Partially, these results are published at [4, 6, 7].

This work was funded by Russian Science Foundation Project No. 22-42-04404.

References:

[1] A.M. Balagurov, I.S. Golovin "Neutron scattering in studies of Fe-based functional alloys (Fe-Ga, Fe-Al)" Physics-Uspekhi 64 (7) (2021) 702-721.

[2] A.M. Balagurov "High resolution Fourier diffraction at the IBR-2 reactor" Neutron News 16 (2005) 8–12.

[3] A.M. Balagurov, S.V. Sumnikov, J. Cifre, V.V. Palacheva, D.G. Chubov, I.S. Golovin "In situ study of order-disorder transitions and anelasticity in Fe-26Al alloy" J. Alloys and Comp. 932 (2023) 167663 (1-8).

[4] T.N. Vershinina, N.Yu. Samoylova, S.V. Sumnikov, A.M. Balagurov, V.V. Palacheva, I.S. Golovin "Comparative study of structures and phase transitions in Fe-(31-35)Ga alloys by *in-situ* neutron diffraction" J. Alloys and Comp. 934 (2023) 167967 (1-10).

[5] A.M. Balagurov, N.Yu. Samoylova, S.V. Sumnikov, V.V. Palacheva, I.S. Golovin "Structural and magnetic phase transitions in Fe3Ge: A neutron diffraction study" Phys. Rev. Mat. 7 (2023) 063603 (1-10).

[6] T.N. Vershinina, I.A. Bobrikov, S.V. Sumnikov, A.O. Boev, A.M. Balagurov, A.K. Mohamed, I.S. Golovin, Crystal structure and phase composition evolution during heat treatment of Fe-45Ga alloy, Intermetallics, 131 (1–5) (2021) 107110.

[7] T.N. Vershinina, I.A. Bobrikov, S.V. Sumnikov, A.M. Balagurov, A.K. Mohamed, I. S. Golovin, Structure evolution of as-cast metastable Fe-38Ga alloy towards equilibrium, J. Alloys Compd. 889 (2021) 161782.

Abstract ID: 134

M2-CT5

Oxide Ion Conducting Materials Containing Tetrahedral Moieties: Structures and Conduction Mechanisms

Presenter: Xiaoyan Yang (Guilin University of Technology)

Keywords: Oxide ion conductors, Tetrahedra units, Solid oxide electrolytes, Solid oxide fuel cells.

This presentation presents an overview from the new sight of the tetrahedral chemistry on various oxide ion conducting materials containing tetrahedral moieties, which have received continuous growing attention as key component candidates for various devices including solid oxide fuel cells and oxygen sensors, due to the deformation and rotation flexibility of tetrahedral units facilitating oxide ion transportation. Emphasis is placed on the structural and mechanistic features of various systems covering from crystalline to amorphs materials, which include a variety of gallates, silicates, germanates, molybdates, tungstates, vanadates, aluminates, niobate, titanates, indium-oxides and the newly reported borates. They contain tetrahedral units in either isolated or linked manners forming different polyhedral dimensionality (0 to 3) with various defect properties and transport mechanisms. The development of the oxide ion conductors containing tetrahedral moieties and the elucidated roles of tetrahedral units on oxide ion migration have demonstrated diverse opportunities for discovering superior electrolytes for solid oxide fuel cells and other related devices and provides useful clues for uncovering the generically key factors directing fast oxide ion conduction.

References:

[1] Y. Feng, X. Pang, K. Feng, Y. Feng, Z. Li, Journal of Materials Research and Technology 15 (2021) 5597-5607.

[2] H. Freiße, A. Langebeck, H. Köhler, T. Seefeld, Dry Metal Forming Open Access Journal 2 (2016) 001-006.

[3] X.X. Zhang, J.R. Kornmeier, M. Hofmann, A. Langebeck, S. Alameddin, R.P. Alessio, F. Fritzen, J.R. Bunn, S. Cabeza, Strain (2023) e12457.

[4] H. Köhler, K. Partes, J.R. Kornmeier, F. Vollertsen, Physics Procedia 39 (2012) 354-361.

[5] H. Köhler, V. Jayaraman, D. Brosch, F.X. Hutter, T. Seefeld, Physics Procedia 41 (2013) 502-508.

[6] G.A. Webster, A.N. Ezeilo, International Journal of Fatigue 23 (2001) S375-S383.

Abstract ID: 21

M2-CT6

Hierarchy of interactions in Dzyaloshinskii-Moriya helimagnets and skyrmion lattice

Presenter: Sergey Grigoriev (NRC "Kurchatov Institute" - Petersburg Nuclear Physics Institute)

Keywords: Skyrmion Lattice, Dzyaloshinskii-Moriya interaction

The cubic noncentrosymmetric structure of the B20 compounds produces the helical (homochiral) structure with the wave vector *k* balanced by the competition of antisymmetric Dzyaloshinskii-Moriya (DM) interaction and the ferromagnetic exchange interaction. The application of the magnetic field *H* transforms the helix into cone structure that is collapsed into the field induced ferromagnet at *Hc2*. The wave vector *k* of the Skyrmion Lattice (SkL) practically equal to that of the helix showing that the SkL is built on the same hierarchy of interactions. The SkL is realized under applied magnetic field within the narrow field corridor and close to Tc only. It is shown that SkL is energetically favorable as compare to the conical structure close to H = 0.4 *Hc2*. We propose the model for the appearance and stability of the SkL. It is dipole interaction and the demagnetization field that makes the SkL more favourable as compared to the conical phase. The model is validated experimentally on the series of the helimagnetic compounds MnFeSi and FeCoSi. Thus it is experimentally confirmed that the whole (H-T) phase diagram in the helimagnets with DM interaction can be drawn on the basis of the hierarchy of interactions determining the energy landscape of the magnetic system: the FM exchange interaction, DM interaction as well as dipole interaction, important for stability of SkL.

Abstract ID: 162

M2-CT7

Spin dependent electronic transport properties of Mn-based antiperovskites

Presenter: Sihao Deng (Spallation Neutron Source Science Center)

Keywords: Magnetic structures, Spin chirality, Electronic transport properties, Antiperovskites

Mn-based antiperovskite compounds with triangular magnetic lattice show a variety of magnetic structures accompanied by some fascinating physical properties, including a large magnetocaloric effect, giant magnetoresistance, giant barocaloric effect, baromagnetic effect, negative thermal expansion, and anomalous hall effect etc. Among them, face-centered magnetic atoms (such as Mn) and body-centered N (C) atoms can form NMn_6 or CMn_6 octahedra, and six magnetic atoms Mn are located at the six corners of the octahedron, which is prone to magnetic frustration. Thereby it generates the abounding magnetic structures. Here, we investigate the chiral spin states and their associated electronic transport properties in antiperovskite materials. For $Mn_{3.33}Ni_{0.67}N$, in addition to the Γ5g triangular antiferromagnetic configuration, there is also a weaker ferromagnetic component perpendicular to the Γ5g plane, which in turn shows non-zero scalar spin chirality values. By cooling with an external magnetic field, the ferromagnetic component is frozen, thereby realizing the manipulation of the chirality of the magnetic structure. Experimentally, we have discovered a vertical shift of the magnetization curve and to an asymmetrical magnetoresistance, and observed the chiral Hall effect. For $Mn_3Zn(Ge)N$ with zero scalar spin chirality, the spontaneous changes occur in the longitudinal and transverse resistivity at low temperatures indicating a magnetic phase transition between different non-collinear phases. Our findings open interesting prospects for tailoring specific materials properties for the development of future chiral spintronic devices.

Abstract ID: 165

M2-CT8

Local structural features of medium-entropy garnet with ultra-long cycle life

Presenter: Wang Hay Kan (Institute of High Energy Physics, Chinese Academy of Sciences)

Keywords: Garnet, PDF, Mid-entropy, Electrolyte, Lithium-ion batteries

High-entropy ceramics (HECs) have gained great attention as one of the rapidly growing families of high-entropy materials. Increasing the species yields enhanced properties owing to high configurational entropy and elemental synergies, alluding to the potential of HECs in designing materials with tailored properties. However, the question is obscure as to whether the multiple elements show priority in the arrangement in the structure, as well as how they regulate the bond length. Here, we synthesize a medium-entropy garnet-structured electrolyte $Li_6La_3Zr_{0.5}Hf_{0.5}Ta_{0.5}Nb_{0.5}O_{12}$ (ME-LLZO) and elucidate its short-range structure based on the calculated supercell and neutron pair distribution function (PDF) refinement. Extended bottleneck size, elongated Li-O bond length, and local clustering of 16a sites, where tetravalent ions prefer to be the first-nearest octahedrons of pentavalent ions, are observed. Differences between the multiple cations inevitably influence the short-range structure, and our study provides a new paradigm for future exploration of HEC-based solid-state electrolytes.

Abstract ID: 171

M2-CT9

Structure Evolutions in Layered Oxide Cathodes

Presenter: Enyue Zhao (Songshan Lake Materials Laboratory)

Keywords: Li-ion Battery, Cathodes, Neutron-based Characterizations

The development of large-scale energy storage technologies such as electric vehicles and smart grids has put forward higher requirements for the energy density of lithium-ion batteries. Lithium-rich cathode materials have attracted much attention due to their high energy density. Unlike the traditional cathode materials, there is not only redox reactions of transition metals but also lattice oxygen redox (O^{2-}/O^{n-}) to provide the charge compensation in lithium-rich layered oxides (chemical formula can be shortened to $Li_{1+x}TM_{1-x}O_2$, TM represents transition metal). This extra lattice oxygen charge compensation not only leads to a high theoretical capacity of Li-rich cathode materials, but also affects the stability of ion-storage structure. Compared with X-rays and electrons, neutrons are more sensitive to light elements lithium and oxygen, and can also readily distinguish transition metal neighbor elements. Here, using multiple neutron scattering techniques including neutron powder diffraction (NPD), neutron pair distribution function (nPDF), and small-angle neutron scattering (SNAS), we systematically studied the local structure and nanostructure evolutions of Li-rich cathode materials related to lattice oxygen charge compensation from different structural dimensions and spatial scales.

Abstract ID: 88

M2-CT10

Study of 3*d* transition metal thin films by combination of neutron and X-ray reflectometry

Presenter: Vasilii Matveev (Petersburg Nuclear Physics Institute named by B.P. Konstantinov of National Research Centre «Kurchatov Institute»)

Keywords: Thin metal films, Neutron reflectometry, X-ray-reflectometry

The metal thin films are widely used for the structural and functional applications, especially in microelectronics industries, aerospace, light and neutron optics and coating technology [1-4]. The chemical and physical properties of thin metal films may substantially differ from those of the bulk, since the portion of the near-surface volume in such films is considerable. The electronic states are perturbed by local symmetry breaking and are subject to the influence of the environment (substrate, atmosphere , etc.).

Neutron reflectometry (NRR) and X-ray reflectometry (XRR) are non-destructive methods that provide information about the thickness and roughness of thin films and multilayers. Both methods are based reflection of neutron or X-ray from the interfaces of different materials. The reflection of X-ray is determined by the difference in electron density. The neutron reflection of is determined by the difference concentration of atoms and their isotopic compositions. Compared with the X-ray, neutrons can penetrate deeper into the inner regions of materials. In this work presents the results of the study of 3*d* transition metal films with thickness 5-100 nm by combination of X-ray and neutron reflectometry. Additionally, some electrical and magnetic properties of thin films of these metals were studied.

References:

1. B. Lin, H. Zhu, et.al. Materials Science Forum. V. 773-774, (2014), P. 616-626.

2. A. Chandrasekaran, Robbert W. E. van de Kruijs, et al. Appl. Mater. Interfaces V. 11 (2019), Issue 49, P. 46311–46326.

3. A. Axelevitch, B. Gorenstein, G. Golan. Physics Procedia V. 32, (2012), P. 1–13.

4. N.K. Pleshanov. Nucl. Instrum. Methods A. V. 853, (2017), P. 61-69.

Abstract ID: 180

M2-CT11

Superior zero thermal expansion alloy via “plum pudding” architecture

Presenter: Chengyi Yu (Institute of Solid State Chemistry, University of Science and Technology Beijing)

Keywords: Zero thermal expansion; In-situ neutron diffraction

Rapid progress in modern technologies demands zero thermal expansion (ZTE) materials with multi-property profiles to withstand harsh service conditions. Thus far, the majority of documented ZTE materials have shortcomings in different aspects that limit their practical utilization. Here, we report on a superior isotropic ZTE alloy with collective properties regarding wide operating temperature windows, high strength-stiffness, and excellent cyclic thermal stability. A boron-migration-mediated solid-state reaction (BMSR) constructs a salient "plum pudding" structure in a dual-phase Er-Fe-B alloy, where the precursor $ErFe_{10}$ phase reacts with the migrated boron and transforms into the target $Er_2Fe_{14}B$ (pudding) and α-Fe phases (plum). The formation of such microstructure helps to eliminate apparent crystallographic texture, tailor and form isotropic ZTE, and simultaneously enhance the strength and toughness of the alloy. These findings suggest a promising design paradigm for comprehensive performance ZTE alloys.

References:

[1] Yu, C., Lin, K., Xing, X. et al. Plastic and low-cost axial zero thermal expansion alloy by a natural dual-phase composite. Nat. Commun. 12, 4701 (2021).

[2] Yu, C., Lin, K., Xing, X. et al. Superior zero thermal expansion dual-phase alloy via boron-migration mediated solid-state reaction. Nat. Commun. 14, 3135 (2023).

Abstract ID: 189

M2-CT12

Pressure-induced polymerization of organic molecular crystals

Presenter: Kuo Li (hpstar)

Keywords: High pressure, Solid state chemistry, Pressure-induced polymerization, Topochemical reaction

Unsaturated molecules (like alkynes and aromatics) tend to polymerize under applied pressure and form more saturated extended structures, including diamond nano-thread, graphane, graphitic nano-ribbon and amorphous carbon materials. Thermodynamically, this process is determined by the volume contraction during the reaction, while the dynamical process is typically topochemical. That is, the movement and bonding process of the atoms are trackable. Such high-pressure addition reactions in crystal are completely different from those in solution at ambient condition due to the highly constrained geometric conformation, and the specific reactions, reaction selectivity, and basic reactions rules in a certain conformation become the key to the precise synthesis of novel crystalline carbon materials. This report will introduce the chemical reactions and the key geometric parameters of the organic molecular crystal in the high-pressure synthesis of diamond nano-thread, graphitic nano-ribbon and graphane, etc., and the theoretical approach in the reaction mechanisms.

Abstract ID: 213

M2-CT13

Neutron powder diffraction for the study of porous materials for adsorption and separation

Presenter: Yong Yan (South China Normal University)

Keywords: MOFs, Neutron powder diffraction, *In-situ* diffraction, Rietveld refinement

Porous metal−organic framework (MOF) materials have attracted increasing research interest because of their potential applications in gas storage, separation, carbon capture, among others.[1] Constructed by bridging metal ions/clusters with organic ligands, crystalline MOFs have the unique advantage of extensive structural diversity and tunability. The crystalline nature of MOFs allows advanced crystallographic analysis of the structural change upon external stimuli and/or the host−guest interactions. These structural insights at a molecular level can effectively direct the design of future MOFs showing optimized capability of binding guest molecules for enhanced storage/separation performance. Hydrogen (H_2) and methane (CH_4) are widely considered to be potential alternatives to fossil fuels for mobile applications because of their environmental benefit and high energy density. However, development of efficient on-board storage systems remains a challenge. In this work, we [2,3] developed a range of high performance MOF materials for H_2 and CH_4 storage. Characterising the preferential adsorption sites in these porous hosts allows deep understanding of the adsorption mechanisms and provides feedback to the materials design. We applied *in-situ* neutron powder diffraction in GEM (ISIS, UK) and MPI in the China Spallation Neutron Source, and the high resolution diffractometer in WISH (ISIS) to study the gas adsorption in these materials. Structural studies successfully revealed the adsorption sites for different guests within these porous hosts.

The 4th Asia-Oceania Conference on Neutron Scattering

Scientific Parallel Session M3. Soft Matter and Life Science

The 4th Asia-Oceania Conference on Neutron Scattering

M3. Keynote Talks

Abstract ID: 91

M3-KT1

Biocompatible Ionic Liquid based Stimuli-Responsive Sof Assemblies for the On-demand Drug Delivery

Presenter: Naved Anjum MALEK (Ionic Liquid Research Laboratory, Department of Chemistry, S.V. National Institute of Technology (SVNIT), Surat-07, India)

Keywords: ionic liquids, soft assemblies, hydrogel, stimuli-responsive hydrogel

Circumventing the limitations of traditional cancer therapeutics with more safer, effective and targeted delivery vehicles for drugs is the prime focus in recent times. The vehicle should increase the efficiency of the drug, reduce its side effects on the healthy cells, and helps in the prevention of cancer recurrences. We at Ionic Liquid Research Laboratory work on the development of various stimuli-responsive therapeutic scaffolds that have ability to transport not only hydrophilic but also hydrophobic chemo drugs to the targeted site in a regulated and sustained fashion. We rely on the excellent physicochemical properties of Ionic Liquids that also have ability to aggregate in their pristine form as well as through synergistically interacting with the external additives to form various morphological aggregates such as micelles, vesicles, coacervates, and hydrogels to carry the drugs, irrespective to their polarity. We have designed various ILs with stimuli-responsive character that form the soft assemblies capable to transport the chemo drugs and deliver as on demand through adjusting the stimuli. We use Small Angle Neutron Scattering (SANS) to not only justify the size and shape of the soft assemblies but also the transport mechanism necessary for the drug delivery at the tumour sites. We have recently designed the pH and temperature responsive hybrid hydrogels through synergistic interaction between the ILs and biocompatible polymers. These hybrid hydrogels show excellent mechanical properties that can be tuned judiciously and other important properties including the unique self-healing behaviour that are required for the new age drug delivery vehicles. We also perform the in vitro cytotoxicity and in vitro drug release study to confirm the role of the hydrogel in the targeted delivery of chemo drugs at physiological condition and more effective in killing the cancerous cells. We are striving to design yet better therapeutic scaffolds with still better performance.

Abstract ID: 81

M3-KT2

Neutron Scattering for Understanding Tribology

Presenter: Tomoko HIRAYAMA (Kyoto University, Japan)

Keywords: tribology, lubrication engineering, lubricant, interface

Neutron scattering is an extremely useful tool for understanding tribological phenomena. Lubricants are used on mechanical sliding surfaces to reduce their friction, and lubricants contain functional molecules called 'additives'. Additives adsorb onto sliding surfaces to reduce friction, and the frictional properties change according to the structure of the adsorption layer. Our group is investigating the relationship between the additive molecules and the coefficient of friction in terms of the structure they adopt in the lubricant, the density and thickness of the adsorption layer on the surface, and how the adsorbed molecules affect the dynamics of the lubricant. Specifically, SANS, NR, QENS and other methods are used, and they bring a lot of scientific knowledge to the field of tribology, which has been developed as an engineering discipline. In this talk, I will present some of the applications of neutron scattering in the field of tribology.

Abstract ID: 51

M3-KT3

Probing Block Copolymer/Homopolymer Blend Films by Grazing-Incidence Small Neutron Scattering and Neutron Scattering

Presenter: Ya-Sen SUN (Department of Chemical Engineering, National Cheng Kung University, Tainan 701, Taiwan)

Keywords: grazing-incidence small-angle neutron scattering, neutron reflectivity, thin film, block copolymer, blend

Neutron reflectivity (NR) and grazing incident small-angle neutron scattering (GISANS) are surface-sensitive tools for characterizing polymer-based surfaces and interfaces. The first part of this talk is to introduce how we probe spatial distributions of deuterated homopolystyrene (dPS) chains within hexagonally perforated layers in blend films of polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) by NR and GISANS. With GISANS and NR, we found that dPS chains preferentially segregate on the surface and within PS-rich layers in thin films regardless of annealing temperature. However, thick films exhibit a different segregation behavior. Surface preference can be prohibited by annealing at 270 °C so that dPS chains can distribute within PS-rich layers and PS perforations. The second part demonstrates how we probe chain conformations at the interface of lamellae-forming PS-b-PMMA films on a cross-linked PS layer. The cross-linked PS layer comprised deuterated homo-polystyrene chains of varied chain lengths. With NR, we found that short cross-linked dPS chains cannot prevent chain inter-diffusion and inter-penetration with the top layer of PS-b-PMMA. As a result, the lamellae in PS-b-PMMA films cannot perfectly orient with a perpendicular orientation. Instead, parallel lamellae form as defects in certain regions with chain inter-diffusion and inter-penetration.

Abstract ID: 56

M3-KT4

Bulk heterojunction morphology of organic photovoltaics – a study based on grazing-incidence X-ray and neutron scattering

Presenter: Xinhui LU (Chinese University of Hong Kong, China)

Keywords: organic photovoltaics, bulk heterojunction, grazing incidence

Nowadays, solar industry becomes the fastest growing industry due to the rising demands to solve the energy crisis and environmental problems. Third-generation solar cells, especially organic solar cells are all relying on a semiconducting thin-film active layer to harvest the solar energy. The bulk morphology of the active layer in terms of crystal structure, orientation and nanophase separation behaviors is known to be critical to the organic solar cell device performance. Here, we will present our recent studies on the process-structure-device correlation of organic solar cells. In these studies, state-of-art grazing incidence scattering techniques using X-rays and neutrons were employed for various purposes, such as grazing incidence wide-angle/small-angle X-ray scattering (GIWAXS/GISAXS), grazing incidence transmission small-angle X-ray scattering (GTSAXS), grazing incidence neutron scattering (GISANS). These techniques can also be applied in material science, chemistry, biology and condensed matter physics studies. By modifying the wavelength of the probing beam and the experimental geometry, a variety of sample types, such as solutions, powders, surfaces and thin films, can be studied, covering wide length scales as well as versatile dynamic and kinetic behaviors.

M3. Invited Talks

Abstract ID: 24

M3-IT1

Understanding the morphology of the proton-exchange membranes over an extended length scale between local and long-range characteristic sizes by simultaneous contrast variation small- and wide-angle neutron scattering

Presenter: Aurel Radulescu (Forschungszentrum Jülich GmbH)

Keywords: SANS, WANS, pinhole, TOF, PEM, conductivity

The outstanding properties of polymer electrolyte membranes (PEM) used in energy applications derive from the microphase separation of hydrophilic ionic material, that promotes the ion conductivity, from the hydrophobic substance, that provides the mechanical strength and limit the dimensional changes of the membrane during swelling. Therefore, to design new PEM systems or to improve the ones under current consideration for such applications, one should not only consider the molecular architecture itself, but also thoroughly understand their microphase-separated structures, such as the crystalline domains and hydrated regions and the distribution of the ionic groups and water in conducting paths. To assess the relationship between the conductive, mechanical strength and durability properties on the one side and the microstructure and morphology on the other side, the molecular organization of the membrane between the local length scale of a few Å (crystal structure) and the mesoscopic length scale (hundreds of nm) should be characterized under relevant conditions for applications, such as humidity (RH), temperature (T) and chemical stress. Here I discuss methodological aspects of neutron scattering experiments on energy-relevant materials at pinhole and TOF-SANS-WANS diffractometers with tunable resolution at the neutron sources in Garching, Germany, and Tokai, Japan. Microstructural analyses of a PEM model system at different temperatures and degrees of hydration, the functionalized syndiotactic polystyrene (sPS) with sulfonated hydrophilic amorphous phase and co-crystalline phase with small organic molecules, are then presented in detail. The use of uniaxially deformed films allowed the identification and characterization of different structural levels with sizes between a few Å (crystal structure) and the mesoscopic scale (hundreds of nm). The neutron scattering length density of the crystalline regions was varied using the guest exchange procedure between toluene isotopologues incorporated as guests in the sPS lattice, while the scattering properties of the hydrated amorphous regions were varied using different H_2O / D_2O vapor mixtures. A direct understanding of conductive pathways is possible following the analysis of the relationship between the morphology of hydrated domains and proton conductivity measured under different conditions.

Abstract ID: 125

M3-IT2

Functional Molecular Granular Materials

Presenter: Panchao Yin (South China University of Technology)

Keywords: Molecular cluster, Topological interaction, Structural Evolution, Relaxation dynamics, Structure-property relationship

Molecular granular materials (MGMs) are constructed with sub-nanoscale molecular clusters (MCs) as the building units and they have recently been observed to possess enriched functionalities distinct from granular materials of colloid nanoparticles. Herein, the birth and recent research advances in MGMs are summarized with the topics covering the precise synthesis of MC assemblies with target topologies, the hierarchical relaxation dynamics and tunable viscoelasticity, impact-resistant capacity, and proton conductivity performance. The extremely small size of MC renders them two features: bulk diffusive dynamics with energy scale close to thermal fluctuation energy and the dominant volume fraction of surface structures. This finally leads to the hierarchical relaxation dynamics and broadly tunable viscoelasticity of MGMs although the structural units are with small sizes and low Mw. Therefore, MGMs have been applied as impact resistant materials and proton conductors for the highly tunable relaxation dynamics.

Abstract ID: 42

M3-IT3

Quasi-Elastic Neutron Scattering Studies on Hydration Water in the Vicinity of Biomolecules and Biocompatible Molecules

Presenter: Hideki Seto (IMSS/J-PARC, KEK (High Energy Accelerator Research Organization))

Keywords: Molecular cluster, Topological interaction, Structural Evolution, Relaxation dynamics, Structure-property relationship

Biological molecules are surrounded by water and their biological functions can only be realized in relation with water. The importance of elucidating the structure and dynamics of water molecules near biological molecules is widely recognized. In this viewpoint, we have investigated the water dynamics of lipid bilayers by quasi-elastic neutron scattering (QENS). [1] The results revealed that the hydration water could be categorized into three types: (1) free water, whose dynamics is similar to that of bulk water; (2) loosely bound water, whose diffusion coefficient is one order of magnitude less than that of free water; and (3) tightly bound water with lipid molecules. We also investigated the effect of adding salt and found that the number of tightly bound water differs depending on the binding sites of divalent cations. [2]

Next, we investigated the hydration water dynamics in the vicinity of synthetic polymers known as biocompatible polymers in order to verify the existence of “intermediate water”, which has been thought to be a key component for their bio-inert properties. The QENS experiments on aqueous solutions of poly(ethylene oxide) (PEO), which is a typical example of biocompatible polymer, were performed, and the significant amount of slow mode water were identified. [3] These results suggested that an existence of slow hydration water is a common feature in biological molecules and biocompatible polymers. In this presentation, we will show further QENS results obtained by the "Mode Distribution Analysis" method developed by one of the authors. [4] From this, the detailed picture of the hydration water in the vicinity of biocompatible materials will be given.

References:

[1] T. Yamada, H. Seto, et al., J. Phys. Chem. B, 121, 8322 (2017).
[2] H. Seto and T. Yamada, Appl. Phys. Lett., 116, 133701 (2020).
[3] T. Tominaga, H. Seto, et al., J. Phys. Chem. B, 126, 1758 (2022).
[4] T. Kikuchi, et al., Phys. Rev. E, 87, 062314 (2013).

Abstract ID: 153

M3-IT4

Universal dynamical transition of hydration water

Presenter: Liang Hong (institute of natural sciences and department of physics & Astronomy, shanghai jiao tong university)

Keywords: hydration water, low-temperature dynamics, biopreservation

Interfacial water remains liquid and mobile much below 0 °C, imparting flexibility to the encapsulated materials to ensure their diverse functions at subzero temperatures. However, a united picture that can describe the dynamical differences of interfacial water on different materials and its role in imparting system-specific flexibility to distinct materials is lacking. By combining neutron spectroscopy and isotope labeling, we explored the dynamics of water and the underlying substrates independently below 0 °C across a broad range of materials. Surprisingly, while the function-related anharmonic dynamical onset in the materials exhibits diverse activation temperatures, the surface water presents a universal onset at a common temperature. Further analysis of the neutron experiment and simulation results revealed that the universal onset of water results from an intrinsic surface-independent relaxation: switching of hydrogen bonds between neighboring water molecules with a common energy barrier of ~35 kJ mol^{-1}.

References:

L. Zheng, Z. Liu, Q. Zhang, S. Li, J. Huang, L. Zhang, B. Zan, M. Tyagi, H. Cheng, T. Zuo, V. G. Sakai, T. Yamada, C. Yang, P. Tan, F. Jiang, H. Chen, W. Zhuang, L. Hong, Universal Dynamical Onset in Water at Distinct Material Interfaces Chemical Science, 2022, 13, 4341.

Abstract ID: 46

M3-IT5

Cholesterol Content of Model Bilayers: Is it Really What we Expect? Answers from Neutron Reflectometry

Presenter: Stephen Holt (Australian Nuclear Science and Technology Organisation)

Keywords: Cell Membrane, Phospholipids, Cholesterol, Ergosterol, Neutron Reflectometry

Cell membranes are complex bilayer assemblies that perform the contradictory functions of separating the internal constituents of the cell from the cytoplasm but also enabling transfer of molecules across the membrane to perform functions essential to life. The major constituents of the membrane being phospholipids, sterols and proteins. Even this is a very reductionist view with there being many variations in size, shape, charge and function possible within this group of compounds. The simplest model employed consists of a single phospholipid assembled, in some manner, into a bilayer system. Even then there is the choice of working with saturated, unsaturated, branched tails and charged, neutral or extended headgroups to name but a few variations. Beyond combining different lipid molecules into the model system, the next step is usually the addition of cholesterol. It has been well established that cholesterol is important to the properties of cell membranes with there being many cholesterol dependant interactions/processes studied.

While the presence of cholesterol is crucial to the 'activity/function' of many model cell membranes it seems that the cholesterol content of model systems is not well defined or quantified. Many model systems are produced via a self-assembly process, often from vesicles and there is an implicit assumption that the ratio of phospholipid to cholesterol prepared in the bulk solution represents both the vesicle composition and the final structure deposited as a single bilayer at an interface. This may not always be the case.

This presentation will describe experiments undertaken with neutron reflectometry at a solid/liquid interface using deuterated/hydrogenous mixtures of phospholipids, cholesterol, ergosterol and buffer solution to quantify the bilayer composition. Cholesterol is the predominant sterol in mammalian cell membranes whereas ergosterol is the dominant sterol in fungal membranes. The results obtained from vesicle fusion (self-assembly) will be compared to those from Langmuir / Schaeffer deposition methods where the monolayer film composition is clearly defined prior to transfer to the substrate. The calculated average area per molecule from the scattering experiments is compared to that determined from molecular dynamics simulations.

Abstract ID: 120

M3-IT6

Electrostatic Interactions in Salt-Doped Polymers Revealed by Scattering Experiment and Theoretical Analysis

Presenter: Weichao Shi (Nankai University)

Keywords: Electrostatic interaction, Phase separation, Phase diagram, Concentration fluctuation

Electrostatic interaction of ions plays a significant role in polymer phase separation. However, the electrostatic interaction cannot be accurately analyzed at high salt concentrations, because of complicated interactions from segment-segment, ion-dipole, ion-ion and even ion clusters. We carry out experiments in the lithium salt-doped polystyrene/poly(ethylene oxide) (PS/PEO) blends, where the salt concentration is extremely low ([Li+]/[EO] = 0.0005) but effective. At this extremely low salt concentration, the effects of ion-ion Coulombic interaction, ion clusters and the entropy of dissociated ions are all trivial and can be neglected. From the small-angle neutron scattering and theoretical analysis, we get the interaction parameter $\chi=\chi_0+\chi_1+\chi_{sol}$, where χ_0, χ_1, χ_{sol} denote the segment-segment, cation-segment and anion-segment interactions, respectively. From the small-angle laser scattering, we find that the electrostatic interaction promotes phase separation significantly and deflects the phase diagram to the low volume fractions of PEO. Our study provides a reliable method to measure the electrostatic interactions in salt-doped polymers

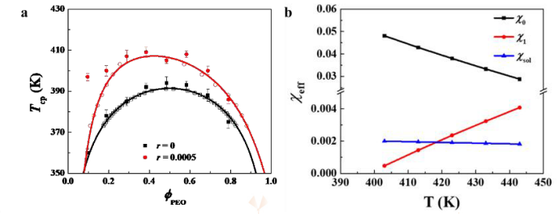


Fig. 1 Electrostatic effect on phase separation of PS/PEO blends. (a) shows the phase boundary is shifted upward and becomes asymmetric with addition of LiTFSI. (b) shows the temperature dependence of interaction parameters.

References:

[1] Wu, X.; Zhou, Y.; Song, T.; Chen, X.; Shen, L.; Jiang, H.; Ke, Y.; He, C.; Yang, H.; Shi, W. Macromolecules 2023, 10.1021/acs.macromol.3c00012.

[2] Wu, X.; Song, T.; Wei, Z.; Shen, L.; Jiang, H.; Ke, Y.; He, C.; Yang, H.; Shi, W. Polymer 2022, 260: 125307.

Abstract ID: 127

M3-IT7

Self-Assembly of Colloidal Nanoparticles into Supercrystals

Presenter: Sung-Min Choi (Department of Nuclear and Quantum Engineering, KAIST)

Keywords: Self-assembly, Nanoparticles, Supercrystals

The self-assembly of colloidal nanoparticles into supercrystals is of great interest as a unique strategy for fabricating materials with emergent properties. The emergent properties of nanoparticle supercrystals (NPSCs), which originate from the collective interactions among nanoparticles, provide new opportunities for applications of these materials in various fields such as plasmonics, photonics, electronics, magnetics, and catalysis. Different types of intermolecular forces, such as van der Waals forces, hydrogen bonds, and electrostatic interactions between nanoparticles have been used to fabricate NPSCs with different crystal symmetries and lattice parameters. Recently, we developed two new different approaches to form NPSCs: a spherical micelle-assisted method [1] and a covalent bonding interaction mediated method [2,3]. The spherical micelle-assisted method forms exceptionally ordered NPSCs which are inherently sensitive to environmental conditions. Upon mixing functionalized gold nanoparticles (AuNPs) with a nonionic surfactant micellar solution, NPSCs of different symmetries ($NaZn_{13}$, $MgZn_2$, and AlB_2-type) are formed in a tunable way. The NPSCs formed by this method show thermally reversible order-order ($NaZn_{13}$–AlB_2) and order-disorder ($MgZn_2$–isotropic) symmetry transitions. The covalent bonding mediated method forms highly ordered NPSCs with superior structural stability than those formed by intermolecular forces. Model solution phase anhydride and aldol reactions are used to form covalent bonds between molecules grafted on the surface of gold nanoparticles, resulting in three-dimensional NPSCs. The NPSCs are very stable in solvents of different polarity, in dried conditions, and at temperatures as high as 160 °C. In this talk, these two new methods for self-assembling nanoparticles into supercrystals will be presented with small angle scattering measurements.

References:

[1] Jae-Min Ha, Sung-Hwan Lim, Jahar Dey, Sang-Jo Lee, Min-Jae Lee, Shin-Hyun Kang, Kyeong Sik Jin, and Sung-Min Choi, Nano Letters 19, 2313 (2019)

[2] Jahar Dey, Sang-Jo Lee, Jiwhan Kim, Sung-Hwan Lim, Jae-Min Ha, Min-Jae Lee, and Sung-Min Choi, Nano Letters 21, 258 (2021)

[3] Jiwhan Kim, Jahar Dey, Aminah Umar, Jae-Min Ha, Sang-Jo Lee, Jehan Kim, and Sung-Min Choi, Chemistry of Materials 34, 15, 6744–6752 (2022)

Abstract ID: 114

M3-IT8

Understanding the molecularly heterogeneous interfaces of nanoparticles

Presenter: Zhi Luo (Southern University of Science and Technology)

Keywords: SANS, surface, proteins, nanomaterials

Interfaces, specifically solid-liquid interfaces, play important roles in many scientific fields. For example, protein functions rely largely on its complex surface structure, which is composed of nanoscale hydrophilic and hydrophobic domains. Likewise, the structured surface determines the self-assembly, molecular recognition, catalysis, and numerous other applications of nanomaterials. To date, the nanoscale interfacial structure-property relationship is still poorly understood. In this talk, I will focus on a specific type of nanoparticle that presents a molecularly heterogeneous surface through the self-organization of small molecules. A series of characterization techniques will first be introduced to reconstruct the 3D structure of these materials. With these tools, I will also explain some nonadditive interfacial properties of these nanoparticles, which deviates from the conventional continuum thermodynamic theories. Finally, the talk will end with discussions on how these results could help us better understand complex biological interfaces and regulate their solution behaviour.

Abstract ID: 132

M3-IT9

Multimodal Multiscale Neutron Measurements on Batteries

Presenter: Howard WANG (China Spallation Neutron Source)

Keywords: Multimodal, Multiscale, neutron, SANS, Batteries

A critical need for advancing battery technology is quantifying the distribution and transport of active ions in functioning batteries over wide temporal and spatial scales in real time. We have carried out critical *in-situ* neutron measurements on Li distribution and transport in electrodes and electrolytes during the battery operation and gain new insights in the function and failure of battery systems. Multimodal neutron measurements, including neutron reflectivity (NR), small angle neutron scattering (SANS), neutron depth profiling (NDP), and neutron imaging (NI), have been used to quantify the Li composition over length scales from sub-nanometers to centimeters. Data have revealed that heterogeneities in structures and transport occur at all scales and play a critical role in battery operation and health. We show that *in-situ* neutron diagnoses offer new opportunities in revealing mechanisms affecting the performance and lifetime of secondary batteries.

Abstract ID: 78

M3-IT10

Unraveling the solution aggregation structure of conjugated polymer blends

Presenter: Long Ye (Tianjin University)

Keywords: solution-state aggregation, conjugated polymers, molecular ordering, phase separation, organic solar cells

The best-performing active layers for organic photovoltaics generally include semi-paracrystalline polymers. However, the solution aggregation and molecular order of these photovoltaic blends and how they control the photovoltaic performance and stability remain elusive. Here, we show that the crystalline-amorphous interaction parameter plays a crucial role in determining the structure and performance of organic photovoltaic blends featuring semi-paracrystalline polymers. Solution small-angle neutron scattering and microstructure results reveal that the high molecularly ordered 2D semi-paracrystalline polymer system P5TCN:Y6 achieves stronger aggregates rigidity in the blend solutions and inherits in the films to form "locked" crystalline domains and intercrystalline links, which lead to the top-tier values and excellent thermal stability for polythiophene solar cells. By establishing correlations between various interaction parameters and solution structure parameters, we provide a comprehensive understanding of changes in aggregate rigidity of semi-paracrystalline polymers upon blending with nonfullerene acceptors and relationships between solution aggregation and performance of solar cells.

Abstract ID: 35

M3-IT11

Contrast variation and *in-situ* SANS studies on the correlation between properties and hierarchical structures of filled rubber

Presenter: Dong Liu

Keywords: Small-angle neutron scattering; China Mianyang research reactor; Contrast variation; Silicone rubber; Nanocomposites

In this report, we will discuss the progresses and applications of small-angle neutron scattering (SANS) spectrometer Suanni [1, 2] on the correlation between properties and hierarchical structures of silicone rubber. The hierarchical structures of series silica-filled silicone rubbers have been investigated by utilizing contrast variation-SANS (CV-SANS) with an established three-level unified Guinier-exponential/power-law approach, with which the correlation among formula, hierarchical structure, and performance of the composites were discussed [3]. Recently, for unveiling the 'microstructure-property' relationship of silicone rubber, systematical investigations were conducted with combining contrast variation, chain labeling, *in-situ* Rheo-SANS (time-resolved) techniques [4-7]. Accordingly, the roles of matrix, interface, and filler networks as well as their interactions on the origin of the softening/hysteresis, Mullins effect, etc. of the composites were discussed.

Reference:

[1] M Peng*, et al., Nucl. Instrum. Meth. Phys. Res., Sect. A, (2016), 810: 63-67.

[2] J Chen, et al., Nucl. Instrum. Meth. Phys. Res., Sect. A, 1051 (2023) 168228

[3] Y Shui, et al., Comp. Sci. and Tech. 215 (2021) 109024.

[4] Y Shui, et al., Composites Communications, 23 (2021) 100547

[5] TT Yang, et al., Composites Part B 242, (2022), 110100

[6] JJ Han, et al., Composites Part A 172 (2023) 107586

Abstract ID: 159

M3-IT12

Investigation of Protein Dynamics and its Relation with Enzymatic Activity by Neutron Scattering

Presenter: Xiangqiang Chu (City University of Hong Kong)

Keywords: QENS, SANS, NSE, Protein Dynamics

Proteins undergo sophisticated motions in space and time, which are believed to govern the biological function and activities of the proteins ultimately. Quasi-elastic neutron scattering (QENS) provides exceptional tools for studying the dynamics of proteins in the time range of 10ps to 1ns at the molecular level. In this talk, based on our recent work on different biological systems studied by QENS and other techniques, such as SANS, INS, and NSE, I will discuss the possibility of combining these techniques to directly connect the dynamic behavior of proteins with their activities or functions.

References:

[1] Z. Wang, et al, "Experimental Evidence for the Role of Dynamics in pH-Dependent Enzymatic Activity", submitted.

[2] U. R Shrestha, et al, "Experimental Mapping of Short-wavelength Phonons in Protein as Precursor to Bioactivity", The Innovation, 3 (1), 100199 (2022).

[3] Shrestha et al., Proc Natl Acad Sci USA, 112 (45): 13886-13891 (2015).

Abstract ID: 75

M3-IT13

Solution Self-assembly of Peptoid Polymers Investigated by Small Angle Scattering

Presenter: Naisheng Jiang (University of Science and Technology Beijing)

Keywords: Block Copolymer, Solution, Self-assembly, Crystallization, Scattering

Amphiphilic block copolymers (BCPs) have been widely recognized for their ability to self-assemble in solution, offering a versatile approach to engineer nano- and meso-structures with tailorable sizes and functionalities. In this study, we investigate the solution self-assembly of peptoid diblock copolymers and triblock terpolymers bearing various crystalline blocks. A series of well-defined peptoid nanostructures has been created in solution, ranging from one-dimensional (1D), two-dimensional (2D) to multi-dimensional hierarchical assemblies. Small-angle X-ray/neutron scattering allowed us to unveil the fundamental relationships between chemical structure, molecular arrangement, phase structure, and solution aggregation of these polymers, thereby providing a better understanding of the self-assembly process within the relevant length and time scales.

The 4th Asia-Oceania Conference on Neutron Scattering

M3. Contributed Talks

Abstract ID: 10

M3-CT1

Combining neutron scattering and selective deuteration to study the dynamics of surrounding matrix of soft materials

Presenter: Zhuo Liu (Shanghai Jiao Tong University)

Keywords: elastic incoherent neutron scattering, selective deuteration, mutual coupling effect, hydrogen bond relaxation, energy barrier

The surrounding matrix of soft materials plays an important role on their structure, dynamics, and function. Therefore, a deep understanding on the interplay between soft materials and their surrounding matrix is crucial for storage and application of soft materials. To elucidate their interdependence, a direct experimental characterization on the dynamics of each component is imperative. It is well known that water is a ubiquitous surrounding matrix on soft materials, and interfacial water can exert a remarkable impact on the dynamics and function of materials, such as enhancing proton conduction of graphene oxide and improving enzymatic activity of proteins. Here, by combining neutron scattering and selective deuteration, we probed the dynamics of water and the underlying substrates independently below 0°C across a broad range of soft materials. The onset of the rapid increase of mean squared displacement with increasing temperature marks the harmonic-to-anharmonic transition in the mixture, namely the dynamical onset. Surprisingly, while the function-related anharmonic dynamical onset in the materials exhibits diverse activation temperatures, the surface water presents a universal onset at a common temperature, i.e., ~200 K. Our analysis of the neutron experiment and simulation results revealed that the universal onset of water results from an intrinsic surface-independent relaxation: switching of hydrogen bonds between neighboring water molecules with a common energy barrier of ~30 kJ/mol. This result implies that the surrounding matrix can have an intrinsic property that is independent on the soft materials.

A further question is whether the energy barrier can be altered by adding some cosolvents in the binary mixture of soft materials and water. To address this question, we extended our research to a more complicated system, which is the ternary mixture of protein, water, and glycerol. Glycerol, as a cryoprotectant, has been extensively investigated to unveil the protective mechanism of surrounding matrix on biomacromolecules. Specifically, it is quite difficult to experimentally distinguish the dynamics of water and cosolvents in a ternary mixture. Fortunately, the combination of neutron scattering and selective deuteration allows us to characterize the individual motions of each component in the protein-water-glycerol mixture. Consequently, we observed the consistent dynamic onset temperatures of protein, water, and glycerol, revealing the mutual coupling effects among the three components. Furthermore, our experimental and simulation results showed that the hydrogen bond relaxation energy barrier in the ternary system is ~43 kJ/mol, whereas in the protein-water binary system, it is merely ~30 kJ/mol. Therefore, we suggest that glycerol can enhance hydrogen bond interactions in the ternary system through the mutual coupling effect, thereby serving as one of the protective mechanisms of protein preservation by glycerol.

In summary, we combined neutron scattering and selective deuteration to study the dynamics of surrounding matrix of soft materials. In the binary system of soft materials and water, we found a universal dynamical onset in water at distinct material interfaces, and the dynamical onset results from a surface independent relaxation process in water with an approximately universal energy barrier of ~30 kJ/mol. Furthermore, we observed a mutual coupling effect between protein, water, and glycerol in the ternary system. More importantly, our study on the dynamics of surrounding matrix showed a higher hydrogen bond relaxation energy barrier in the protein-water-glycerol ternary system, i.e., ~43 kJ/mol. Based on these observations, we propose that the addition of glycerol to aqueous protein solutions can enhance hydrogen bond interactions in the ternary system through the mutual coupling effect, representing one of the protective mechanisms of protein preservation by glycerol. Thus, our investigation on the dynamics of surrounding matrix of soft materials have not only revealed the individual dynamics in both binary and ternary systems by experiment, but also elucidated the effect of glycerol on the hydrogen bond interactions in the ternary system, enlightening the development of more effective cryoprotectant.

Abstract ID: 195

M3-CT2

Screening, characterization and application of self-assembled targeting peptides

Presenter: Weizhi Wang (Beijing Institute of Technology)

Keywords: Targeting peptide, molecular recognition, self-assembly

Targeting peptides are promising for biomedical and other applications due to their designability, high affinity and biocompatibility, et al. However, the number of available targeting peptides is too limited to meet the demand for applications. In addition, small molecule peptides are difficult to bind stably to their targets and are susceptible to enzymatic degradation and loss of their activity. Therefore, there is an urgent need to develop targeting peptides with novel sequences and the ability to bind stably to the target. Self-assembly is a special property possessed by peptide. Under the action of a series of non-covalent bonds, sequence-specific peptide molecules can form long-range ordered nanostructures, which not only greatly improve the enzymatic stability of the peptide, but also facilitate multivalent binding to the targets. Based on the above research status, we designed a peptide library using the de novo design approach, and then used combinatorial chemistry to synthesize peptides with a capacity of 105-108. In order to efficiently obtain targeting peptides with high affinity for any target, we have developed a microfluidic screening platform that enables peptide library screening in several hours. For cancer, we have screened a series of high-affinity, self-assembling targeting peptides using immune checkpoints (PD-L1, CD47) and tumor-associated proteins (DDR2, Rbm38) as targets. The peptide assembly behaviors and morphological parameters were further investigated by SANS, AFM, and MD, and verified at cellular, in vivo level to have potent anti-tumor effects.

Abstract ID: 185

M3-CT3

Small angle neutron scattering studies on wood bio-composites

Presenter: Pan Chen (Beijing Institute of Technology)

Keywords: cellulose, plant cell wall, nanocomposites

Transparent wood bio-composites based on polymethyl methacrylate (PMMA) combine high optical transmittance with excellent mechanical properties. One hypothesis is that despite poor miscibility between hydrophobic PMMA and hydrophilic hydroxy group on the cellulose surface, the polymer is distributed at the nanoscale, inside the cell wall. Small-angle neutron scattering (SANS) experiments are performed to test the hypothesis, using bio-composites based on deuterated PMMA. The wood cell wall nanostructure is quantified in terms of the correlation distances d between the center of elementary cellulose fibrils. This distance is slightly increased for bio-composites based on deuterated PMMA, showing that the polymer is indeed distributed in the cell wall at the scale of nanometers. Results are verified by complementary small-angle neutron scattering with contrast matching and X-ray scattering (SANS/SAXS) data. The specific processing method used for transparent wood explains the nanocomposite nature of the wood cell wall and can serve as a nanotechnology for cell wall impregnation of polymers in large wood biocomposite structures.

Abstract ID: 188

M3-CT4

Neutron Backscattering Spectrometer (NuBS) at CSNS

Presenter: Hongyu GUO (Institute of High Energy Physics)

Keywords: Backscattering Spectrometer, dynamics

NuBS at CSNS is the only Backscattering Spectrometer in China. The preliminary design of NuBS has been finished recently. Hopefully, we can deliver it by the end of 2027. NuBS can provide very fine energy resolution, as low as 3.0μeV, at the elastic peak. This requires a long initial guide section of 90 m from moderator to sample in order to achieve the timing resolution necessary for obtaining the desired energy resolution. In fact, NuBS is the longest instrument at CSNS. NuBS also provides an excellent dynamic range near the elastic peak of about plus and minus 300 μeV in the standard high-intensity operation regime, which, if needed, could be extended to plus and minus 600 μeV and beyond. NuBS will be used to probe dynamic processes in various systems on the pico- to nanosecond time scale. It is well suited for study of Soft Matter and Life Science.

Abstract ID: 167

M3-CT5

The structure change of SARS-CoV-2 nsp8 studied by Small Angle scattering

Presenter: Jiang Xin (City university of Hong Kong)

Keywords: Small Angle Neutron Scattering, RNA-dependent RNA polymerase, nsp8, protein structure change

As an RNA virus, the replication process of SARS-CoV-2 is mediated by RNA-dependent RNA polymerase (RdRP). The nsp12-nsp7-nsp8 is the smallest complex with RdRP activity. Nsp8 both has the primase activity for de novo RNA synthesis, and regulates the polymerase activity of nsp12, which plays a key role in the replication of the SARS-CoV-2. In addition, the nsp8 is highly conserved, so the inhibitors targeting nsp8 are expected to be broad-spectrum antiviral drugs and have important therapeutic application potential. Many research focus on the structure of RdRP complex by cryo-EM and diffraction technology, which laid solid foundations for understanding RdRP complex [1-2]. We further characterize the structure of nsp8 in a solution state by Small Angle Neutron Scattering (SANS) technology and study its conformational changes in response to changes in the cellular environment, so as to understand its dynamic structure of nsp8.

Our previous research demonstrates that the phase separation of nsp8 in cell and regulated by salt concentration, and the conformational change of nsp8 mediates by salt concentration regulation through SANS experiment [3]. In this work, we further investigated the structural changes of nsp8 dimers and tetramers in response to temperature changes and binding to RNA. We found that nsp8s tend to fold into a denser state at higher temperatures to protect the active center of the protein against heat stress. In addition, we further studied the conformational changes of nsp8 dimer and tetramer binding to RNA in solvents with different proportions of D_2O by SANS contrast matching strategy.

In conclusion, we studied the two stable aggregation states of nsp8, dimer and tetramer by SANS technology and Molecular Dynamics simulation. We found that nsp8 tetramer has more exposed active centers, which induce structural changes to better bind RNA and in response to temperature changes, thus regulating the process of viral RNA synthesis, which help to understand the molecular mechanism of viral replication process and further guide the design of anti-viral drugs.

Reference

[1] Wang Q, Wu J, et al. Structural Basis for RNA Replication by the SARS-CoV-2 Polymerase. Cell. 2020 Jul 23;182(2):417-428.e13.

[2] Gao Y, Yan L, et al. Structure of the RNA-dependent RNA polymerase from COVID-19 virus. Science. 2020 May 15;368(6492):779-782.

[3] Xu J, Jiang X, et al. Multiscale characterization reveals oligomerization dependent phase separation of primer-independent RNA polymerase nsp8 from SARS-CoV-2. Commun Biol. 2022 Sep 7;5(1):925.

Abstract ID: 182

M3-CT6

In-situ observation of structural transformation of photo-responsive materials with small-angle neutron scattering

Presenter: Hanqiu Jiang (China Spallation Neutron Source)

Keywords: time resolved small angle neutron scattering; *in-situ* light irradiation system; photo-responsive materials

Upon light irradiation, the molecular conformational change of photo-responsive materials can be integrated and amplified through the microscale assemblies, and lead to distinct macroscopic properties. Understanding the transition pathway of the assembled microstructures during the photo-responsive cycle is crucial for the establishment of a dynamic structure-property relationship and achieving precise control of macroscopic behaviors of photo-responsive materials.

Small-angle neutron scattering (SANS) is a powerful technique for studying the structure and inhomogeneity of a sample in the nanometer scale. The isotope sensitive feature of neutron, especially the large scattering length difference between hydrogen and deuterium, has made SANS indispensable for the study of the structure and dynamics of hydrogen-rich materials such as polymers and biological macromolecules. Time-resolved small angle neutron scattering experiment allows for capturing of the transient structures down to seconds. However, due to the limitation of neutron flux, direct acquisition of statistically usable scattering data of such high time-resolution is not really feasible.

In this presentation we present a newly developed *in-situ* photo-irradiation device with synchronized photo irradiation and neutron data acquisition. Higher time-resolution can be achieved through careful extraction, alignment and stacking of the data from repeated measurements. The preliminary results from a photo-responsive rotaxane dendrimer sample and a traditional micelle sample will be presented.

Abstract ID: 190

M3-CT7

The *in-situ* tensile apparatus in small angle neutron diffractometer at China Spallation Neutron Sources and its application in different materials

Presenter: Zhenhua Xie (Spallation Neutron Source Science Center)

Keywords: small angle neutron scattering, *in-situ* tensile, microstructures evolution

The nanoscale microstructures and their evolution under multi-field coupling condition are important to materials' property and service stability. However, most of the "structure-property" studies were carried out for *ex-situ* condition, because it is difficult to *in-situ* investigate the microstructures evolution under complicated fields. Small angle neutron scattering (SANS) has been widely used to probe the nanoscale structures in different materials. Due to the high penetration of neutrons, it is a powerful technique for *in-situ* experiments with complicated sample environments, such as load frame and furnaces. Based on small angle neutron diffractometer at China Spallation Neutron Sources (CSNS), we build up an *in-situ* stress-temperature loading apparatus. Its maximum load capacity is 10 kN, and the available temperature range is from -70 to 400 ºC. In-situ SANS experiments on composites, polymer networks, hydrogels and alloys under thermal-mechanical coupled field loading conditions were carried out by using this apparatus. The SANS 2D scattering pattern was found to evolve from isotropic to anisotropic with stress loading, which reveals the morphology and spatial orientation change of the nanoscale aggregation in the specimen.

Abstract ID: 130

M3-CT8

Nanoparticle dispersion in PMMA/SiO_2 nanocomposite films studied using the small-angle X-ray and neutron scattering

Presenter: Che-Yi Chu (Department of Chemical Engineering, National Chung Hsing University)

Keywords: polymer nanocomposite, nanoparticle dispersion control

Our previous study has investigated the effect of the polymerization rate on the nanoparticle dispersion in the nanocomposites formed by poly(methyl methacrylate) (PMMA) and silane-modified silica (M-SiO_2) nanoparticles via free radical polymerization, where the tethered silanes were capable of polymerizing with the MMA monomer (Macromolecules 2019, 52, 8312-8322). It was found that, at slower polymerization, the nanoparticles could self-organize to form a mass-fractal network structure with an average fractal dimension of 2.7, in which the M-SiO2-rich clusters by interparticle bridging were organized into a hierarchical fractal network by intercluster bridging. By contrast, the nanoparticles exhibited a dispersed morphology when the polymerization proceeded at a faster rate. It is noting that the aforementioned structural change revealed by small-angle X-ray scattering (SAXS) studies was proposed to be correlated to the interfacial property between the polymer matrix and nanoparticles. Thus, in this work, the role of the interfacial density profile in dominating the nanoparticle dispersion of the PMMA/M-SiO_2 nanocomposites is further characterized by means of the contrast-variation method with different H/D ratios of the PMMA phase using small-angle neutron scattering (SANS), through which the localization of the PMMA chains in the fractal-forming nanocomposite can be identified as well.

Abstract ID: 163

M3-CT9

The investigation for static structures and dynamical behaviors for polystyrene during glass transition

Presenter: Zehua Han

Keywords: glass transition, small angle neutron scattering, molecular dynamics simulation

The phenomenon of glass transition has long stood as a profound, intriguing, and unresolved puzzle in the field of soft matter physics. Understanding the changes in static structures and dynamic behaviors during glass formation and transition is crucial. Yet, one of the key challenges lies in the difficulty of directly observing the molecular origins of this process.

In our research, we successfully employed a combination of small-angle neutron scattering (SANS) and molecular dynamics (MD) simulation to directly visualize the most probable all-atom structure of polystyrene (PS) during the glass transition. PS, chosen as our sample due to its simplicity and representativeness, enabled our analysis to delve into both static structures and dynamical behaviors. This approach allowed us to decipher the events from melting to the glass state, uncovering the profound and intrinsic reasons behind this phenomenon.

Concerning static structures, we identified the characteristic structures of PS and observed their changes during glass formation and transition. Polymers typically exhibit broad peaks in the range of 0.5-2 $Å^{-1}$, reflecting their inherent structures. During the glass transition, these peaks change, providing crucial insights into the process. We discovered specific peaks in PS related to the glass transition: one at 0.6 $Å^{-1}$ from segment-segment interactions and another at 1.4 $Å^{-1}$ from phenyl-phenyl interactions. Below the glass formation temperature, both peaks remain constant in heights and shapes. While during glass formation, they exhibit jumps, revealing configuration variation and phenyl flipping in the melting state.

To further analyze the dynamical behaviors of PS during glass formation, we employed temperature-dependent MD simulations. Utilizing various theories, including free volume, dynamic heterogeneities, and cooperative rearrangement, we gained significant insights. Close to glass formation, the polymer is confined within tubes, whose diameter corresponds to the main chain-main chain distance. This model explains the kinetic pathway dependence of Williams-Landel-Ferry (WLF) free volume. Notably, this is a statistical concept and cannot be observed in any single frame of static structure. Therefore, we turned to the theory of cooperative rearrangement, which is reasonable due to confinement during glass formation. From MD simulation results, we identified Cooperative Rearrangement Regions (CRRs) in real space and explored their characteristics. CRRs grow over extended time and length scales, typically moving through loosely occupied space. Our observations unified the concepts of free volume and cooperative rearrangement. We propose that statistical averaging leads to the formation of a polydisperse "static cage", providing the foundation for CRR formation and offering loose space for their movements.

Through our study of both static structures and dynamic behaviors of PS, we unraveled the events during glass formation and transition. Importantly, we believe this approach, combining neutron scattering and computer simulations, can open new avenues for directly investigating and analyzing atomic details in disordered macromolecular systems.

Abstract ID: 166

M3-CT10

A high performance small-angle scattering simulation method with GPU acceleration

Presenter: Mu Li (Institute of Advanced Science Facilities, Shenzhen)

Keywords: small-angle scattering; simulation; fast Fourier transform; GPU acceleration

Particle-solution system is one of the main research objects of small-angle neutron scattering (SANS). Benefits from the unique features of neutrons, SANS can characterize the morphology and internal structure of particles in solution *in-situ*, which has important applications in soft matter and life science, such as studies of proteins, nanoparticles, polymer solutions etc. The interpretation of solution SANS data highly depends on model fitting. Model fitting requires the derivation of corresponding scattering equations for possible geometrical structures in order to calculate the theoretical scattering curves, which is often difficult for complex structures. At present, there are several methods and software capable of calculating the one-dimensional theoretical scattering curves from particle structures, including Debye equation method (e.g., FoXS), spherical harmonics expansion method (e.g., CRYSON) etc. However, the computation time of these methods is usually in the order of seconds to minutes, which didn't reach the practical level in scenarios such as data fitting and large-scale batch computation. Based on the basic principle of small-angle scattering (SAS), we developed a high-performance SAS simulation method based on fast Fourier transform (FFT) algorithm. The method conducts spatial Fourier transform on the scattering length density (SLD) distribution of the whole particle, and then obtaining scattering intensity by sampling and interpolating directly in the reciprocal space. In order to take advantage of modern high-performance GPUs, the computation flow is optimized to use GPU acceleration, which greatly improves the speed. With similar or better accuracy, our method achieves better performance less than a second, which can serve as an important basis for the subsequent developments of SANS data analysis.

Abstract ID: 196

M3-CT11

Mechanism study on the structural and mechanical properties of triblock copolymer hydrogels using *in-situ* SAXS and SANS

Presenter: Mengze Lu (South China University of Technology)

Keywords: Amphiphilic triblock polymer hydrogel; Mechanical property; SAXS; SANS

Hydrogels are a class of soft and wet materials composed of a hydrophilic three-dimensional polymer network and water. As hydrogel materials find increasingly wide-ranging applications in areas such as medical devices, tissue engineering, and flexible electronic devices, there is a growing demand for understanding and enhancing their mechanical properties. This study presents a novel approach in the design of physically cross-linked hydrogel materials through self-assembly of amphiphilic triblock copolymers (ABA or BAB). The hydrophobic segments of the copolymer form crosslinking points in an aqueous environment, thereby maintaining the material's structure and imparting elasticity. The weak interactions between the hydrophilic segments function as dynamic bonds that can be broken under load, absorbing energy and conferring toughness to the material. Upon unloading, these dynamic bonds reform, endowing the material with self-healing properties. In this research, we employed synchrotron s small-angle X-ray scattering (SAXS) and small-angle X-ray scattering (SANS) to analyze the structural organization of the block copolymer self-assembly in the hydrogel. Additionally, *in-situ* SAXS and SANS techniques were utilized to monitor the structural evolution of the hydrogel during the tensile deformation, enabling the establishment of a relationship between the internal structure and the macroscopic mechanical properties of the hydrogel. Preliminary findings suggest the presence of numerous microscale continuous pore structures within the hydrogel material, with the copolymer forming a lamellar phase. This lamellar structure undergoes evolution as the material undergoes deformation. The study extensively discusses the impact of polymer molecular weight and compositional constituents on the formation of the gel phase structure and explores the effects of internal structural evolution on the macroscopic mechanical performance of the material.

Abstract ID: 158

M3-CT12

Complementary use of molecular dynamics, SANS and SAXS methods

Presenter: Alexey Shvetsov (Petersburg Nuclear Physics Institute named by B. P. Konstantinov of NRC «Kurchatov Institute»; Research Center "Kurchatov Institute" Institute; Peter the Great St. Petersburg Polytechnic University)

Keywords: MD, GROMACS, SANS, SAXS

SANS and SAXS methods are widely used to study various types of biological systems. However, in general, small-angle scattering methods provide only limited insight into the structure of biomacromolecular complexes in solution. In this case, small-angle scattering can be used in combination with other methods, such as molecular modeling and molecular dynamics taking into account the influence of the solvent, which in some cases can make it possible to construct detailed all-atomic models of the biomacromolecular complex under study in solution.

The use of SAXS, SANS and molecular dynamics methods requires a direct comparison of data obtained by small-angle scattering methods and molecular dynamics data. In this case, the correct consideration of the contribution of the solvent remains an important factor, especially in the case of using contrast methods. We used our developed method for calculating SANS curves[1] for a number of multicomponent biological systems, such as the RecA::ssDNA, RecA::RecX::ssDNA[2] complexes, various influenza A virus RNP complexes[3], lactoferrin and other biomacromolecular systems. In some cases, the use of such a combined approach even makes it possible to find new, previously unknown complexes in solution or shed light on some interesting effects with parameters observed from SANS data.

Reference:

[1] Shvetsov A.V. et.al. doi:10.1134/S1027451013060372

[2]Shvetsov A.V. et.al. doi:10.1016/j.febslet.2014.01.053

[3]Shvetsov A.V. et.al. doi:10.1080/07391102.2020.1776636

Abstract ID: 48

M3-CT13

Introducing a software that uses small-angle neutron scattering experiments to analyze three-dimensional structures at the nanoscale

Presenter: Changli Ma (Institute of High Energy Physics)

Keywords: small-angle neutron scattering, three-dimensional structures at the nanoscale

Using the inverse Monte Carlo method, we developed an analysis software to reconstruct the nanoscale three-dimensional structure of experimental samples based on small-angle neutron scattering experimental data. The software uses GPU-accelerated technology to analyze systems containing millions of particles. The software uses OpenGL to display the analysis results directly.

Abstract ID: 187

M3-CT14

Conformation and aggregation of conjugated polymers in solution

Presenter: Guoming Liu (Institute of Chemistry, Chinese Academy of Sciences)

Keywords: Conjugated polymers, Conformation, Scattering

Conjugated polymers have been intensively investigated as the base material for optoelectronic devices owing to their excellent solution processability. Theories have correlated charge mobility with persistence length. More rigid backbones, among which coplanar ones, with maximized overlapping of wave functions, should facilitate a pathway for carrier transport. However, a direct link between chain rigidity and optoelectronic properties has not been established yet. In this presentation, I will introduce the recent results of the measurement of the persistence length of conjugated polymers by static/dynamic light scattering and small angle neutron scattering techniques, using several conjugated polymers as examples, covering semiflexible chains to rod-like chains. The process of aggregation from individual chains in solution with time and temperature is a typical feature of those polymers. A rod-like conformation can effectively reduce the disorder in the melt state of aromatic planar extended polymers.

Abstract ID: 154

M3-CT15

The multi-slit very small angle neutron scattering instrument in China Spallation Neutron Source

Presenter: He Cheng (spallation neutron source science center)

Keywords: small angle neutron scattering, neutron focusing, multi-slit

A multi-slit Very Small Angle Neutron Scattering (MS-VSANS) instrument has been finally accepted in China Spallation Neutron Source (CSNS). It is the first VSANS instrument based on a spallation neutron source. MS-VSANS has a good signal-to-noise ratio, and can cover a wide scattering vector range from 0.00028 $Å^{-1}$ to 1.4 $Å^{-1}$. In its primary flight path, a combined curved multichannel beam bender and sections of rotary exchange drums are installed to minimize the background at downstream of the instrument; an exchangeable multi-slit beam focusing system is integrated into the primary flight path, enabling a minimum scattering vector of 0.00028 $Å^{-1}$. MS-VSANS has three modes, i.e., conventional SANS, polarizing SANS and VSANS modes. In SANS mode, three motorized high efficiency 3He tube detectors inside the detector tank cover the scattering angle from 0.12 to 35 degrees simultaneously; in polarizing SANS mode, a double-V cavity provides highly polarized neutrons and a high-efficiency ^{3}He polarization analyzer allows full polarization analysis; in VSANS mode, an innovative high resolution GEM detector covering the scattering angle from 0.016 to 0.447 degrees. The absolute scattering intensity of standard samples are obtained by using the direct beam method. Effectiveness of the method is verified by testing standard samples and comparing the results from a benchmark instrument. The instrument is designed to be flexible and versatile, and all the designed goals have been achieved.

The 4th Asia-Oceania Conference on Neutron Scattering

Scientific Parallel Session M4. Engineering and Industrial Applications

The 4th Asia-Oceania Conference on Neutron Scattering

M4. Keynote Talks

Abstract ID: 68

M4-KT1

Development and application of pulsed neutron imaging at J-PARC MLF

Presenter: Takenao SHINOHARA (Japan Atomic Energy Agency, Japan)

Keywords: neutron imaging, energy-resolved imaging, pulsed neutrons

Neutron imaging is regarded as a fundamental technique to observe the interior of a bulk object non-destructively or to study behavior of substances composed of light elements by using the neutron's large penetration power and high sensitivity to light elements. The conventional neutron imaging method simply dealt with attenuation of the white neutron beam. However, the analysis of energy dependent neutron transmission spectra position by position enables us to map and visualize spatial distribution of physical information of the object, such as crystallographic information, elemental or thermal information, magnetic information, and so on. The utilization of a short-pulsed neutron beam in this imaging technique offers significant advantages, not only in its fine energy resolution but also in its high efficiency. This is particularly advantageous in the quantification of analyzed data. In J-PARC, we have constructed the energy-resolved neutron imaging system, named "RADEN", as the dedicated beamline for energy-dependent neutron imaging experiments. This instrument was designed to fully conduct Bragg edge imaging, neutron resonance absorption imaging and pulsed polarized neutron imaging together with the state-of-the-art conventional neutron imaging.

RADEN is now used by users in various scientific and industrial fields. Especially industrial applications on the hydrogen fuel cells and Li ion batteries for the electric vehicles are intensively conducted to improve their performance due to the recent movement toward carbon neutrality.

In this presentation, development of pulsed neutron imaging techniques at J-PARC will be introduced and results of application studies will be discussed.

Abstract ID: 49

M4-KT2

Fatigue Properties of Entropy Alloys Manufactured by Hot-Rolling and Additive Manufacturing

Presenter: Soo Yeol LEE (Chungnam National University, Korea)

Keywords: entropy alloy, fatigue, hot rolling, additive manufacturing

In this work, we report low-cycle-fatigue properties of CoCrFeMnNi and CoCrNi entropy alloys manufactured by direct-energy-deposited (DEDed) and hot-rolled (HRed) processes. The CoCrNi medium entropy alloy exhibits superior tensile and fatigue properties in comparison with CoCrFeMnNi high entropy alloy. The DED process offers advantages in terms of fatigue strength and toughness. However, the fatigue life of the DEDed samples was inferior to that of HRed samples. A dislocation slip mode is primarily activated in both HRed and DEDed CoCrFeMnNi alloy during fatigue deformation, forming a dislocation cell structure. On the other hand, nano-twins are significantly developed in CoCrNi alloys due to lower stacking fault energy (SFE) and a localized stress concentration. Especially, multiply deformed microstructures, such as stacking faults, nano-twins, and hexagonal close-packed (HCP) phase, are generated in DEDed CoCrNi alloy. These are attributed to low effective SFE and high capacity of strain energy density. These diverse microstructures improved fatigue resistance by acting as obstacles by impeding crack propagation and promoting crack branching. Meanwhile, anisotropic microstructural evolution of HRed and DEDed CoCrNi is due to leading and trailing partial dislocations depending on crystallographic orientation. The current research demonstrates that the alloy can be effectively applied to different industrial fields by tuning the fatigue characteristics via a control of the manufacturing process.

Abstract ID: 86

M4-KT3

Using Neutron Diffraction Investigating Fatigue Behavior of Advanced Metallic Systems

Presenter: E-Wen HUANG (National Yang Ming Chiao Tung University, Taiwan)

Keywords: entropy alloy, fatigue, hot rolling, additive manufacturing

High-entropy alloys and additive manufacturing are emerging topics for the advanced metallic systems. In this talk, few selected cases are summarized to demonstrate the unique neutron diffraction methods to examine the fatigue behavior of the advanced metallic systems. The samples were measured by *in-situ* neutron-diffraction experiments subjected to continuous loading, such as tension-compression cyclic loading at different temperature. With spallation neutron, the evolutions of multiple diffraction peaks are collected simultaneously in the axial loading direction and radial direction of the cylindrical dog-bone specimen for lattice-strain measurement and peak profile analysis. In one of the representative cases, recorded temperature variations during fatigue cycles are compared with the thermodynamics-model predictions based on lattice structural changes. The discrepancy between the modeled and measured temperature evolution indicates the evolution of the microstructure during fatigue deformation, which is validated from the microscopic examination.

Abstract ID: 136

M4-KT4

Engineering and Industrial Research at the Australian Centre for Neutron Scattering

Presenter: Max AVDEEV (ANSTO, Australia)

Keywords: neutron scattering, engineering and industrial applications

Wide available range of energies, high penetration, and centimetre size beams make neutron scattering an invaluable tool for engineering and industrial research, as materials and components can be studied in real-life size and under real-life conditions. The suite of instruments installed at the OPAL research reactor (ANSTO) enables non-destructive probing of structural and dynamic properties of materials in a wide range of scale, from atomic structure and defects to microstructure (texture, stress) to macro level (imaging). Even more insights are gained when several neutron scattering techniques are used in combination.

I will present an update on capabilities and recent highlights of diverse applied research at the Australian Centre for Neutron Scattering.

The 4th Asia-Oceania Conference on Neutron Scattering

M4. Invited Talks

Abstract ID: 61

M4-IT1

Neutron diffraction analysis method to elucidate deformation mechanisms of metals with multimodal-structures and -deformation modes

Presenter: Stefanus Harjo (J-PARC Center, Japan Atomic Energy Agency)

Keywords: Metals, Deformation, *In-situ*, Stress, Phase transformation

In-situ neutron diffraction during deformation becomes the well-known probe to elucidate the deformation mechanisms of various metals, bridging the microscope-microstructural information with the mechanical properties. However, for advanced materials with excellent mechanical properties, the analysis procedure becomes very complicated and it is difficult to understand the detailed deformation mechanisms. Many advanced metallic materials composed of not only multiphases but also multi-morphological structures within one of the constituent phases, so-called multimodal structure metallic material. On the other hand, in addition to dislocation glide, so-called multimodal deformation modes such as phase transformation, stacking faults, twinning, and serrated deformation accompany many advanced metallic materials to express their excellent mechanical properties. In this presentation, we will introduce and discuss our methods to understand the deformation behavior in metallic materials with multimodal structure and multimodal deformation mode, using two cases: (i) Strengthening of αMg and long-period stacking ordered phases in a Mg-Zn-Y alloy by hot-extrusion with low extrusion ratio, and (ii) Quantitatively evaluating the huge Lüders band deformation in an ultrafine grain stainless steel by combining *in-situ* neutron diffraction and digital image correlation analysis.

Abstract ID: 191

M4-IT2

Characterisation of Residual Stress, Intergranular Strain and Microstructure by Neutron Techniques

Presenter: Bo Chen (University of Leicester)

Keywords: Residual stress, Microstructure, Creep, Fatigue, Diffraction, Small-angle scattering, Bragg-edge transmission imaging

Structural integrity is a multidisciplinary field that encompasses various disciplines, including physical metallurgy, mechanical engineering, and chemistry, among others. A reliable assessment procedure for the structural integrity requires a thorough understanding of materials characterisation and testing, manufacturing processes, and stress analysis, not only during construction but also throughout the service life. This talk aims to demonstrate the engineering applications of neutron techniques, including diffraction, small-angle scattering, and Bragg-edge transmission imaging, from a user's perspective. The experiments were primarily conducted using beamlines at the ISIS pulsed neutron source, such as ENGIN-X, ZOOM, LARMOR, and IMAT. The selected engineering problems revolve around three main themes: residual stresses induced by materials processing, intergranular strains and micromechanics related to monotonic, fatigue, and creep loading scenarios, and the characterisation of nano-precipitates in bulk samples non-destructively. The first part of the talk aims to outline the principles of neutron techniques and data reduction. In the second part, we will describe the engineering problems, elucidate the solution derived through neutron techniques, and highlight the key research findings. Below, you'll find concise one-sentence summaries of the research topics in this talk:

• Neutron diffraction is employed to characterise the triaxial residual stress state, shedding light on the role of microstructure in stress relaxation during thermal exposure.

• A combination of neutron diffraction and simulated post-weld heat treatment is used to measure changes in residual stress in a steel pipe with circumferential welds.

• Intergranular strains are measured under various loading scenarios, including tension-compression, creep, and fatigue.

• Microstructural stability in bulk nanostructured titanium is studied through *in-situ* neutron diffraction, coupled with fatigue loading at both room and cryogenic temperatures.

• The evolution of composition and size in nanoparticles in additively manufactured tool steel is investigated through a combination of small-angle neutron scattering and advanced microscopy.

• Bragg-edge neutron transmission imaging is used to map residual strains induced by several processing methods in aluminium alloys.

Abstract ID: 230

M4-IT3

Residual stress measurement of titanium weld blade by neutron and synchrotron X-ray diffraction techniques

Presenter: Shilei Li(Institute for High Energy Physics, CAS)

Keywords: Residual stress; X-ray diffraction; Neutron diffraction

A systematic assessment of the three-dimensional residual stress distribution in welded, heat-treated, and machined titanium alloy blades was conducted using the General Purpose Powder Diffractometer at the China Spallation Neutron Source and BLS12W beamline Station of Shanghai Synchrotron Radiation Facility. During the welding process, the temperature of the blade weld area is significantly higher than that of the base body. During the subsequent cooling process, the weld seam shrinks. Due to the obstruction of the base material, a high residual tensile stress is formed, up to more than 760 MPa. The residual stress decreases rapidly away from the weld, and the residual stress in the matrix area is very low. During the heat treatment process, the metastable β phase undergoes phase transformation under the action of residual tensile stress and temperature, and the volume expansion of the α phase offsets the residual tensile stress. Measuring neutron diffraction stresses in titanium alloy blades poses several challenges, including weak diffraction signals and difficulties in positioning. Through preliminary literature research, microstructural analysis, optimization of measurement parameters, and meticulous data processing, better results for residual stresses can be obtained, showing good consistency with results obtained from other neutron sources.

Abstract ID: 227

M4-IT4

Recent Progress of Neutron Scattering Instrumentations and Applications in China Mianyang Research Reactor (CMRR)

Presenter: Guangai Sun (China Academy of Engineering Physics)

Keywords: CMRR, Neutron scattering, Residual stress analysis spectrometers

As a reactor based neutron source, CMRR and its neutron scattering facilities are available since 2014.With reactor power of 20 MW, CMRR provides a thermal neutron flux about 2.4×1014 n/(cm^2·s) and cold neutron flux about 109 n/(cm^2·s), similar to NCNR. Currently, CMRR has 13 neutron scattering instruments, the annual operation day is around 200, about 50% open to the public totally for free. Researchers both from China and the world come to do experiments every year with high quality fruits produced.

This report will firstly give a brief introduction of the capabilities of CMRR, especially on some recent progress, including the accomplishment of Spin Echo Small Angle Neutron Scattering(SESANS) spectrometer and Longitudinal Neutron Resonance Spin Echo Spectrometer(LNRSES), and also the long small angle neutron scatter spectrometer-LUOSHU under construction. Then information of the three residual stress analysis spectrometers will be given, some recent applications on engineering components and metal materials will be illustrated in details, such as the stress measurements of rail, turbine blades and 316LN stainless steel.

Abstract ID: 206

M4-IT5

Effect of heat treatment and Er element on the microstructure and properties of AlSiMg alloy prepared by SLM forming

Presenter: Runxia Li (Dongguan University of Technology)

Keywords: Al-Si-Mg alloy, Er element, SLM forming, Heat treatment

AlSi10Mg alloy samples were prepared by SLM forming technology. The optimal process parameters were laser power 360 W, scanning speed 1200 mm/s, scanning spacing 120 μm and the layer thickness 50 μm. The compressive strength, compression rate, microhardness, and density of the alloy were 608 MPa, 30.5%, 138.7 HV0.5, and 99.8%, respectively. The effect of annealing treatment on the microstructure and properties of AlSi10Mg alloy formed by SLM was studied. When the annealing temperature was 180℃, the mechanical properties of the alloy showed a trend of first increasing and then decreasing within the range of 0-8 h. When treated at 180 ℃ for 2h, the mechanical properties of the alloy were the highest, with tensile strength, yield strength, and microhardness of 449 MPa, 339 MPa, and 139.0 HV0.5, respectively, which were 12.0%, 23.2%, and 5.9% higher than those of the untreated alloy. The AlSi10Mg alloy with Er addition was prepared by SLM technology, and the mechanical properties of the alloy were further improved. The yield strength, tensile strength, and elongation were 301 MPa, 439 MPa, and 9.4%, respectively, which were 9.5%, 9.5%, and 9.3% higher than the AlSi10Mg alloy without Er addition, and the grain size of the alloy has decreased from 7.2 μm to 6.6 μm, the Al combined with Er to form an Al_3Er strengthening phase.

Abstract ID: 229

M4-IT6

Reconfigurable lattices in a high-entropy alloy with three-dimensional honeycomb cellular regions

Presenter: Gang Wang (Shanghai University)

Keywords: High-entropy alloy

The various dissimilarities in atomic sizes and bonds render high-entropy alloy (HEA) lattice severe distortion and manifold configurations with changing distortion, each varies in potential energy. Upon external heat or force stimuli, the HEA distorted lattice is sensitive to distortion change. Here, through an *in-situ* tension synchrotron X-ray diffraction technique, we report that the degree of lattice distortion oscillates with increasing the stress in an Al0.1CrFeCoNi HEA with three-dimensional honeycomb cellular regions: the marginally (Al, Cr, Ni)-enriched and severely-distorted cellular-wall, and mildly (Fe, Co)-rich and slightly-distorted cellular-core regions. This unusual behaviour uncovers a novel deformation mode–lattice reconfiguration manifested as the reciprocating lattice configuration state alternation in the distorted lattices. The reconfigurable lattices allow for promoting dislocation planar slip, facilitating stack faulting, nano-twinning, and transformation from the face-centered-cubic to hexagonal-close-packed structure, and local releasing of stress-concentration. These enable a significant ductility enhancement by the magnitude more than one third without sacrificing strength directly in the as-cast state, even compared to the unreconfigurable-lattice counterpart in the recrystallized state. The strategy of engineering reconfigurable lattice ductilizes highly distorted materials, beating classical solid-solution hardening ‘Achilles’s heel’ vulnerability in compromising ductility.

Abstract ID: 226

M4-IT7

Internal mechanical mechanisms and materials design

Presenter: Yu Xiao (University of Science and Technology of China)

Keywords: Internal measurement, Mechanical mechanisms, CT, Materials design

Along with the development of technology, the requirements for material performance are increasing day by day. Material optimization design is an important way to improve material performance and meet the needs of high-performance materials in key fields. Due to the complexity of material parameters and the diversity of material properties, the traditional trial-and-error method of material design is difficult to meet the needs. The internal mechanical evolution mechanism of materials under the action of external parameters is the key bridge connecting material parameters and material properties. Therefore, using advanced light sources for internal measurement to reveal the internal mechanical evolution mechanism is an important basis for achieving controllable mechanical design. This article starts from the two ends of material parameters and material properties. In terms of material parameters, the mechanisms of material damage and failure based on representative simplified models wear revealed. In terms of material performance, the toughening and strengthening mechanisms of high-performance natural biological materials were studied. It was revealed that strain is an important bridge connecting material parameters and material properties. Based on strain control, material design was carried out to improve material performance.

Abstract ID: 225

M4-IT8

The archeometallurgical study on metal arrows through non-destructive neutron techniques

Presenter: Fengyan Zhao

Keywords: The Western Han Dynasty, Arrows, Neutron diffraction, Neutron tomography

The manufacturing process and corrosion features are important contents of the ancient metal research. In this work, we present the analysis of archaeological bronze and iron arrows based on non-destructive neutron methods. The arrows unearthed from a tomb near the archaeological site of Han Chang'an Cheng and date back to the Western Han Dynasty (202 BC-AD 8). Neutron diffraction and neutron tomography have been used to determine the mineralogical composition and the structure of arrows. The results provide useful information on their manufacturing techniques and corrosion features. It is meaningful for the application of neutron techniques in cultural heritage in China.

Abstract ID: 80

M4-IT9

In-situ neutron scattering study of plastic deformation mechanism in a high-entropy alloy with nanoscale structure heterogeneity

Presenter: Si Lan (Nanjing University of Science and Technology)

Keywords: High entropy alloys, Neutron diffraction, Small-angle Neutron Scattering

Like elements gather together and form nanoscale structure heterogeneity in compositionally complex alloys, i.e., high-entropy alloys. The role of chemical heterogeneity in the plastic deformation of a CoCrFeNiPd alloy has been studied using *in-situ* neutron diffraction and small-angle neutron scattering. The FCC single-phase CoCrFeNiPd alloys show much more substantial nanoscale heterogeneity (~30 nm) than the CoCrFeNiMn Cantor alloy. Moreover, lattice strain analysis reveals that the stacking fault probability is much lower in CoCrFeNiPd alloy than that of Cantor alloy due to increased stacking fault energy by chemical heterogeneity. Analysis of diffraction and microscopy data confirms that dislocations interactions and propagations, rather than stacking faults or twinning, play an essential role at the early stage of plastic deformation in CoCrFeNiPd, leading to higher yield strength without compromising strain hardening and tensile ductility than those in Cantor alloy.

Abstract ID: 96

M4-IT10

Introduction to the Engineering and Scientific Stress Diffractometer at China Advanced Research Reactor and its application

Presenter: Xiaolong Liu (China Institute of Atomic Energy)

Keywords: Residual stress, Engineering and scientific stress diffractometer, Engineering component

A new neutron residual stress instrument-Engineering and Scientific Stress Diffractometer(ESSD) at China Advanced Research Reactor was built and put into service. Here the neutron optic and the main components of ESSD will be introduced including neutron guide, doubly focusing Si(400) monochromator, monochromator shielding, sample stage, first slit/radial collimator , area detector and sample environment. The flux at the sample position was accurately measured using neutron Au activation method. The neutron flux at the sample position is 3.0×10^7 n cm^{-2} s^{-1} at wavelength 1.64 Å with full reactor power, which indicates that ESSD is a world-class instrument.

ESSD has been used to measure the 3D residual stresses in typical engineering components. The day-one experiment was measuring the inner residual stresses of the full-size high-speed train wheels. The largest penetrating thickness was 41mm with gauge volume 3 mm × 3 mm × 3 mm. 3D residual stress mapping were obtained, which was used to assess the structural integrity. Another typical experiment is SiCp/Al matrix composites. The macro stress measured by user showed to be about zero. Neutron diffraction illustrated the micro stress of aluminum and SiC, especially the total macro stress of aluminium phase and SiC phase was near to be zero, which proved the advantages of thermal neutrons. Also large aluminium alloy forging pipe, superalloy disks, superalloy ring pieces and steel welding will be introduced.

Abstract ID: 219

M4-IT11

Construction and application progress of Energy Resolved Neutron Imaging Instrument (ERNI) of CSNS

Presenter: Jie Chen (Institute for High Energy Physics, CAS)

Keywords: Energy resolved, Neutron imaging, Time-of-flight

In July 2023, the construction of Energy-Resolved Neutron Imaging Spectrometer (ERNI) of China Spallation Neutron Source (CSNS) was completed and successfully passed the acceptance tests. The performance parameters of ERNI include: the best wavelength resolution is better than 0.4%, the wavelength range is from 0.03 to 18 Å, the neutron imaging field of view can reach 20 cm ×20 cm, and the flux at the sample location can reach 10^7 $n{\cdot}s^{-1}cm^{-2}$. In China, ERNI is the first and unique pulsed neutron source-based instrument that combines high spatial-resolution neutron imaging with neutron diffraction. Compared with X-ray imaging, neutron imaging has the advantages of deep penetration and sensitivity to light elements. ERNI can detect structural information of several centimeters deep inside materials and components. Neutron radiography and tomography can provide structure information about defects, holes, and cracks inside samples; Time-of-flight (TOF) Bragg-edge neutron imaging and neutron diffraction can obtain the spatial distribution of crystallographic structure, magnetic structure, and stress & strain inside the material. Preliminary tests were carried out on a 20 cm long knife of the Western Han Dynasty by using Neutron diffraction and CT experiments. The rust cracks, fractures and wooden shell structures of iron artifacts are clearly displayed.

Abstract ID: 93

M4-IT12

Neutron imaging of hydrogen in nuclear fuel claddings

Presenter: Weijia Gong (Northwestern Polytechnical University)

Keywords: Neutron imaging, Nuclear fuel cladding, Zirconium alloys, Hydrogen, Diffusion

In light water reactors, the nuclear fuel of UO_2 pellets is encapsulated in cladding rods, consisting of a zirconium alloy. The cladding is the first barrier to prevent the release of highly radioactive fission products; thus, the cladding integrity is of utmost importance. During operation in reactor, the fuel rods, bundled in fuel assemblies, reside in the cooling water. The high temperature at the cladding surface leads to the cladding oxidation, and a part of the created hydrogen diffuses into the cladding material. When the solubility limit for hydrogen is exceeded, hydrides are formed. As the hydrides are brittle, they can affect the mechanical properties of the cladding. This is relevant during operation, for instance during fast transients or when a cladding is pre-damaged, and after operation, when the cladding cools down and more hydrides are generated. A specific interest is in handling and transportation of used fuels after intermediate dry storage.

An excellent tool to analyze the distribution of hydrogen and hydrides concentrations is neutron attenuation imaging. While zirconium has a very low cross section for neutrons, for hydrogen it is very high. At the spallation neutron source SINQ (PSI), the so-called neutron microscope is utilized to detect hydrogen in claddings with a sub 10 µm spatial resolution and hydrogen concentrations from very few ten wppm up to several thousand wppm, with a concentration resolution of 10 wppm. Non-homogeneous hydrogen/hydrides distributions can lead to critical, weak spots or areas. It is relevant to know under which conditions and kinetics hydrogen and hydrides accumulate. In principal, the gradient of mechanical stress, temperature, electrochemical potential (in a wider sense, like inhomogeneity in material composition), and hydrogen concentration itself are decisive for the diffusion.

In the present work, quantitative and qualitative examples for the different factors are presented, leading to effects like hydrogen accumulation at stress raisers or in cladding liners, in the cladding oxide layer, and hydrides reorientation or delayed hydride cracking. Tests have been performed with non-irradiated hydrogenated cladding as well as with claddings irradiated in Swiss nuclear power plants.

The obtained results can find their way into fuel modelling with respect to cladding mechanical behavior, for situations after operation of the fuel rods or during accidental transients. Further, the results can be combined with methods of standard post-irradiation examination comprising metallography, scanning electron microscopy or electron probe microanalysis, or with advanced methods like synchrotron investigations, allowing, for instance, acquiring local crystallographic information related to hydrides.

Reference:

[1] Liang S, et al., “Hydride precipitation dependence on α-parent orientation and plastic deformation in zirconium alloys”, Acta Mater Vol.259pp.119292(2023)

[2] Gong W, et al., “Hydrogen diffusion and precipitation under non-uniform stress in duplex zirconium nuclear fuel cladding investigated by high-resolution neutron imaging”, J Nucl Mater Vol. 570pp.153971(2022)

[3] Trtik P, et al., “Sample container for high-resolution neutron imaging of spent nuclear fuel cladding sections”, Review of Scientific Instruments Vol.91pp. 056103(2020).

[4] Gong W, T et al., “Hydrogen diffusion and precipitation in duplex zirconium nuclear fuel cladding quantified by high-resolution neutron imaging”, J Nucl Mater Vol.526pp.151757(2019)

[5] Gong W, et al., “Hydrogen diffusion under stress in Zircaloy: High-resolution neutron radiography and finite element modeling”, J Nucl Mater Vol.508pp.459-464(2018)

Abstract ID: 231

M4-IT13

Atmospheric neutron irradiation spectrometer and its industrial application

Presenter: Hu Zhiliang (Institute for High Energy Physics, CAS)

Keywords: ANIS, Methodology research, Industrial application

With the wide application of nano-scale VLSI, high integration of electronic equipment and complex operation logic, the challenge of single event effect caused by ubiquitous atmospheric neutrons is becoming more and more serious. The accelerator-based ground simulation test is the most basic and effective way to study atmospheric neutron irradiation effect.

This report will briefly introduce the facility of ANIS, its performance parameters, methodology research and the application of ANIS in aviation, power grid, new energy vehicles and other industries.

Abstract ID: 222

M4-IT14

The influence of fractal structure on the deformation mechanism of Ti alloy

Presenter: Juan Mu (Northeastern University)

Keywords: Fractal structure, Martensitic transformation, Mechanical properties

The fractal concept is a discipline that studies the complexity and self-similarity of structures, offering a novel perspective to facilitate a profound comprehension of the essence of natural and artificial systems. The fractal theory has been widely used in diverse domains such as mathematics, physics, chemistry, mechanics, economics, computer science, etc. In the field of materials science, it provides a new perspective and methodology for structural characterization, performance analysis, functional design, and application development. By employing the fractal concept, scientists can delve into the intricacies and diversities of materials, thus laying a robust foundation for the innovation and application of materials. Dendrites formed by the solidification process are typical fractal structures that generally influence the mechanical behavior of materials. However, the fundamental understanding of the influence of dendrites' fractal nature on mechanical properties remains insufficient, and the precise relationship between fractal structures and microstructure evolution is still unclear.

This work revealed the critical role of the fractal structure in governing the deformation mechanisms of Ti alloy through numerical simulations and experimental investigations. The fractal structure yields distorted interface and multiscale microstructures, leading to a stable martensitic nucleation that is much different from a continuous martensitic nucleation and growth in BMGCs without fractal structures. The stable martensitic nucleation and stagewise deformation mechanisms play a crucial role in overcoming the strength−plasticity trade-off. Furthermore, we have also employed the fractal induced stable martensitic nucleation and stagewise mechanisms to guide preloading treatments aimed at achieving improved mechanical properties.

Abstract ID: 100

M4-IT15

Origins of internal stress during phase transformation in carbon steels

Presenter: Yanxu WANG (Institute of Metal Research, CAS)

Keywords: Phase transformation, In-situ neutron diffraction, Eignestrain

The evolution of internal stress during phase transformation is a topic of continuous debate. However, direct observation of phase transformation has been attempted using various experimental techniques and new findings have been reported. Neutron diffraction, which has a high transmission capacity, is appropriate for experiments in which austenite is processed at high temperatures followed by rapid cooling, and other methods are difficult to use. In this study, we attempted time-resolved measurements of displacive transformation behavior using practical steels.

Neutron diffraction was used to study the isothermal bainite transformation in a 0.4 C low alloyed steel from 773 to 623 K to provide a clearer basis for discussion regarding the change in the austenite lattice parameter. According to diffraction profile analysis, fresh bainite possesses a body-centered tetragonal structure, and its c/a ratio decreases rapidly over time. The austenite lattice parameter increases or decreases depending on whether the transformation temperature is above or below the nose of the Time-Temperature-Transformation (TTT) curve. This isothermal transformation behavior can be divided into two categories: above and below the nose of TTT curve, which correspond to the upper and lower bainites, respectively. The internal stresses caused by the transformation strains are relaxed by dislocation motion and vacancy formation. The yielded dislocations and vacancies not only affect the broadening of both austenite and bainitic ferrite diffraction peaks but also the lattice parameter. The first-principles calculations demonstrate that the austenite lattice parameter decreases as the vacancy density increases, which may account for the experimental observation in lower bainite.

Abstract ID: 228

M4-IT16

Neutron diffraction gradient stress measurement and life evaluation of induction hardened railway S38C axles

Presenter: Shengchuan Wu (Southwest Jiaotong University)

Keywords: Neutron diffraction method, Gradient residual stress, Finite element modeling, Fatigue crack propagation, High-speed railway S38C axles

Gradient compressive residual stress with a depth of several millimeters exists in railway S38C hollow axles subject to surface induction hardening, which is a challenging problem for structural integrity assessment. To address this, the axial, hoop, and radial residual stress values inside the axles are measured by neutron diffraction technology. By integrating the limited neutron diffraction data, an innovative nodal stress based coordinate assignment (INSCA) approach was then proposed, to numerically reconstruct the global initial residual stress field in three dimensions for S38C axles. The comparison between simulations and experiments clearly show that approximately 515 MPa (axial), 710 MPa (hoop), and 43 MPa (radial) compressive residual stresses were retained underneath the induction hardened martensite layer, which also validates the newly-developed INSCA method. By including the measured axial- and hoop-direction residual stresses, the crack propagation behavior of railway S38C axles were investigated, in terms of fracture mechanics. It was clearly shown that the presence of compressive residual stress leads to a lower driving force of crack propagation, in terms of stress intensity factor range (ΔK). Such a smaller ΔK also indicates that this compressive residual stress can effectively prolong the service lifetime of high-speed railway axles subjected to induction hardening treatment.

M4. Contributed Talks

Abstract ID: 233

M4-CT1

The current status of neutron imaging project at CARR

Presenter: Prof. HE, Linfeng (China Institute of Atomic Energy)

Keywords: CARR; neutron imaging

The China advanced research reactor (CARR) of the China Institute of Atomic Energy is a 60 MW multipurpose research reactor. The neutron imaging project include two dedicated neutron imaging facilities which have been developed: the thermal neutron imaging instrument located in H8 port of reactor and the cold neutron imaging instrument located at the end of CNGC guide in the guide hall. The construction of thermal neutron imaging instrument has been completed at the end of 2021 and the first neutron radiography measurements were performed in January of 2022. The measured neutron flux at the sample position is 6.4 ×108 / cm^2 / s (L/D = 180). The cold neutron imaging instrument has been completed recently this year. In addition, neutron imaging facility based on the compact neutron source has been developed, and the preliminary experimental results verify its good performance.

In recent years, we have successfully established a test station for neutron imaging, and developed several imaging methods, which have been used to investigate various objects of interest, such as water management of fuel cell, concrete and rock imbibition, spent fuel element and steel welding, archaeology etc.

Abstract ID: 57

M4-CT2

Residual stress measurements on dissimilar metal welding pipe for nuclear power plant

Presenter: GAO, Jianbo (Centre of Excellence for Advanced Materials)

Keywords: Residual stress, dissimilar metal welding, neutron diffraction

In nuclear power plants, the main connection method for key equipment and systems in the primary and secondary circuits is welding. Among them, dissimilar metal welding (DMW) is a typical application for connecting ferritic vessel nozzles and austenitic piping systems in nuclear power plants, and the structural integrity of dissimilar metal welds during their service life is crucial for the safe operation of nuclear power plants. Residual stresses directly affect the quality, safety, and lifespan of welded components. Accurately quantifying the magnitude and distribution of residual stresses in dissimilar metal weld structures is of significant reference value for optimizing welding and heat treatment processes, evaluating and predicting service safety, and ensuring the safe operation of nuclear power plants.

Three sizes of nuclear safety end samples were designed and manufactured for the precise measurement of residual stresses. Temperature, strain, and displacement were collected during the sample preparation process, and numerical simulations were conducted based on the collected data to determine the residual stresses. The wall thickness of the three samples was 12.7 mm, 20 mm, and 30 mm, respectively.

Comparing the magnitude and distribution of circumferential residual stresses obtained from neutron diffraction, contour method, and numerical simulations, there is good correlation among the three methods. The obtained residual stress data can be used for subsequent structural integrity evaluation.

Abstract ID: 210

M4-CT3

Characterization of the Microstructure of Cement-Casing and Cement-Rock Interfaces Using Nano-CT

Presenter: YANG, Xinxiang (Zhejiang Ocean University)

Keywords: nano-CT; microstructural variation; cement; greenhouse gas emission

Mitigating greenhouse gas emissions from oil and gas wells is an industry-wide challenge. Microstructural variations across the cement-rock and cement-casing interfaces are agreed upon as the main contributors to leakage pathway formation. In this study, microstructures of interfacial regions were investigated using the nano-CT scanning technique and downscaled samples simulating casing-cement-casing (CCC) and rock-cement-casing (RCC) interfaces. The main objectives were to: 1-) visually characterize variations of microstructures and; 2-) quantify the porosity distribution across the CCC and RCC interfaces. Downscaled CCC and RCC samples were prepared using stainless steel pipes, core samples collected from Alberta reservoirs, and two real-world cement blends. The samples were cured at ambient temperature (~ 21 ℃) and 1500 psi for 7 days, and then scanned by Xradia Versa 620 nano-CT at a resolution of 6.8 μm. Radial and axial porosity distributions were quantified by analyzing the CT data. Results show that phenomena such as cement migration in formation rocks and slurry sedimentation can be visually captured by the nano-CT. The radial porosity distributions in RCC and CCC samples are significantly varied. The results enhance the understanding of factors affecting gas leakage pathways from wells, and the proposed methodology can be used to optimize cement blends for effective wellbore barriers.

Abstract ID: 232

M4-CT4

Nanostructure of Phase Separation in Stainless Steels Studied by SANS

Presenter: Xin Xu (Sun Yat-sen University)

Keywords: SANS, phase separation, stainless steel, nanostructure

Ferrite or/and martensite containing stainless steels have different applications in chemical, gas and oil industries, and are promising candidates in the next generation nuclear power plants due to their excellent corrosion resistance and mechanical properties. Fe and Cr in martensite and ferrite are prone to demixing inside the miscibility gap, forming nanostructure consisting of Fe-rich bcc (α) and Cr-rich bcc (α′) phases, namely the phase separation phenomenon. Phase separation increases the hardness and reduces the toughness of the alloys and the embrittlement rate is fastest at about 475 ℃. Phase separation limits the service temperature of, e.g., duplex stainless steels, to ~280 ℃. Different factors, including temperature, composition, initial microstructure and external fields, affect the mechanisms and kinetics of the nanostructural evolution due to phase separation. In order to understand the effects of different factors and the mechanisms, characterization of the nanostructural evolution is necessary. Small-angle neutron scattering (SANS) is a powerful technique to characterize the nanostructure of phase separation. This presentation is on the effects of initial microstructure and applied stress on the evolution of phase separation nanostructure studied by SANS combining other experimental techniques. It has been found that both initial microstructure and applied stress have significant effects on phase separation and the kinetics of the nanostructural evolution depends on the inhomogeneity of the initial microstructure and stress level. The mechanisms of the effects will be discussed.

Abstract ID: 211

M4-CT5

Progress of Neutron Imaging at Institute of Nuclear Physics and Chemistry

Presenter: Hang Li (Institute of Nuclear Physics and Chemistry, China Academy of Engineering Physics)

Keywords: Neutron Imaging; China Mianyang Research Reactor; Accelerator.

Based on China Mianyang Research Reactor (CMRR) and accelerator neutron sources, several neutron imaging facilities have been developed at Institute of Nuclear Physics and Chemistry (INPC), China Academy of Engineering Physics (CAEP). In recent years, INPC has completed the development of the large view field thermal and exceeding-cadmium neutron imaging facility, and high resolution cold neutron imaging facility based on CMRR. A moveable thermal and fast neutron imaging facility, and a new high neutron yield fast neutron imaging facility based on accelerator D-T neutron sources have also been developed. These neutron imaging facilities have been applied in metal bonding quality detection, aero engine turbine blade detection, irradiated high radioactive samples detection, aerospace heat pipe two-phase flow state detection, lithium ion battery detection and so on. In addition, new techniques such as polarized neutron imaging, fission neutron imaging, and neutron imaging coupled with Prompt Gamma-rays Neutron Activation Analysis (PGNAA) have also been studied at INPC.

Abstract ID: 60

M4-CT6

弹性安定条件下焊接残余应力的分布规律研究

Presenter: 吴, 桂毅 (Centre of Excellence for Advanced Materials)

Keywords: 残余应力，弹性安定，对接接头，角接接头、疲劳

船舶是水上运输的重要交通工具，是水面上的漂浮建筑和经济实体。船体拥有众多焊接接头，在其龙骨架上的角焊缝处存在疲劳裂纹扩展和失效的风险。焊接残余应力在这些焊接关节处是及其复杂的，拉伸残余应力会降低焊接接头的疲劳寿命，从而对船舶的结构完整性造成影响。船舶在海上经受复杂的风、浪、流等疲劳载荷的影响，其残余应力在复杂环境载荷下会发生释放或重分布，但至今没有一个明确的答案，这些船舶结构完整性的准确评估带来重大挑战。弹性安定是材料对循环载荷的其中一种常见行为，即材料在初始几个载荷周期内发生一定量的塑性形变。本报告采用中子衍射的方法，对船上用钢的对接接头和角接接头在不同的循环载荷周期下，进行内部三维残余应力的测量，从而获得了焊接接头在弹性安定疲劳载荷下的重新分布规律。通过该研究，可对弹性安定的极限载荷值做出规定，避免棘轮效应的发生，大大降低了船舶疲劳失效的可能性。

Abstract ID: 200

M4-CT7

Optimization of Titanium Alloy Materials, Processes, and Service Performance for Deep-sea Pressure Shell Based on Neutron Method

Presenter: WANG, Qian (Institute of metal research, Chinese Academy of Sciences)

Keywords: Titanium alloy; Deep-sea engineering; Two-phase stress partitioning; Welding residual stress; Hydrogen diffusion behavior

Titanium alloys are ideal materials for manufacturing deep-sea facilities due to their high specific strength and excellent corrosion resistance to seawater. The full-process and full-chain optimization design on the material, processes and service performance of large-scale titanium alloy pressure-resistant shells is carried out with the help of China spallation neutron source large scientific device. Two-phase stress partitioning behavior of different titanium alloys is investigated by the method of *in-situ* tensile experiment. β phase with larger proportion can coordinate more stress, thereby improving the toughness of the material. Different detection methods (contour method, deep-hole drilling and neutron diffraction) are used to compare and analyze residual stress at welds prepared by different electron beam welding processes. Preheating welding can significantly reduce weld residual stress and improve toughness. Hydrogen is a key factor causing stress corrosion cracking in deep sea service. Hydrogen diffusion behavior in titanium alloys is studied using neutron imaging technique. The inhibitory effect of alloying elements on hydrogen diffusion from strong to weak is Mo, V, Cr, Fe.

Abstract ID: 161

M4-CT8

The new Engineering Material Diffractometer (EMD) at China Spallation Neutron Source CSNS

Presenter: Xiaohu Li (the Institute of High Energy Physics, CAS)

Keywords: residual stress analysis, engineering material

The new engineering material diffractometer, located at beam line 8 of CSNS, is designed for measuring residual stress, analyzing texture, and studying phase transformations kinetics in metallic materials. It completed construction in 2022 and successfully underwent physical calibration and data reduction in April 2023. Currently, there is ongoing development of a high-precision 3D positioning system for residual stress measurement, as well as integration of a servohydraulic test system with the diffractometer. There are plans to officially incorporate these systems into the proposal system and make them available to users worldwide next year.

Abstract ID: 22

M4-CT9

High-precision neutron diffraction measurement using an industrial robot at the STRESS-SPEC instrument

Presenter: WANG, Lijiu (Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich (TUM), Lichtenbergstr. 1, 85748 Garching bei München, Germany)

Keywords: industrial robot; neutron diffraction; high accuracy; sample environment

Components and materials from new production processes, i.e. additive manufacturing (AM), require a highly flexible sample positioning system for residual stress diffraction experiments. Therefore, the STRESS-SPEC group has pioneered the use of industrial robots for sample handling and positioning at neutron diffractometers [1, 2]. However, for samples with high stress gradients and gauge volumes down to the size of 1 mm³, the absolute positioning accuracy of the current robot is insufficient for the experiment. To overcome this issue, we will present a robot control system which tracks the sample position with an optical metrology system and actively compensates any occurring motion errors. This improves the sample positioning accuracy of our robot to better than 50 µm, enabling highly accurate stress and local texture measurements.

To fully explore the measurement possibilities using the industrial robot and to accommodate to the weight-carrying capacity of the robot, we will also present a dedicated lightweight laser furnace with a large neutron acceptance angle for elevated sample temperatures up to 1200 °C. Finally, we will give an outlook on the development of a lightweight mechanical tensile testing machine with a force up to 50 kN, that can also be mounted on the robot.

Reference:

[1] H.-G. Brokmeier et al., Mater. Sci. For. 652 (2010) pp. 197–201. DOI: 10.4028/www.scientific.net/MSF.652.197

[2] C. Randau et al., Nucl. Instr. Meth. A 794 (2015) pp. 67–75. DOI: 10.1016/j.nima.2015.05.014

Abstract ID: 218

M4-CT10

Imaging System and CT Algorithm Development in Energy-Resolved Neutron Imaging Instrument (ERNI) of CSNS

Presenter: WANG, Shengxiang (Institute of High Energy Physics, CAS)

Keywords: neutron CT, imaging

The imaging capabilities of ERNI encompass various techniques, including traditional neutron computed tomography (CT), neutron energy spectrum CT, neutron grating interferometry imaging, and *in-situ* X-ray micro-CT. Consequently, algorithmic research on three-dimensional CT reconstruction plays a crucial role in the software infrastructure development of imaging spectrometers. In three-dimensional reconstruction, artifacts often arise due to physical factors such as high noise levels, tilted rotation axes, or incomplete data. To address this, we have also conducted research on artifact correction algorithms. This work presents an overview of the construction of imaging systems and the associated work on artifact correction.

Abstract ID: 220

M4-CT11

Constitutive modeling and strengthening mechanism of gradient nanostructured 304H stainless steel based on Bragg-edge neutron imaging

Presenter: Yonggang Wang (Spallation Neutron Source Science Center)

Keywords: gradient nanostructured； 304H stainless steel ； Constitutive model； strengthening mechanism； Bragg-edge neutron imaging

The conventional tensile curve can only reflect the overall mechanical response of the gradient structure material, but the gradient change of the mechanical properties of the material unit in the gradient nanostructured (GNS) material is limited by the sample size and microstructure complexity, and there is no suitable material constitutive to describe its non-uniform deformation response mechanism. However, the neutron Bragg-edge imaging technology has high spatial resolution (25 μm), which can obtain two-dimensional stress and strain distribution of any structural unit in gradient nanostructured materials. Therefore, the macroscopic elastic-plastic constitutive relationship of any structural unit in GNS 304H is established based on the neutron Bragg-edge imaging technique. The stress and deformation states of gradient nanostructured materials are revealed, and the formation and evolution of multiaxial stress state, stress and strain gradients during uniaxial tension are clarified. Combined with the quantitative characterization of tensile deformation microstructure, the strengthening and toughening mechanism of GNS 304H under multi-factor synergy is analyzed.

Abstract ID: 217

M4-CT12

Understanding the high-temperature oxidation resistance of heat-resistant austenitic stainless steel with gradient nanostructure

Presenter: WEI, Liangliang (Spallation Neutron Source Science Center)

Keywords: SMRT; Gradient nanostructured; Heat-resistant stainless steel; Oxidation resistance; Precipitates; Diffusivity

Alloys with gradient nanostructured (GNS) surface layer generally exhibit superior high temperature oxidation resistance compared to homogeneously structured counterparts, although their high density of grain boundaries promote diffusion of reactive elements which are expected to accelerate high temperature oxidation. In this study, we study the underlying reasons as to why the heat-resistant austenitic stainless steel with GNS surface layer exhibits better oxidation resistance and thereby reveal the underlying mechanism through systematic analysis of microstructure and composition. The improved high temperature anti-oxidation property of the GNS austenitic stainless steel was ascribed to the formation of pronounced (Mn, Cr, Fe)$_3O_4$/(Mn, Cr)$_3O_4$ spinel oxides and high-density precipitates. Nanoscale oxide crystals together with GNS layer provided plenty of diffusion paths for the outward diffusion of Mn and promoted Cr-Mn spinel oxide formation, which effectively suppressed elemental diffusion and formation of volatile CrO_3. High level of residual stress in the GNS layer facilitated the formation of high-density precipitates at the oxide/matrix interface and grain boundaries, which hindered the inward growth of oxide scale and diffusion of reactive elements. The enhanced high temperature oxidation resistance of the GNS stainless steel was the synergy result among spinel oxides, precipitates, and high-density grain boundaries. Moreover, outward diffusion of alloying elements in the GNS surface layer reduced the thermal stability of nanograins and led to abnormal grain growth. High density precipitates formation together with grain growth resulted in the softening of GNS surface layer.

Abstract ID: 141

M4-CT13

Time-of-flight neutron diffraction study of residual stress and grain refinement mechanism in rapidly solidified pure Ni

Presenter: Dandan Zhao (Spallation Neutron Source Science Center, Dongguan 523803, China)

Keywords: Rapid solidification, High undercooling, Neutron diffraction, Residual stress; Grain refinement

Rapid solidification of high undercooling, which include high cooling rate and high undercooling, is an advanced non-equilibrium solidification technology. Grain refinement during rapid solidification of a highly undercooled liquid has been a hot topic in the field of non-equilibrium solidification processing of materials in the past sixty years. In literature, dendrite fragmentation [1] and recrystallization [2] have been proposed to interpret grain refinement observed in various materials. Although dendrite fragmentation during solidification has been observed *in-situ* using synchrotron X-rays [3], the possibility of recrystallization-induced grain refinement during rapid solidification at low undercoolings cannot be precluded. Moreover, some researcher proposed that the plastic deformation and dynamic recrystallization may occurred in the highly undercooled sample, and then induced grain refinement [4]. Therefore, there must be stress in the undercooled sample after rapid solidification if the recrystallization mechanism is reasonable. Normally, stress is the driving force for recrystallization, so residual stress should be present in the undercooled sample. In addition, thermal stress may occur during solid state cooling stage after slow solidification. Consequently, the residual stress could be confirmed by nondestructive measuring the strain in the rapid solidified sample, and further confirm the recrystallization refinement mechanism.

To study these issues, neutron diffraction is used for characterize strains and texture stored in bulk samples of pure Ni throughout rapid solidification processing at high liquid undercoolings and effects of post-solidification annealing. Moreover, the back-scattered electron diffraction is used to characterize the grain morphology, distribution of grain size, texture and orientation as well as crystal defects such as twins in these samples. The results indicated that grain refinement at low undercooling is caused by dendrite fragment, grain refinement at medium undercooling is caused by dendrite fragment and recrystallization, while grain refinement at high undercooling is mainly caused by recrystallization. The driving force of recrystallization is the intergranular stress.

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References:

[1] Schwarz M, Karma A, Eckler K, et al. 1994, 73(10): 1380–1383.

[2] Powell G L F. Australian INST Metals J, 1965, 10(3): 223–230.

[3] Mathiesen R H, Arnberg L, Bleuet P, et al. Metallurgical and Materials Transactions A, 2006, 37(8): 2515–2524.

[4] Liu F, Yang G C. Journal of Crystal Growth, 2001, 231(1–2): 295–305.

The 4th Asia-Oceania Conference on Neutron Scattering

Scientific Parallel Session M4. Engineering and Industrial Applications

M5. Keynote Talks

Abstract ID: 151

M5-KT1

Upgrade history of cold-neutron disk-chopper spectrometer AMATERAS

Presenter: Seiko OHIRA-KAWAMRA (J-PARC Center, Japan Atomic Energy Agency, Japan)

Keywords: chopper spectrometer, AMATERAS, sample environment

The cold-neutron disk-chopper spectrometer, AMATERAS, installed at the Materials and Life Science Experimental Facility (MLF) in J-PARC, is an instrument designed for inelastic and quasielastic neutron scattering experiments within an energy range from cold to sub-thermal [1]. The original concept of AMATERAS aims to achieve both high flexibility in neutron intensity and energy resolution by utilizing a combination of monochromating and pulse-shaping choppers. While AMATERAS has been operated in two main conditions, referred to as high-resolution modes and high-intensity/low-resolution modes, depending on the research field during its early years of operation, subsequently other intermediate conditions are also effectively used for wide research fields. With changing trends of research, the instrument group has also developed various sample environments. In addition to the closed-cycle refrigerators with low background dedicated to this instrument, we have introduced specific pieces of low-temperature and magnetic-field equipment shared among some instruments in the MLF. This presentation will cover the upgrade history of AMATERAS in response to the research trends including the sample environment shared in the MLF.

Reference:

[1] K. Nakajima et al., J. Phys. Soc. Jpn. 80 (2011) SB028.

Abstract ID: 89

M5-KT2

Bilby – and Australian time-of-flight Small Angle Neutron Scattering instrument: its complexity, benefits and successful stories

Presenter: Anna SOKOLOVA (ANSTO, Australia)

Keywords: small angle neutron scattering, time-of-flight scattering, nanostructure

Bilby [1] is a Time-of-Flight (ToF) small angle neutron scattering instrument at the Australian Center for Neutron Scattering, Australian Nuclear Science and Technology Organization (ANSTO).

Bilby is also equipped with a monochromatic option, though a majority of the experiments for the eight years of its operation have been performed in the ToF mode. The design of Bilby opens the possibility to vary wavelength resolution in a wide range (from 4% to 30%). Two arrays of position-sensitive detectors in combination with utilizing of wide wavelength range (from ~2Å to ~20Å) provide the capability to collect scattering data of wide angular range without changing the experimental set-up. The instrument can cover Q (momentum of transfer) range from 1 x 10^{-3} to 1.8 $Å^{-1}$, with the most common settings allowing simultaneous data collection in the range between 1 x $10^{-3}Å^{-1}$ and $1.0Å^{-1}$. Offered instrument design opens the possibility to collect scattering from a wide range of samples, with a unique capability to record fast (at the level of seconds) kinetics data.

The time-of-flight mode has enormous advantages at a price of several complexities as incoherent/inelastic background caused by hydrogen, which require a good understanding to be able to overcome them [2]. Having an instrument that is ideal for the analysis of the issues, we have accumulated some experience in the reduction of heavily contaminated data. We think our results might be useful for scientists operating ToF SANS machines.

We also plan to present several examples of the scattering data from the soft and hard matter systems, all reduced using customized algorithms implemented in Mantid software [3].

Reference:

[1] “Performance and characteristics of the BILBY time-of-flight small-angle neutron scattering instrument”, Sokolova A. et al, J. Appl. Crystlography, 52, p.1-12 (2019), DOI: 10.1107/S1600576718018009

[2] “Small angle X-ray and neutron scattering”, Cy M. Jeffries et al, Nature Reviews Methods Primers, 2021-12, DOI: 10.1038/s43586-021-00064-9

[3] O. Arnold, et al., Nuclear Instruments and Methods in Physics Research Section A. 764 (2014), DOI: https://doi.org/10.1016/j.nima.2014.07.029

Abstract ID: 169

M5-KT3

Fundamental physics with neutrons

Presenter: Kenji MISHIMA (KEK, Japan)

Keywords: nuclear physics, particle physics, quantum physics

The neutron is a unique particle, which is a smallest nucleus, has no charge, and sensitive to four interactions: strong, electromagnetic, weak, and gravity. Thanks to the features, neutrons have been used in a variety of fundamental physics research. In this talk, fundamental physics experiments using neutrons will be reviewed, mainly focused on activities in J-PARC.

The neutron lifetime is an important parameter for elemental particles and astrophysics. So far, the neutron lifetime measured by counting decay of thermal neutron and storing ultra-cold neutrons (UCNs) gives different results. It is so-called “neutron lifetime puzzle”, and not yet unsolved. The present situation is introduced.

Neutron interferometry using Si single crystals has been a great success in the field of fundamental physics. Recently, a neutron interferometer with multilayer mirrors has been successfully demonstrated with the pulsed neutron at J-PARC. It can be applied for measurements of scattering lengths of nuclei, and going to try to be further sensitivity for new physics.

In order to explain the matter-dominated universe, the search for time-reversal symmetry breaking has been vigorously conducted. The search is being conducted using UCN and epi-thermal neutrons. A pulsed UCN source using a Doppler shifter is in operation at J-PARC, used for R&D of new coming neutron EDM experiment.

Abstract ID: 76

M5-KT4

A complimentary suite of cold neutron inelastic spectrometers designed for new materials research

Presenter: Wei BAO (City U of Hong Kong, China)

Keywords: spectrometers

Despite increasing power in the new generation of neutron reactors or spallation sources, neutron flux is still much short of our expectation in material physics research fields. Novel design ideas have been developed constantly and utilized to deliver more efficient measurement of scattered neutrons. Here we report the design and construction of two cold neutron inelastic spectrometers as a National Key Research Infrastructure Project at China Advanced Research Reactor (CARR). The Boya multichannel spectrometer could simultaneously measure hundreds of points in the (E, ***k***) phase space, suitably for search for excitation signal in a new material speedily. The Xingzhi triple-axis spectrometer is equipped with a velocity selector to screen off higher order neutrons, providing flexible selection of Ei or Ef of the cold neutron beam, and equipped with the full polarized neutron analysis capacity. Cryostats, furnace, magnets and high pressure cells have been equipped to provide wide choices of the sample environment.

The 4th Asia-Oceania Conference on Neutron Scattering

M5. Invited Talks

Abstract ID: 107

M5-IT1

Design and performance of a TOF single crystal diffractometer SENJU at J-PARC

Presenter: Yoshihisa Ishikawa (Neutron Science and Technology Center, CROSS)

Keywords: J-PARC, SENJU, neutron diffraction

"SENJU" is a time-of-flight (TOF) neutron single crystal diffractometer installed at MLF/J-PARC in Japan. This diffractometer is designed for a crystal and magnetic structure analysis of inorganic and organic materials in various measurement environments. With the upgrading of the accelerator beam power in recent, it can get enough peak intensities using the small single crystal size less than 1.0 mm3 [1]. SENJU has installed 41 area detectors, arranged a cylindrical geometry from the sample position. Since such multiple area detectors cover a large three-dimensional reciprocal space, it can measure for collecting many Bragg reflections for crystal structure, as well as for searching of super-lattice reflections caused from a phase transition.

SENJU is also developing a data processing system using the software "STARGazer". A series of data processing processes, such as peak search, peak indexing, and peak integration for every Bragg reflection, are handled remotely in cloud computing via a web user interface. These integration intensity data can be applied to typical crystal structural analysis software (Jana2020, Shelx, Fullprof, and GSAS-II). In the presentation, the authors show the details of sample environment devices and data-handling system in SENJU.

Reference:

T. Ohhara, R. Kiyanagi, K. Oikawa, T. Kawasaki, I. Tamura, A. Nakao, T. Hanashima, K. Munakata, T. Moyoshi, T. Kuroda, H. Kimura, T. Sakakura, C-. H. Lee, M. Takahashi, K. Ohshima, T. Kiyotani, Y. Noda, M. Arai, (2016). J. Appl. Cryst., 49, 120.

Abstract ID: 181

M5-IT2

Development of Neutron Optics Devices and Sample Environment at China Advanced Research Reactor

Presenter: Yuqing Li (China Institute of Atomic Energy)

Keywords: Neutron Optics Devices, Sample Environment, China Advanced Research Reactor

The China Advanced Research Reactor (CARR) is a high-flux and multipurpose reactor, located at China Institute of Atomic Energy(CIAE) in Beijing. This reactor is a tank-in-pool inverse neutron trap type reactor with a maximum power of 60MW. The maximum undisturbed thermal neutron flux in heavy-water reflector is about 8.0×1014 n/cm2/s. The main applications of the CARR are neutron scattering and neutron imaging, radioisotopes production, material irradiation, neutron transmutation doping silicon, neutron activation analysis, etc.

The neutron optical devices and sample environments are the core components of the neutron spectrometer, which are related to the performance and research field of the spectrometer.

In this presentation, the research and development of optical devices and sample environments at CARR-Neutron Science Center will be briefly introduced, including Double focusing neutron monochromator, Neutron Soller and Radial collimators, Double crystal graphite monochromator, High-temperature sample environment, Stretching sample environment, High-temperature creep sample environment, Radioactive sample environment, Neutron polarization device etc. In addition, the Germanium hot pressing process and equipment have been developed, which have the preparation ability of germanium single crystal.

Abstract ID: 63

M5-IT3

Status of neutron optics using novel concepts and substrate materials

Presenter: Christian Schanzer (SwissNeutronics AG)

Keywords: Neutron optics, guides, NMO, WAPA

Efficient neutron transport using neutron guides is the basis for a high performance of modern neutron scattering instruments. The combination of special guide profiles and supermirror coatings with high reflectivity makes it possible to adapt the properties of the neutron beam to the needs of the experiments. In addition, a variety of substrate materials (various glasses, various metals, silicon) offer expanded options in terms of precision, shielding and service life (perhaps also mention something regarding cost optimization). Recently, new concepts for focusing (nested mirror optics) and wide-angle polarization analysis (tWAPA) have been developed that utilize advanced supermirror technology in new sophisticated geometric arrangements.

In our presentation we report on the state of the art and the latest developments in these areas at SwissNeutronics. In particular, we will demonstrate the capabilities and performances of neutron guides made from metallic substrates with highly reflective supermirror coatings (e.g. R = 83% @ m = 4). Similar coatings are used on very thin silicon substrates (t = 0.15 mm). Such substrates are used to build compact Nested Mirror Optics (NMO), which make it possible to transfer the high brilliance of modern neutron sources to experiments or to focus large beams with a defined phase space (beam size and divergence) on very small samples. In addition to transporting and focusing neutron beams, polarizing supermirror coatings have often been used in special configurations, for example V-cavities for polarizing the incident neutron beam and polarizing benders in transmission geometry. These devices are easy to use, to align, and maintenance-free. Advantages that are highly appreciated for the polarization analysis of scattered neutrons, where devices are required that can cover a large solid angle. The concept of tWAPA (transmission Wide Angle Polarization Analyzer) is proposed. Prototyping such a device provided proof of this highly advanced concept.

Abstract ID: 119

M5-IT4

Development of next-generation triple-axis spectrometer HODACA in JRR-3

Presenter: Hodaka Kikuchi (ISSP, UTokyo)

Keywords: Inelastic neutron scattering spectrometer, HODACA

A new multiplex-type inelastic neutron scattering spectrometer, HOrizontally Defocusing Analyzer Concurrent data Acquisition spectrometer (HODACA), was recently developed and built at the C1-1 cold neutron beam port in JRR-3. The spectrometer is suitable for dynamics measurements in the energy range of -1 meV < ħω < 7 meV, catering to a broad array of research fields in physics and material science. HODACA combines 24 detectors and 132 pieces of analyzer crystals and has an estimated measurement efficiency that is 70 times greater than the existing conventional triple-axis spectrometer at the C1-1 beam port.

Abstract ID: 150

M5-IT5

Polarized neutrons, polarized ^{3}He, and new physics beyond the Standard Model

Presenter: Haiyang Yan (China Academy of Engineering Physics)

Keywords: 极化中子、极化 3He、自旋相关的新相互作用、标准模型之外的新物理

To be decided.

Abstract ID: 106

M5-IT6

Polarized ^{3}He neutron spin filters at J-PARC

Presenter: Takashi Ino (KEK)

Keywords: ^{3}He neutron spin filter, spin-exchange optical pumping, polarized neutron scattering

In the last twenty-some years, polarized ^{3}He neutron spin filters (NSF) have been recognized their effectiveness in polarized neutron scattering worldwide. Particularly in ^{3}He nuclear polarization via spin-exchange optical pumping or SEOP, technical advances have boosted the gas volume of highly polarized ^{3}He, which has made larger area and angle coverage for neutron beam polarization as well as neutron spin analysis possible. Such developments in SEOP include alkali-hybrid optical pumping, high-power diode laser arrays, volume Bragg gratings (diffractive optical elements), homogeneous magnetic cavities, non-magnetic electrical heaters, loss-less ^{3}He spin flipping techniques, etc.

We present our *in-situ* polarized ^{3}He NSF system and polarized neutron scattering with ^{3}He NSF at J-PARC.

Abstract ID: 193

M5-IT7

Status of the neutron detectors for instruments at China Spallation Neutron Source

Presenter: Jianrong Zhou (Spallation Neutron Source Science Center)

Keywords: Imaging detector, Large area coverage, High detection efficiency, High spatial resolution，High counting rate

Neutron science and technology plays an irreplaceable role in national defense and industry. China spallation neutron source (CSNS) is a major science and technology platform for multidisciplinary applications. As one of the most expensive core equipment of neutron instruments, the neutron detector plays a very important role in the construction and operation of neutron instruments at CSNS. Based on the requirements of the instruments, many common key technologies of neutron detectors have been studied and the detector system of large-scale engineering application has been preliminarily established. A professional and young team has been cultivated to be engaged in developing the advanced neutron detectors. The team has completed the construction of neutron detectors for General Purpose Powder Diffractometer (GPPD), Small Angle Neutron Scattering (SANS), Multifunctional Reflectometer (MR), Multi-Physics Instrument(MPI), Energy Resolved Neutron Imaging instrument(ERNI), High Energy Direct-Geometry Inelastic Neutron Scattering Spectrometer(HD), Very Small Angle Neutron Scattering Instrument(VSANS) and Engineering Material Diffractometer (EMD). We have successfully developed a large area of scintillator detector (Fig.1 (a)), a large area of 3He tube array detector (Fig.1 (b)), an energy resolved neutron imaging detector (Fig.1 (c)) and a ceramic GEM neutron detector (Fig.1 (d)). These detectors are under the final commissioning for operation. At the present, CSNS II will start to be constructed in this winter. Many kinds of detectors will be further developed to realize better performances including larger area, higher spatial resolution, higher detection efficiency and higher integration.

Abstract ID: 199

M5-IT8

A Flexible Electronics System for the Readout of MTPC and MCP Detectors at CSNS Back-n

Presenter: Changqing Feng (University of Science and Technology of China)

Keywords: MTPC, CSNS Back-n, Neutron Resonance Imaging, Neutron Sensitive Microchannel Plate

The Back-n White Neutron Source at CSNS (China Spallation Neutron Source) has advantages of high flux and wide energy spectrum, which makes it a powerful facility for nuclear data measurement and neutron resonance transmission imaging. To promote both the applications, two projects, with the equipment of a Multi-purpose Time Projection Chamber (MTPC) and a Boron doped Microchannel Plate (MCP) system respectively, have been proposed.

The MTPC, using Micromegas (one type of Micro-Pattern Gas Detectors, MPGDs) as its readout cap, is planned mainly for the measurements of neutron-induced charged particle emission reaction and fission reaction, as well as for neutron beam measurement and neutron resonance photography. Meanwhile, the MCP system is aimed for the study of neutron resonance imaging technology.

This presentation will introduce an optical fiber-based flexible readout electronics system, that is intended to provide a general readout solution for the MPGD and MCPs at CSNS Back-n.

The function of its front-end electronics is mainly implemented by low noise pre-Amplifiers (ASICs or discrete components) and multi-channel digitizing modules with the waveform sampling rate of 40 or 80 MSPS, and a 12-bit precision.

With the assistance of Giga-bit optical links, data streams from the front-end electronics are collected to the Data Concentration Module (DCM) and afterwards transferred to PC or computer servers. By configuring the number of optical fibers, the readout system can be easily scaled up to thousands of channels.

This electronics system has been installed with both prototype-MTPC and MCP detectors. Several experiments have been successfully conducted.

Abstract ID: 197

M5-IT9

Photonic glass and fiber for radiation detection

Presenter: Shifeng Zhou (South China University of Technology)

Keywords: Scintillating glass, fiber, radiation detection, neutron detection

Scintillating glasses and fibers are considered to be the important material candidates for radiation detection. In this talk, the recent progress in designs, fabrications and applications of selected materials for multicomponent optical glasses and fibers is introduced. The results about the relation between the glass microstructure and its scintillating properties are introduced. The glasses and fibers for various scintillating functions including high-energy rays and neutrons detection are highlighted.

Abstract ID: 39

M5-IT10

About a Test of the Relativity Principle in a Free Neutron Beta-Decay

Presenter: Vadim Skoy (Joint Institute for Nuclear Research)

Keywords: Neutron Beta Decay, Relativity, Parity Violation

A hypothesis of neutron life time dependence on its helicity is proposed. It is shown that this effect contradicts with relativity principle and thus may be a test of it in a weak interaction. The numerical model of effect is built and the experiments for it measurement are considered as well as discussion and consequences.

Abstract ID: 8

M5-IT11

Development of neutron instrument components by NRC "KURCHATOV INSTITUTE" - PNPI

Presenter: Evgenii Altynbaev (Deputy head of engineering department of National research center ”Kurchatov Institute” - B.P. Konstantinov’s Petersburg Nuclear Physics Institute)

Keywords: Neutron instrumentation, Scientific instrument development

In Accord to the current strategic plan of the Russian Federation “On approval of the Federal Scientific and Technical Program for the Development of Synchrotron and Neutron Research and Research Infrastructure” (hereinafter –FSTP) More than 250 billion rubles have been allocated for the development of the modern research Mega-science infrastructure on the territory of the Russian Federation. Modern research infrastructure means the commissioning of a number of neutron and synchrotron sources and research equipment:

- PIK Research Reactor Complex, Gatchina
- Pulsed neutron source “Omega”, Protvino
- Synchrotron “SILA”, Protvino
- Synchrotron “KISI-Kurchatov-2”, Moscow
- Siberian ring photon source “SKIF”, Novosibirsk
- Synchrotron “RIF”, Vladivostok

Such an intensive growth in demand for high-tech scientific instruments and its components opens up opportunities for effective development and implementations of new technologies. In particular, thanks to targeted mechanisms to support the R&D in the field of scientific instrumentation, the NRC “Kurchatov Institute”- PNPI actively and effectively implements projects in the field of creating components of neutron optics, monochromators, detectors, sample environment for neutron instrumentation and other components of scientific equipment.

The report will represent the recent achievements of NRC “Kurchatov Institute”- PNPI in the field of neutron instrumentation including the presentation of sputtering facility for neutron optics and other developed technologies.

Abstract ID: 36

M5-IT12

A semiempirical Hartree Fock method to calculate the neutron scattering function

Presenter: Anton Stampfl (Australian Nuclear Science and Technology Organisation)

Keywords: inelastic neutron scattering, Hartree-Fock approximation, neutron scattering function, neutron vibrational spectroscopy

The scattering function, S (Q, ω), representing the interaction between the incident neutron and the pseudopotential representing an ensemble of atoms may be determined in a variety of ways: Via classical force-field approaches, through electronic structure calculations, through analytical approaches and through a combination of one or both of the first two approaches and applying molecular dynamics to study systems under non-equilibrium conditions. Electronic structure calculations quickly become computationally intensive once more than several hundred atoms are involved in a cluster or unit cell that represents the system under investigation.

In the case of neutron spectroscopy many systems investigated are dominated by hydrogen vibrations as the total scattering coefficient, $\sigma_{total} \sim 82$ Barn is approximately an order of magnitude larger than most total scattering coefficients from other elements. Scatter from hydrogen is mainly incoherent and therefore may be considered localised allowing potentially simple molecular models to be employed in the study of hydrogenous materials. Here a well known Hartree-Fock semiempirical calculation scheme is presented that is lightning fast for small molecules and adequate for large molecules, clusters, and dynamical studies.

Force constants are obtained by diagonalisation of the mass-weighted Hessian matrix to obtain the vibrational frequency for each mode assuming that each atomic-pair vibrates in a simple-harmonic fashion. The scattering function, $S(Q, \omega)$, is then calculated firstly assuming a one-atom oscillator and then secondly more thoroughly for each atom-pair vibration within the molecule/cluster. A number of benchmark molecules are reported on. Interestingly these rapid calculations give a very good estimation of the scattering function that can be used for initial peak identification and further analysis of the detailed electronic and vibrational structure.

Abstract ID: 113

M5-IT13

Search for new gravity-like interaction in the sub-micron range with small-angle neutron scattering

Presenter: Tatsushi Shima (Research Center for Nuclear Physics, Osaka University)

Keywords: Neutron scattering, Gravity, Hierachy problem, Extra dimensions

Unknown gravity-like interactions, i.e. new interactions coupling to mass, with sub-millimeter ranges are recently attracting considerable interests, since it is suggested by the large-extra-dimension (LED) models which provide a possible solution for so-called hierarchy problem in the elementally particle physics[1]. So far, such new interactions have been searched with Cavendish-type experiments using torsion pendulum or atomic-force microscope. The sensitivities of those experiments, however, are drastically lost in the range below a few micrometers due to serious background caused by inter-molecular forces whose strength is proportional to the electric polarizabilities of the test objects. The small-angle neutron scattering (SANS) is considered useful to obtain high sensitivity to new gravity-like interactions in sub-micron range thanks to an extremely small electric polarizability of the neutron. Previously, SANS experiments with noble gas targets were performed[2,3]. The sensitivities of those experiments are however still far from the theoretically predicted strength of new interactions, and therefore improvement on experimental sensitivity is required to verify the theories. For that purpose we are promoting the SANS experiment using the targets made of nanoparticles[4] in the series of the experiments 2019A0225, 2019B0339, 2020B0416, 2022A0253, and 2022B0333 at Materials and Life-science experimental Facility (MLF) of Japan Proton Accelerator Research Complex (J-PARC). In the case of neutron scattering with nanoparticle target, since the coherent scattering intensity is enhanced by a factor of ˜106 which corresponds to the number of atoms contained in a particle, a drastic improvement of the sensitivity to new interactions is expected. The key to the present method is the suppression of the background caused by the nuclear coherent scattering which is also enhanced. Therefore, we are developing the nanoparticles made of the elements or isotopes with opposite signs of coherent scattering length. This paper will report the present status of the target development and the SANS experiment. In this talk the development of nanoparticle target and recent result of SANS experiment will be presented.

Reference:

[1] N. Arkani-Hamed, S. Dimopoulos, G. Dvali, Physics Letters B429, 263–272 (1998)

[2] N. Arkani-Hamed, S. Dimopoulos, G. Dvali, Physical Review. D59, 086004 (1999).

[3] Y. Kamiya et al., Physical Review Letters 114, 161101 (2015).

[4] C.C. Haddock, et al., Physical Review D97, 062002 (2018).

[5] M. Hiromoto et al., JPS Conf. Proc. 33, 011118 (2021).

Abstract ID: 25

M5-IT14

^{3}He neutron PSD prototype for the wide-angle option of the KWS-2 SANS diffractometer with extended Q-range at the Jülich Centre for Neutron Science

Presenter: Aurel Radulescu (Forschungszentrum Jülich GmbH)

Keywords: SANS, WANS, pinhole, TOF, detectors, ^{3}He

KWS-2 is a classical small-angle neutron diffractometer (SANS) at which, after recent improvements, the pinhole mode with different neutron wavelengths and detector distances using the ^{3}He multi-MHz main detector can be combined with the focusing mode with MgF_2 lenses and a high-resolution secondary detector (1 mm position resolution) to achieve a broad Q range between $2x10^{-4}$ and 1.0 $Å^{-1}$.

To improve the performance of the instrument for structural analyses at very short length scales of a few Å further improvements of the detection system are currently underway. A wide-angle detection option (WANS), which will be beneficial for characterization of semi-crystalline materials and small biological morphologies, is currently being designed for at KWS-2. Given the great versatility of the instrument, which is equipped with two types of chopper systems, the resolution double-disk chopper and the background single-disk chopper, WANS and SANS measurements are being sought on KWS-2 in various combinations of standard and TOF modes.

Several types of detection systems are being considered for the WANS option. The main candidate for this purpose is the well-established position-sensitive ^{3}He tube detector (PSD) with fast readout electronics. The new innovative Solid-State Neutron Detector (SoNDe), a scintillation-based neutron detector, might be considered as a complement to the ^{3}He PSDs. A versatile geometrical arrangement of the two types of detectors may be taken into consideration.

In a first approach, two WANS detectors, each consisting of an array of 80 position-sensitive ^{3}He tube detectors (PSDs) with compact fast readout electronics, will be mounted above and below the beam axis at a distance of 1.25 m downstream from the sample position, in a tilted position with respect to the direction of the beam, which offers the possibility to record the scattered neutrons in a wide angular range up to $2\theta_{max} = 50°$. In combination with short wavelength neutrons ($\lambda = 2.8$ Å), this provides scattering data up to $Q_{max} = 2.0$ $Å^{-1}$. In addition, it is possible to record the scattered neutrons in the high Q range of the instrument in TOF mode, if required, and to discard the inelastic component when measuring hydrogenated samples, to improve the signal-to-noise ratio.

The ^{3}He PSD tubes have a thickness of 6.4 mm and an active length of 60 cm and are grouped in packs of 8 together with fast readout electronics in a compact arrangement that can

be operated in vacuum, air, or He atmosphere. The latter configuration would not require a cooling system for the readout electronics, as demonstrated by the use of the same detection system for the WANS detection benches in BL-15 TAIKAN, J-PARC, Japan, and would help avoid technical complications associated with operation in vacuum. By minimizing the air path between the sample and the detectors, a low background is also achieved. A prototype of such an 8-pack module was tested at MLZ in Garching using a stationary ^{252}Cf neutron source and a borated mask with narrow slits.

The test provided the pulse height spectra and gave the expected position resolution of about 4-5 mm in the middle and at the end of the PSD tubes. Further tests with high intensity neutron beams at a stationary source (BNC reactor, Budapest) in continuous and pulsed (chopper) TOF modes are currently underway.

We will report here in detail on the planned WANS upgrade of the instrument and the test of the ^{3}He PSD prototype.

M5. Contributed Talks

Abstract ID: 152

M5-CT1

High Pressure Instrument at CSNS

Presenter: Le KANG (Institute of High Energy Physics, China)

Keywords: high pressure, instrument, neutron scattering

Based on the major needs of high-pressure neutron scattering instrument in research of new energy field, functional materials, condensed matter physics, geophysics and life sciences, a high pressure instrument had been planned to be built at CSNS through cooperation with SUStech. Through the combination of neutron diffraction and imaging, research on major materials under extreme sample environment is possible.

In order to fulfill the requirement, the physical design of the instrument had been done. DWM had been chosen to act as neutron source. We use elliptical focusing guide to obtain reasonable flux gain as well as to achieve the 0.6% best resolution at 90 degree. T0 chopper together with disk choppers will be used to select required wavelength range. Helium 3 detectors act as main detectors just to achieve high neutron capture efficiency. Standard pressure equipment like PE cell, Zap cell, gas or liquid press cell combined with exclusive three axis large press will be accommodated in our instrument. Meanwhile, sample environment such as temperature and magnetic field is available.

Abstract ID: 102

M5-CT2

Development of time-of-flight neutron diffraction technique based on compact neutron source towards stress measurement

Presenter: Chihiro IWAMOTO (RIKEN, Japan)

Keywords: Compact Neutron Source, Neutron Diffraction, Strain Measurement, Time-of-Flight Method

Neutron diffraction is a powerful non-destructive measurement method for assessing the microstructure and internal stresses of metals. In order to perform on-site neutron diffraction stress measurements in laboratories and factories on a frequent or even daily basis, the time-of-flight neutron diffraction measurement and analysis methods are being improved by utilizing the accelerator-driven Compact Neutron Source (RANS) at the Institute of Physical and Chemical Research, Japan (RIKEN). First, we proposed an analysis method to decompose the original diffraction peaks from the delayed neutron component by defining a model function that describes the shape of the delayed neutrons. Second, a new collimator system, as-called decoupled collimator, is developed to reduce the number of delayed neutrons.

Recently, the diffraction angle dependence of the above function has been calculated using a neutron ray-trace simulation package McStas and the quantitative evaluation of the function parameters have been carried out. Here, we will report the comparison between the simulation and measurement of BCC Fe powder sample. The further analysis result including strain evaluation will be reported in the poster.

Abstract ID: 144

M5-CT3

Present Status on DNA ToF backscattering spectrometer in MLF, J-PARC

Presenter: Yukinobu KAWAKITA (J-PARC Center, Japan Atomic Energy Agency, Japan)

Keywords: backscattering spectrometer, ToF, J-PARC

DNA is a time-of-flight backscattering spectrometer installed at the Materials and Life Science Experimental Facility (MLF) in Japan Proton Accelerator Research Complex (J-PARC), Tokai, Japan. Its purpose is revealing pico to nano second dynamics in a wide field of sciences and industrial applications including soft matter, bio-molecules, chemical molecules, battery, catalyst, and magnetism [1,2]. A pulse-shaping chopper equipped at the 7.75 m position from the coupled moderator makes this instrument relatively short in the neutron guide length (42 m from the moderator to the sample position). Its maximum rotation speed of 300 Hz provides us fine energy resolutions up to 1.4 micro second for a sample with dimension of 1 cm wide and 1cm tall. Changing phases of the slit opening of the chopper enables us to select energy bands and even to scan a wide energy transfer range with the highest resolution. Two types of analyzer mirrors of Si111 and Si311 cover large momentum transfer ranges of 0.08 to 1.98 $Å^{-1}$ and 1.79 to 3.39 $Å^{-1}$, respectively. Frequently used measurement modes are a high-flux mode without rotating the chopper and a high-resolution mode with 225 Hz. Those provides 12 and 3.6 micro eV energy resolutions for a large sample of 1.4 cm wide and 4 cm tall. The back-coat by neutron absorber such as Gd and Gd_2O_3 for Si analyzer mirrors serves us in realizing extremely high signal-to-noise ratio of 105, which allows us to obtain QENS spectra from a tiny amount of sample or a dilute protein solution. Various conditions of sample environment are available; cryo-furnaces (4 K to 700 K), a 2K cryostat, a top-loading sample stick for applying electric field, a humidity control system, a cryostat with a samples changer for three samples, an inner atmosphere controller for cryo-furnaces and so on. A high temperature furnace up to 1000 K, 3.5 Tesla cryo-magnet and a sample changer for 20 samples are under commissioning.

Reference:

[1] K. Shibata et al., JPS Conf. Proc. 8, 036022 (2015).
[2] Y. Kawakita et al., EPJ Web of Conference 272 (2022) 02002

Abstract ID: 234

M5-CT4

Status of Sample Environment at China Spallation Neutron Source

Presenter: Bai Bo (IHEP)

Keywords: Sample Environment, China Spallation Neutron Source

As one of the important auxiliary devices for neutron scattering instruments, sample environment provides various experimental conditions to enhance the research capabilities of the instruments. The sample environment at the Chinese Spallation Neutron Source (CSNS) has been providing *in-situ* experimental services since the commissioning of the instrument in 2018. It has evolved from initially serving as a cryostat to now supporting a wide range of sample environments, including low temperature, high temperature, high pressure, and magnetic field, catering to different user needs. The development has enabled the transition from single-sample environment experiments to multiple-sample environment experiments, showcasing the progress from 0 to 1 and from 1 to many in terms of experimental applications. This article primarily introduces the operation and usage of the sample environment at CSNS. It also highlights recent developments and optimizations in sample environment. Additionally, some experimental applications conducted in collaboration with users are also presented.

Abstract ID: 66

M5-CT5

Current status of a newly high-resolution stress and texture neutron diffractometer HETU at China Mianyang Research Reactor

Presenter: Baihua WANG (School of Materials Science and Engineering, Shanghai Jiao Tong University, China)

Keywords: Neutron stress diffractometer, high instrument resolution, high neutron flux

Recent progress of a newly high-resolution stress and texture neutron diffractometer “HETU” constructed by the Neutron Science Research Center at Shanghai Jiao Tong University, based on the C12 port at neutron guide hall of China Mianyang Research Reactor, is presented. The “HETU” diffractometer enables a high instrument resolution measurement mode using a double-focusing perfect single-crystal silicon monochromator or a high neutron flux mode using a highly-oriented pyrolytic graphite monochromator, dedicated to the analysis of residual stress and texture of engineering materials or components. The peak width functions showed that “HETU” implements a high instrument resolution at moderate neutron flux. The residual stress experimental results of aluminum round-robin and the texture results of zirconium alloy illustrated that “HETU” has sufficient reliability and precision to perform experiments on residual stress and texture of engineering materials or components. The “HETU” has been completed in 2022 and it is open for both national and international users.

Abstract ID: 184

M5-CT6

Status of polarized neutron in-house development at the China Spallation Neutron Source

Presenter: Tianhao WANG (Institute of High Energy Physics, China)

Keywords: Polarized neutron; polarized ^{3}He

Polarized neutron constitutes an important part of the neutron experiment capability. At the China Spallation Neutron Source, the polarized neutron development continuously expands its in-house development capability to support the growing demand of the existing and upcoming beamlines.

As a major part of the in-house polarized neutron capability, the established off-situ and *in-situ* polarized ^{3}He neutron spin filter systems are set as a routine measure to produce high quality polarized neutron for the CSNS beamlines. Combined with supermirrors, plans are made for commissioning polarized neutron on various CSNS beamlines. Magnetic field simulation and neutron polarization also contribute to the capability and ensures guide fields for neutron, spin flippers and precession devices can be designed and manufactured. Lastly, the neutron technology development beamline provides an important beamtime for the testing and calibration on all CSNS related polarized neutron devices.

Recently, the polarized neutron development efforts focus on novel techniques including polarized neutron imaging, strong magnetic field compatible shielding solutions and zero-field environment for polarized neutrons, which will be briefly introduced in the presentation.

Abstract ID: 58

M5-CT7

The possibilities of a compact neutron supermirror transmission polarizer

Presenter: Vladislav SYROMYATNIKOV (Petersburg Nuclear Physics Institute, Russia)

Keywords: transmission neutron polarizer, supermirror, neutron polarization analysis

A new compact neutron supermirror transmission kink polarizer for SANS is proposed in [1, 2]. This polarizer is considerably more compact then a V-cavity! The polarizer consists of a set of plates transparent to neutrons placed in the magnet gap. There are no air gaps between the plates. A polarizing supermirror coating without absorbing underlayers is deposited on the polished surfaces of the plates. Magnetic and nonmagnetic layers of the supermirror coating as well as the material of the plates have nearly equal neutron-optical potentials for spin-down neutrons. There is a considerable difference, however, between neutron-optical potentials of layers in the supermirror structure for spin-up neutrons. This leads to reflection of spin-up neutrons by the supermirror coating and thus to their removal from the original trajectory or, in other words, from a direct beam. In contrast, spin-down neutrons are not reflected by the coating and, consequently, keep their initial trajectories. As a result, that part of the transmitted beam which propagates along the axis of the incoming beam contains vastly larger number of spin-down neutrons what makes this part of the beam highly polarized.

The compact kink polarizer on silicon plates with supermirror CoFe/TiZr (m = 2) coating has been designed and produced at PNPI. First experimental results of measurements of this polarizer obtained on the reflectometers of polarized neutrons SuperADAM and D17 (ILL, Grenoble, France) are presented.

In [3], a more advanced version of this polarizer is considered. At the output of this polarizer, the angular distribution of the neutron beam has almost the same width as at its input, and there are no additional peaks in the angular distribution. The transmitted beam has a high polarization.

The prospects of using this version of polarizer in modern neutron research facilities with polarization analysis will discuss in the report. In particular, the results of calculations of the parameters and main characteristics of this polarizer for using it as a polarizer and analyzer in the inelastic scattering spectrometer of polarized neutrons IN2 are discussed in detail. This facility is part of the instrumental base being created for the PIK reactor (PNPI, Gatchina, Russia).

Reference:

[2] V.G. Syromyatnikov, V.M. Pusenkov. New compact neutron supermirror transmission polarizer. - Journal of Physics: Conf. Ser. 862 (2017) 012028.
[3] V.G. Syromyatnikov. “New neutron transmission supermirror remanent polarizer”. The paper in arXiv:1911.02936 [physics.ins-det].

Abstract ID: 157

M5-CT8

The progress of neutron chopper development for CSNS

Presenter: Ping WANG (Institute of High Energy Physics, China)

Keywords: neutron chopper

Various neutron choppers are key components for the time of flight neutron scattering technique, over the past decade, China spallation neutron source has made significant progress in neutron chopper development. several key technologies have been overcome, leading to the successful development and mass production of T0 choppers, disk choppers, and Fermi choppers, and the neutron chopper technologies are being expanded to the development of X-ray choppers and proton choppers, which will enrich the mechanical particle chopping techniques.

Abstract ID: 221

M5-CT9

Advancements in Readout Electronics for the Detector of Neutron Instruments at China Spallation Neutron Source

Presenter: Hongbin LIU (Institute of High Energy Physics, China)

Keywords: Neutron Detector; Readout Electronics; Neutron Imaging; Data Acquisition

The readout electronics of neutron detectors play a pivotal role in neutron instruments. They are used for amplifying, shaping, and subsequently measuring parameters such as time, position, and energy from the signals produced by neutron detectors. These measurements are then forwarded to backend data acquisition systems for the reconstruction of neutron hit positions and flight time information.

The primary neutron detectors at China Spallation Neutron Source (CSNS) have adopted two major approaches: large-area ^{3}He tube array neutron detector based on position-sensitive 3He tubes, and large-area scintillator neutron detector that integrates scintillator detectors, wavelength-shifting fibers, and SiPMs. Correspondingly, the readout electronics have been developed and implemented in accordance with the requirements and characteristics of these detectors. For the 3He tube array, charge-sensitive preamplifiers are employed to integrate and shape the charges at both ends of the ^{3}He tubes, with digital peak detection and charge division methods utilized to determine the precise neutron hit positions on the 3He tubes.

Addressing the special requirement of placing both the detector and electronics in a vacuum, efforts are actively underway focusing on low-power custom preamplifier ASICs and low-power digitization electronics. For the scintillator-type neutron detector, which possesses a higher channel count, a highly integrated multi-channel ASIC is used for amplifying and discriminating SiPM outputs, with the discriminated signals counted by high-speed FPGAs. Flight time measurements for energy information acquisition are realized by calculating the time difference between global target T0 signals and neutron threshold signals.

Currently, the detector and electronics team at CSNS has successfully accomplished the R&D and implementation of readout electronics for eight neutron instruments start from the CSNS-I project and is now undertaking the construction of electronics for two more neutron instruments. In CSNS - II, the team is set to work on readout electronics for seven neutron spectrometers, including those for ^{3}He tube detectors, scintillator detectors, Multi-Blade detectors, and 3He-GEMs. For ^{3}He tube-type detectors, the readout electronics system can now achieve a position resolution of 7.5 mm for standard 1-meter 3He tubes, comparable with commercial products. Notable advancements have also been made in the development of several preamplifier ASIC chips designed to operate directly in a vacuum and significant progress in low-power digitization electronics. For scintillator-type neutron detectors, a multi-channel preamplifier ASIC and a mature full-chain readout electronics solution have been developed, capable of reading out from scintillator detectors at the level of tens of thousands of channels, meeting the performance requirements for neutron spectrometers in terms of count rate and time measurement accuracy. Additionally, in the field of energy resolved neutron imaging or Bragg-edge imaging, the team is developing a new generation of wide-field, high-resolution energy-resolved neutron imaging devices based on the Timepix4 pixel readout chip invented by the Medipix collaboration.

Abstract ID: 9

M5-CT10

Highly aligned pyrolytic graphite blades for focusing monochromator and analyzer

Presenter: Hongxia Zhang (Laboratory for Neutron Scattering and Beijing Key Laboratory of Optoelectronic Functional Materials and MicroNano Devices, Department of Physics, Renmin University of China)

Keywords: Highly aligned pyrolytic graphite blade, Cleave, Soldering, Neutron monochromator, Neutron analyzer

Highly oriented pyrolytic graphite (HOPG) crystals are often used to monochromatize and analyze incident and scattered neutron beams.[1] Typically several highly aligned pyrolytic graphite blades are used to cover the large cross-section of the neutron beam.[2] To mount small HOPG crystals on the blades without introducing too much misalignment is one of the common technical challenges. Another technical challenge is how to cleave the HOPG crystal to the required thickness without much loss of the precious crystals.

We report the successful fabrication of highly aligned pyrolytic graphite blades from small pieces of HOPG crystals, (see Fig. 1). A special cleavage device and a soldering device are designed which make the fabrication process reliable and with a minimum loss of the precious HOPG crystals. The control parameters of the radio frequency magnetron sputtering technique utilized to deposit indium in the soldering are optimized. The highly aligned pyrolytic graphite blades of a large area coverage, 136 mm wide × 20 mm high, are achieved with minimum increase of the mosaic over that of the original HOPG (see Fig. 2). The peak position, and the miscut angles between the surface and the lattice plane were comparable with the original small-size commercial HOPG crystals.[3]

The devices and procedure reported here could be applied to the development of the low background and high transmission monochromators and analyzers in neutron scattering instruments using a sizable neutron beam.

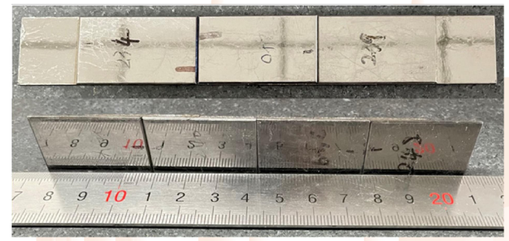

Fig. 1 Photograph of a piece of indium bonded highly aligned pyrolytic graphite blade

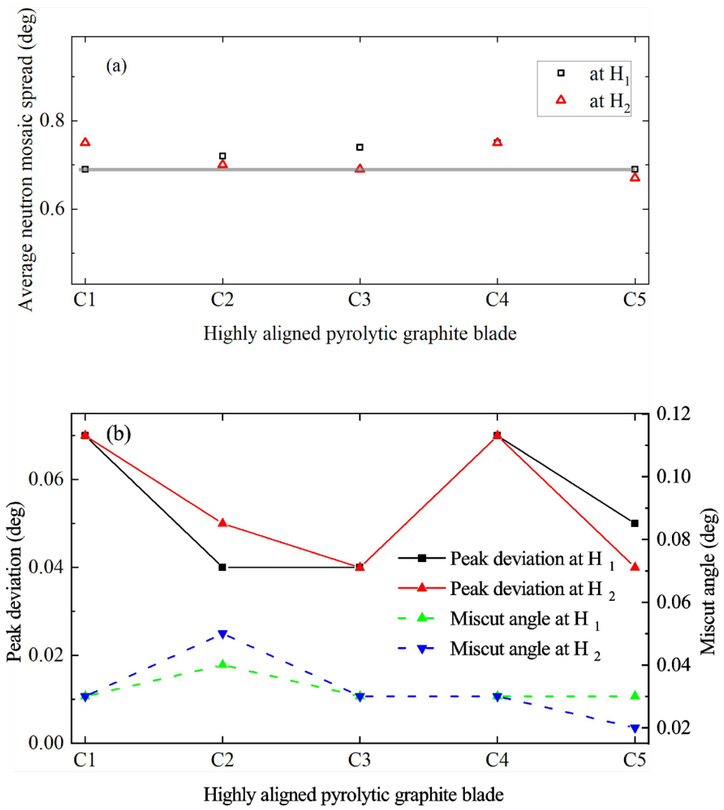

Fig. 2 The averages of mosaic spreads (a), peak position deviations (left axis, b), and miscut angles (right axis, b) of the seven spots measured. The grey line represents the mosaic spread of the original HOPG crystal.

Reference:

1.A.K. Freund, D.H. Yu, Nucl. Instrum. Methods Phys. Res., Sec. A 634, S75 (2011).
2.Michael Schneider, et al., JPS Conf. Proc., 011012 (2018)
3.Hongxia Zhang et al., Highly aligned pyrolytic graphite blades for neutron monochromator and analyzer, submitted to Rev. Sci. Instrum.

Abstract ID: 209

M5-CT11

Introduce to the data system of CSNS

Presenter: Ming TANG (Institute of High Energy Physics, China)

Keywords: data management, cloud analysis, data system

The features of data system at CSNS covers transfer, storage, management and analysis. According to the functions and roles, the whole system can be divided into two parts: online analysis system and offline data platform.

On the online part, a dedicated global ID system was developed for identifying each neutron pulse, which lays the basis for logical experiment runs and parallel data stream processing. Logical run means there is no more start-stop of hardware between runs, hence the beamtime efficiency improved. We achieved high-throughput and real-time data analysis by constructing a memory-based messaging system. This enables the data analysis without sampling and the deep decoupling between components. A web application integrated with WeChat was provided to instrument scientists to monitor the experiment status in quasi real time, anywhere and anytime.

On the offline part, a metadata catalogue system based on ICAT and a storage system based on iRODS are deployed, which enable the full lifetime management of scientific data and the distributed data persistence and data virtualization. This architecture supports heterogeneous storage hardware and disaster recovery backup. A cloud analysis system based on OpenStack was constructed, one can access and analyze data directly in the cloud virtual machine (VM). With the help of integration of shared storage space and CVMFS software distribution repository, we split the data dealing software from the cloud images, so they can be updated independently. It also makes the share of workspace between cloud VM and HPC became available. Finally, a web-based data portal was developed. It integrates all the systems mentioned previously together, and serves as the one-stop application for CSNS users to access, download and analyze their data.

Abstract ID: 244

M5-CT12

A Generic High-Performance Framework for Neutron Spectrometers Data Flow Based on the Distributed Stream-Processing Platform

Presenter: Haiyun Teng (IHEP)

Keywords: stream-processing platform, real-time process, big data sharing

In the recent project of China Spallation Neutron Source (CSNS), a new designed data process framework is applied as the fundamental system on user cooperative instruments, which aims to provide the big data sharing and setup a real-time processing ability for the hierarchical applications. The framework roots in the operation mode of neutron spectrometers, and makes a full-range stipulation from the hardware interface to data flow topology. It also makes best of the open-source Apache Kafka software to setup a distributed stream-processing platform, and coordinates other subsystems to form the adaptive scheme upon it. After all, the system is assembled with modularity and interconnect with standard interface. Users could easily manipulate the experiment data with extensible service and loop-back feeding to other subsystem. This generic technical framework has been verified in the performance and deployment, and is expected to benefit various future advanced experiment methods either.

Abstract ID: 11

M5-CT13

Reactor PIK complex

Presenter: Vladimir VORONIN (NRC Kurchatov Institute - PNPI, Russia)

Keywords: PIK, neutron source

The current status and plans for the organization of the International Center for Neutron Research based on the PIK research reactor (NRC “Kurchatov Institute” - PNPI, Gatchina), will be presented.

The PIK reactor is a neutron source with record parameters. It is a vessel reactor, where light water (H_2O) is used as a coolant, and heavy water (D_2O) as a neutron reflector and moderator. The main design characteristics of the reactor are as follows [1]:

- Thermal power - 100 MW;
- The volume of the reactor core - 50 liters
- Thermal neutron flux in the reflector up to 1.2 10^{15} n/cm^{2}s;

The PIK reactor has been brought to the power mode of operation in 2021. Thermal power of 7 MW [2] has been reached in March 2022. The first 5 neutron scattering stations have been put into operation, and the first experiments are being carried out [3]. The full-scale instrumentational program [4] for the creation of 20 instruments, cold and hot neutron sources are currently under progress.

Reference:

[1] M. V. Kovalchuk, S. L. Smolskiy, and K. A. Konoplev, Research Reactor PIK, Crystallography Reports, 2021, Vol. 66, No. 2, pp. 188–194.
[2] M. V. Kovalchuk, V. V. Voronin, S. V. Gavrilov et al, Research Reactor PIK: The First Experiments, Crystallography Reports, 2022, Vol. 67, No. 5, pp. 729–738
[3] S. Grigoryev, V.V. Voronin, A. Gartvik et al, PIK research reactor put into megawatt-power operation, Neutron New, 2022, DOI: 10.1080/10448632.2022.2126716
[4] Kovalchuk M.V., Voronin V.V., Grigoriev S.V. et al. Instrument Base of the Reactor PIK. Crystallogr. Rep. 66, 195–215 (2021)

Abstract ID: 242

M5-CT14

Physical Design of Radial Collimator for High-Resolution Neutron Diffractometer at China Spallation Neutron Source

Presenter: Zhenhong Tan (IHEP)

Keywords: radial collimator, neutron diffractometer, neutron engineering science

The high-resolution time-of-flight neutron diffractometer at China Spallation Neutron Source is specifically designed for research in materials science, energy science, and life sciences. It achieves a best resolution ($\Delta d/d$) of 0.05%, and it offers wide detector coverage from 5 to 177.3 degrees. However, the broad coverage angles pose a challenge for designing a radial collimator to reduce noise neutrons. Based on the aperture angle, the gauge volume, and the cut-off values, we conducted a systematic and detailed analysis and physical design for the radial collimator.

During the process, we evaluated the shielding effect of the collimator on high- and low-angle banks. Consequently, we abandoned the idea of setting collimator blades to these two banks. Then, we performed the Monte Carlo simulations and theoretical calculations to access the shielding effectiveness. Furthermore, we conducted the calculations related to collimator blade thickness and its efficiency in attenuating noise neutrons.

In this presentation, we will introduce the detailed results of well-designed radial collimator for the diffractometer. The corresponding simulations and calculations results will be also discussed.

Abstract ID: 18

M5-CT15

Small-angle neutron scattering instruments at the PIK reactor

Presenter: Liubov AZAROVA (Petersburg Nuclear Physics Institute of NRC “Kurchatov Institute”, Gatchina, Leningradskaya oblast., Russia)

Keywords: SANS, instruments, PIK, time-of-flight

The Petersburg Nuclear Physics Institute (NRC “Kurchatov Institute” - PNPI) has started work on the construction of small-angle neutron scattering facilities at the PIK reactor complex. Small-angle neutron scattering (SANS) is one of the key and most popular methods used in the study of nanostructures and nanoobjects. Small-angle neutron scattering (SANS) is a non-destructive diffraction method in which neutron scattering occurs on large-scale inhomogeneities (ranging from 1 nanometer to 10 micrometers) and at small angles. This method has found applications in a wide range of scientific disciplines, including physics, chemistry, biology, materials science, engineering, and earth sciences [1].

This report focuses on the development and mathematical modeling [2] of two SANS instruments - "TENZOR" and "MEMBRANA-2". The "TENZOR" instrument is a classic high-flux monochromatic SANS instrument designed to address problems related to magnetism and materials science. The "MEMBRANA-2" instrument is designed as a time-of-flight machine for studies in the field of biology, polymer physics, materials science, and kinetics studies in samples. The presentation will cover the main parameters and characteristics of these mentioned instruments.

Reference:

[1] Schmatz W. et al. Neutron small-angle scattering: experimental techniques and applications //Journal of Applied Crystallography.1974. T. 7. No. 2. C. 96-116.

[2] Lefmann K., Nielsen K. McStas, a general software package for neutron ray-tracing simulations //Neutron news. 1999. T. 10. No. 3. C. 20-23.

Part Two:
Poster Presentations

The 4th Asia-Oceania Conference
on Neutron Scattering

Scientific Poster Session M1.
Condensed Matter Physics

Abstract ID: 7 **M1**

Evolution of the skyrmion lattice in MnGe-based compounds under high pressure

Presenter: Daria Skanchenko (NRC «Kurchatov Institute» - PNPI)

Keywords: manganese germanide, helical spin structure, small-angle neutron scattering, magnetic ordering temperature, skyrmion lattice, quasi-hydrostatic pressure

We have grown $Mn_{1-x}Fe_xGe$ compounds with x = 0.1 and 0.3 using high pressure synthesis [1]. The appearance of the skyrmion lattice (SkX) in MnGe-based compounds with Fe-replacement of Mn atoms was observed under external magnetic field within the wide field range at temperatures far below T_c [2]. The increase of the field range of its presence is accompanied by the linear increase of the DMI in $Mn_{1-x}Fe_xGe$ with increase of Fe concentration [3-5]. The temperature range of the presence of the SkX is most likely connected to the intrinsic instability of the magnetic structure found for MnGe and Fe-doped compounds [6].

Here we report on the evolution of the magnetic system of the $Mn_{1-x}Fe_xGe$ compounds with x = 0.1 and 0.3 under external magnetic field and qasi-hydrostatic pressure up to 1.0 GPa. As the result the (H–T) phase diagram has been plotted for each compound.

With pressure increase all of the critical fields increases at low temperatures for both compounds, while the ordering temperature decreases. The temperature and field ranges of the existence of the SkX decreases with pressure increase. We believe that these facts are connected to the stabilization of the magnetic structure of MnGe-based compounds under pressure. This process is opposite to the Fe-replacement of Mn atoms despite the fact that the lattice constant continues to decrease.

Authors thank for support the Russian Scientific Foundation (Grant No 22-12-00008).

References:

[1] A. V. Tsvyashchenko, J. Less-Common Met. 99, L9 (1984).

[2] E. Altynbaev, et al., Physical Review B vol. 101 N. 100404(R) (2020).

[3] T. Koretsune, et al., Sci. Rep. 5, 13302 (2015).

[4] J. Gayles, et al., Phys. Rev. Lett. 115, 036602 (2015).

[5] T. Kikuchi, et al., Phys. Rev. Lett. 116, 247201 (2016).

[6] E. Altynbaev, et al., Physical Review B vol. 94 N. 17 (2016).

[7] D. Skanchenko, et al., J. of All. and Comp. vol. 865 N. 158606 (2021).

Abstract ID: 17 **M1**

Dispersion relation in amorphous ferromagnets

Presenter: Liubov Azarova (Petersburg Nuclear Physics Institute of NRC “Kurchatov Institute”, Gatchina, Leningradskaya oblast., Russia; St. Petersburg State University, St. Petersburg, Russia)

Keywords: SANS, amorphous magnets, ferromagnets, spin waves, magnons

Amorphous magnetic materials are of considerable interest, both from a fundamental and applied point of view. The low coercive field in an amorphous magnet is an important property for its application as a core material in electrical transformers. The structural and magnetic properties of amorphous magnetic systems can be quite complex. The presence of structural as well as magnetic disorder plays an important role in amorphous systems. However, understanding the formation and growth of spin clusters in amorphous systems is a complex task. The properties of spin clusters in an amorphous system under the influence of an external magnetic field depend on their morphology. Therefore, from the magnetism point of view, interesting aspects are: (1) correlation between structural and magnetic properties; (2) understanding the behavior of spin clusters and (3) investigation of magnetic excitations in such systems. Despite some success in describing the static properties of magnetically soft amorphous magnets [1, 2], their dynamic characteristics and, in particular, the characteristics of the magnon dispersion have not been studied in detail, so the problem of direct measurement of the spin wave spectrum by neutron scattering methods turns out to be relevant.

The dispersion of spin waves in an amorphous ferromagnet can be described through the model of a ferromagnet with random anisotropy: $\epsilon(q) = Aq^2 + g\mu_BH + \delta\omega(q)$, where $\delta\omega(q)$ is a linear in $|q|$ additive [1, 3]. In this paper, we investigate the temperature dependence of the energy characteristics in the spin wave spectrum of the amorphous ferromagnetic alloy $Fe_{48}Ni_{34}P_{18}$ and show that it is possible to obtain information not only about the spin-wave stiffness, but also about the characteristic random anisotropy constant that determines the appearance of the additive $\delta\omega(q)$. We use the method of small-angle scattering of polarized neutrons to prove the significance of the additional term $\delta\omega(q)$ in the dispersion. The measurements were carried out at different values of the external magnetic field H and the neutron wavelength λ. The neutron scattering map is a circle of a certain radius centered at the point $q = 0$. The spin-wave stiffness A is extracted directly from the λ-dependence of the radius of this circle. The spin-wave stiffness A of an amorphous alloy weakly decreases from 140 to 110 meV Å^2 with an increase in temperature in the range from 50 to 300 K. The field dependence of the radius demonstrates the presence of an additive $\delta\omega(q)$ in the kind of an energy gap, which practically does not depend on the field and temperature. The additive value is 0.015÷0.020 meV.

References:

[1] R. S. Iskhakov, S. V. Komogortsev, A. D. Balaev, and L. A. Chekanova, JETP Lett. 72, 304 (2000).

[2] S. V. Komogortsev, R. S. Iskhakov, and V. A. Fel'k, J. Exp. Theor. Phys. 128, 754 (2019).

[3] V. A. Ignatchenko and R. S. Iskhakov, Zh. Eksp. Teor. Fiz. 72, 1005 (1977).

Abstract ID: 32 **M1**

Symmetry Stabilization of Orthoferrite Epitaxial Thin Films

Presenter: Sungkyun Park (Pusan National University, Busan, Korea)

Keywords: Ferromagnetic thin films, Polarized Neutron Reflectomery

The Metal-Oxide-Semiconductor Field-Effect Transistor (MOSFET) is a crucial component widely employed in the semiconductor industry, particularly in applications reliant on oxide systems. To enhance its operational efficiency, energy efficiency improvements and size reduction are imperative. The development of high-k oxide dielectrics is thus of paramount importance for achieving high-capacitance MOSFETs with compact dimensions. Traditional oxide SiO_2 is prone to significant leakage currents, especially in ultrathin configurations. On the other hand, HfO_2, another high-k oxide material, exhibits reliability concerns due to abrupt breakdown when compared to perovskite dielectric materials.

In this presentation, we propose the utilization of $LaFeO_3$ as a novel high-k material in the form of epitaxial thin films. Notably, its tetragonal lattice symmetry has been stabilized to overcome its original bulk orthorhombic phase. $LaFeO_3$ also possesses intriguing characteristics, including its canted antiferromagnetic structure, rendering it multiferroic and suitable for spintronic applications. This property opens up extensive possibilities for magnetoelectric coupling in conjunction with its dielectric properties. Furthermore, our investigation has unveiled a correlation between the lattice constant and dielectric constant, modulated by the control of oxygen partial pressure ($P(O_2)$). Remarkably, the material exhibits the highest dielectric constant when its lattice constant is minimized, and it demonstrates robustness across varying temperatures.

References:

[1] S. Acharya et al., (2010) Multiferroic behavior of lanthanum orthoferrite (LaFeO3) Mater. Lett, 64, 415-418

[2] W. Lin et al., (2022) Evidence for spin swapping in an antiferromagnet, Nat. Phys, 18, 800-805

Abstract ID: 45 **M1**

Multiple magnetic transitions and complex magnetic structures in Fe_2SiSe_4 with the sawtooth lattice

Presenter: Feihao Pan (Renmin University of China); Peng Cheng (Laboratory for Neutron Scattering and Beijing Key Laboratory of Optoelectronic Functional Materials and MicroNano Devices, Department of Physics, Renmin University of China)

Keywords: complex magnetic structures, Neutron Scattering, sawtooth lattice

The sawtooth lattice shares some structural similarities with the kagome lattice and may attract renewed research interest. Here, we report a comprehensive study on the physical properties of Fe_2SiSe_4, an unexplored member in the olivine chalcogenides with the sawtooth lattice of Fe. Our results show that Fe_2SiSe_4 is a magnetic semiconductor with band gap of 0.66 eV. It first undergoes an antiferromagnetic transition at T_{m1}=110 K, then an ferrimagnetic-like one at T_{m2}=50 K and finally a magnetic transition at T_{m3}=25 K which is likely driven by the thermal populations of spin-orbit manifold on the Fe site. Neutron diffraction analysis reveals a non-collinear antiferromagnetic structure with propagation vector q1= (0,0,0) at $T_{m2}<T<T_{m1}$. Interestingly, below T_{m2}, an additional antiferromagnetic structure with q2= (0,0.5,0) appears and Fe_2SiSe_4 exhibits a complex double-q magnetic structure which has never been observed in sawtooth olivines. Density functional theory calculations suggest this complex noncollinear magnetic structure may originate from the competing antiferromagnetic interactions for both intra- and inter-chain in the sawtooth lattice. Furthermore, band structural calculations show that Fe_2SiSe_4 has quasi-flat band features near the valence and conduction bands. Based on the above results, we propose Fe_2SiSe_4 as a new material platform to condensed matter researches.

Abstract ID: 84 **M1**

Yinglong a new thermal triple-axis spectrometer at CMRR

Presenter: Xin Li (Key laboratory of neutron physics and institute of nuclear physics and chemistry)

Keywords: triple-axis spectrometer inelastic neutron scattering

A new thermal neutron triple axis spectrometer named Yinglong was developed and tested at the China Mianyang Research Reactor (CMRR). Instrument design, main components, and test results with neutron beam are present in this work.

By utilizing neutron velocity selector and double-focusing HOPG monochromator, monochromatic neutron beam with flux intensity at sample stage larger than 107 n/(cm^2·s) was achieved. The use of horizontal focused analyzer greatly enhanced the inelastic neutron scattering signal. Yinglong can be typically used to study lattice dynamics and magnetic excitations in solid state physics. Beam time application will keep open to the research community.

Abstract ID: 85 **M1**

Spin-slip magnetic phase in Ho_3Co evidenced by neutron diffraction

Presenter: Andrei Gubkin (M.N. Mikheev Institute of metal physics)

Keywords: neutron diffraction, rare-earth intermetallics, magnetic superspace groups, spin-slip structure

Binary rare-earth intermetallic compounds of R_3T type (R − rare-earth metal, T − transition metal) crystallizes in orthorhombic structure of Fe_3C type described by the space group Pnma. Competition of RKKY-type exchange interactions combined with a low symmetry crystal electric field gives rise to a rich magnetic phase diagram and incommensurate magnetic structures that affect the macroscopic properties in R_3T compounds. In particular, Ho3Co exhibits two successive magnetic phase transitions on cooling [1,2]. Complicated incommensurate magnetic structure described by a combination of two propagation vectors k_{IC}=(0.15 0 0) and k_C=(0 0 0) was observed by neutron diffraction below the Nèel temperature T_N = 22 K. Weak spontaneous magnetization in the incommensurate magnetic phase of Ho_3Co was reported below the spin-reorientation transition at T_t = 9 K though its origin stayed unclear 1. No quantitative description of the low temperature magnetic structure in Ho_3Co was reported up date. In this work, we report a model of the low temperature magnetic structure in Ho_3Co obtained by the Rietveld refinement using magnetic superspace group (MSG) approach. We explain the origin of the weak spontaneous magnetization in terms of the spin-slip effect in the incommensurate magnetic phase of Ho_3Co.

Propagation vectors of the incommensurate magnetic structure in Ho_3Co and corresponding Bragg peaks intensity are plotted as a function of temperature based on the neutron diffraction data measured in a wide temperature range 1.5−300 K (see Fig. 1). It has been found that superposition of two irreducible representations $[k_C]m\Gamma_4^-$ and $[k_{IC}]m\Sigma_4$ giving rise to a magnetic structure of spin-density wave type described with the MSG P$m'cn$(00g)000 at T = 15 K. A future cooling below $T_t \approx$ 11 K results in emergence of both even $2k_{IC}$, $4k_{IC}$ and odd $3k_{IC}$,$5k_{IC}$ harmonics of the incommensurate propagation vector. Odd harmonics imply that squaring-up process of the incommensurate spin-density wave magnetic structure develops below 11 K. Even harmonics may be considered as an evidence of discommensuration process that brings about a periodical disruption of the squared spin-density wave that brings uncompensation of the antiferromagnetic sublattice. This discommensuration is known as a «spin-slip» process [3].

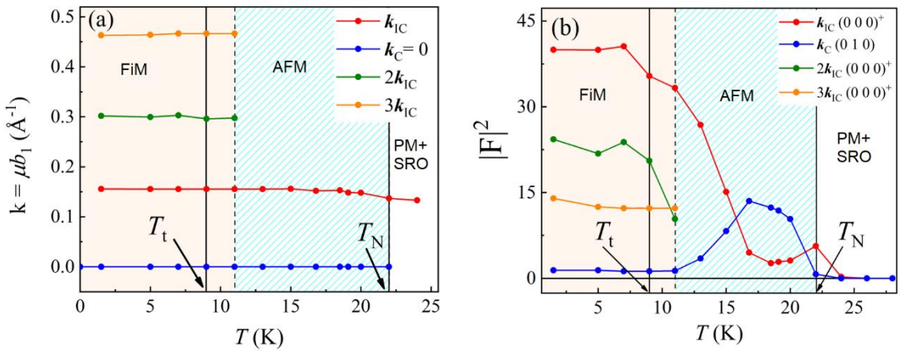

Fig. 1: Magnetic phase diagrams of Ho_3Co plotted as temperature dependence of propagation vectors (a) and structure factor $|F|^2$ of principial Bragg peaks (b). Structure factor $|F|^2$ of the (μ 0 0)$^+$ satellite is reduced by a factor of 90 and of the (0 1 0) magnetic Bragg peak by a factor of 5.

This work was partly supported by the Ministry of Science and Higher Education of the Russian Federation (Project No. № 122021000031-8) and High-end Foreign Experts Recruitment Plan of China, Grant No. G2023014004.

References:

[1] Irreversible field-induced magnetic phase transitions and properties of Ho3Co / N. V. Baranov et al. // Journal of Physics: Condensed Matter 17 (2005) 3445.

[2] Magnetic structures and magnetic phase transitions in Ho3Co / A. Podlesnyak et al. // Journal of magnetism and magnetic materials. 272 (2004) 565-567.

[3] Direct Observation of Spontaneous Weak Ferromagnetism in the Superconductor ErNi2B2C / S.-M. Choi et al // Phys. Rev. Lett. 87 (2001) 107001

Abstract ID: 105

M1

Uncommon magnetism in rare-earth intermetallic compounds: neutron spectroscopy data

Presenter: Pavel Savchenkov (NRC «Kurchatov Institute»)

Keywords: Uncommon magnetism, Inelastic Neutron Scattering, induced magnetism, intermediate-valence

Rare-earth intermetallic compounds are characterised by the presence of a long-range magnetic order due to the interaction of local magnetic moments periodically located within the crystal lattice. This report considers the possibility of forming an ordered state in cases where there is no opportunity to observe the local moment of the f-electronic shell in a traditional sense [1,2].

These are, first of all, systems with a singlet ground state of a rare earth ion. In such systems, under a certain ratio between the dipole matrix element connecting the singlet to the excited state and the magnitude of the interionic interaction at each lattice site, an induced magnetic moment can form and a simultaneous ordering of such moments can occur. This phenomenon, called "induced" magnetism, is discussed in this report using the example of the intermetallic compound PrNi. Some results of experimental investigations of induced magnetism in PrNi and related systems are presented. Primarily, the information extractable from neutron magnetic inelastic scattering spectra is analysed and developed theoretical and model-based representations are discussed.

Special attention is devoted to explaining the influence of defects of various natures in the rare-earth sublattice (nonmagnetic impurity La - $Pr_{1-x}La_xNi$ and intermediate-valence (IV) Ce - $Pr_{1-x}Ce_xNi$) on the conditions for the emergence of long-range magnetic order (see Fig. 1).

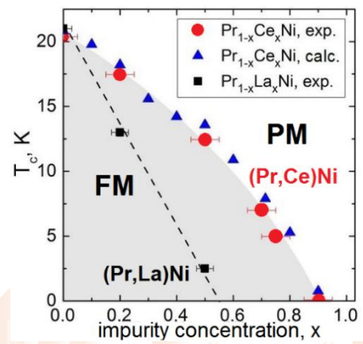

Fig.1 The relationship between Tc and x in Pr1-xLaxNi (black squares) and Pr1-xCexNi (red circles). The blue triangles represent the TC calculations for $Pr_{1-x}Ce_xNi$ using a microscopic state model. The calculation result for $Pr_{1-x}La_xNi$ is presented as dashed line. The grey area indicates the region of the ferromagnetic state of the (Pr, Ce)Ni system, which is significantly larger than for (Pr, La)Ni.

Another type of "unconventional" magnetism explored in the report is the observed

coexistence of magnetic order and fast spin fluctuations in certain intermetallic compounds of Eu. This coexistence initially appears anomalous due to the intermediate valence state of the rare earth ion (see Fig. 2). This report presents the results of experiments investigating the influence of high hydrostatic pressures (up to 15 GPa) on the long-range magnetic order in $EuCu_2Si_2$ and provides evidence for the uniformity of the intermediate valence state of Eu in $EuCu_2(Si_xGe_{1-x})_2$. Based on a comprehensive analysis of the results from a combination of neutron experiments and calculations within the framework of induced magnetism theory, a realistic description of the mechanisms underlying the formation of an ordered antiferromagnetic state against a background of uniform intermediate valence is proposed for $EuCu_2(Si_xGe_{1-x})_2$.

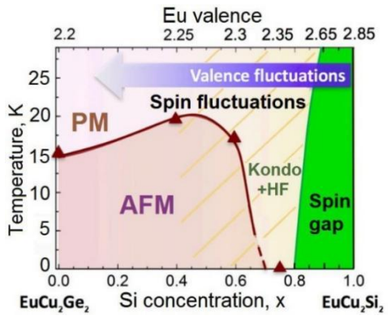

Fig.2 Magnetic phase diagram for $EuCu_2(Si_xGe_{1-x})_2$. The valence values shown on the upper scale. The solid brown line rep-resents the phase boundary between the antiferromagnetic (AFM) and paramagnetic (PM) states. The triangles indicate the values obtained from neutron powder diffraction experiments. The yellow region (Kondo + HF), extending down to x = 0.4 and overlapping with the AFM region, represents the spin-fluctuation regime where a quasielastic response is observed. The green colored region represents the low temperature spin gap regime.

References:

[1] Savchenkov, P. S., & Alekseev, P. A. (2023). Uncommon Magnetism in Rare-Earth Intermetallic Compounds with Strong Electronic Correlations. Crystals, 13(8), 1238.

[2] Savchenkov, P. S., Alekseev, P. A., Podlesnyak, A., Kolesnikov, A. I., & Nemkovski, K. S. (2018). Intermediate-valence state of the Sm and Eu in SmB6 and EuCu2Si2: neutron spectroscopy data and analysis. Journal of Physics: Condensed Matter, 30(5), 055801.

Abstract ID: 123

M1

Phonon coherence induced glass-like thermal conductivity of bismuth-halide $Cs_3Bi_2Br_9$

Presenter: Yongheng Li (School of Aerospace Engineering, Beijing Institute of Technology, Beijing, 100081, China)

Keywords: Phonon coherence, thermal conductivity, anharmonicity

$Cs_3Bi_2Br_9$ emerges as a promising candidate for thermoelectrics, attributed to its ultralow and weak temperature dependent thermal conductivity. The conventional theory, i.e. particle-like thermal conductivity described by the phonon gas model, fails to describe such glass-like behavior of thermal transports. Here, we unearth the significance of phonon coherence in the weak temperature-dependent thermal conductivity of bulk single crystal $Cs_3Bi_2Br_9$.The restrained ability of acoustic phonon bands to carry heat results in the ultralow particle-like thermal conductivity of $Cs_3Bi_2Br_9$, thereby amplifying importance of wave-like thermal conductivity via phonon coherence. The phonons exhibit obvious phonon coherence effect in $Cs_3Bi_2Br_9$, especially for optical phonon modes, and contributes to the wave-like thermal conductivity. The experimental glass-like thermal conductivity of $Cs_3Bi_2Br_9$ is accurately reproduced first-principles calculations, when taking the phonon coherence into account. The wave-like thermal conductivity accounts for ~50% of total thermal conductivity at 300K. This work highlights the importance of phonon coherence in predicting thermal transport properties of strong anharmonic materials.

Abstract ID: 129 **M1**

Bulk and surface phase effects in the Fe-Ga magnetostrictive alloy

Presenter: Sergei Sumnikov (Joint Institute for Nuclear Research)

Keywords: Fe-Ga alloys, neutron diffraction, X-ray diffraction, synchrotron radiation diffraction.

Iron-gallium intermetallic compounds exhibit impressive magnetostrictive properties and are increasingly being used in various industries. However, despite the increasing practical application of such intermetallic compounds, the mechanism of the appearance of the magnetic properties observed in them still remains unclear. The solution of this problem will make available to obtain samples with specified parameters (the main ones are magnetic and mechanical) and to increase the maximum value of magnetostriction. Historically the main method for studying such alloys is X-ray diffraction, which has a small penetration depth and is highly sensitive to surface effects. However, recently, other research methods have become popular, for example, the use of synchrotron radiation and neutrons. Thermal neutrons have a much greater penetration depth and make it possible to obtain more reliable information averaged over the entire volume of the sample. Synchrotron radiation has a colossal brightness, exceeding the brightness of X-ray tubes by millions of times, which makes it possible to determine the presence of phases with a very low concentration. In the presented study, we compared the results obtained using neutron, X-ray and synchrotron radiation diffraction, as well as a comparison of the information obtained with the available literature data. The performed analysis explained a number of mismatches in the phase composition for identical samples in different literature sources, this could be caused by unaccounted for surface effects and possible erroneous interpretation of the results. The works performed [1-3] on a specific practical example showed in which cases it is most expedient to use X-ray diffraction, and in which cases neutron diffraction is an indispensable tool. Thus, the results can be directly used to popularize neutron methods for studying matter.

References:

[1] I. A. Bobrikov, N. Y. Samoylova, S. V. Sumnikov, O. Y. Ivanshina, K. A. Korneeva, A. M. Balagurov and I. S. Golovin, Journal of Applied Crystallography 53 1343-1352 (2020)

[2] A. M. Balagurov, D. Yu. Chernyshov, A. A. Bosak, I. A. Bobrikov, S. V. Sumnikov, I. S. Golovin “In-grain phase separation and structural ordering in Fe-Ga alloys seen from reciprocal space” Intermetallics 128 (2021) 107016 (1-4)

[3] S. V. Sumnikov, I. A. Bobrikov, I. S. Golovin, A. M. Balagurov, Journal of Alloys and Compounds 928 167116 (2022)

Abstract ID: 135 **M1**

Understanding the spin correlations in the $5d^2$ Re-based double perovskites

Presenter: Otkur Omar (University of Science and Technology of China, China)

Institute

Keywords: spin-orbit coupling, double perovskites, neutron scattering

The relativistic spin-orbit coupling (SOC) entangles the spin and angular momenta of electrons and fosters a variety of exotic electronic states. The double-perovskite $A_2BB'O_6$ with the B’ sites occupied by the heavy transitional metal ions is an important family of compounds to study the interplay between electron correlation and SOC. In this study, we determine the magnetic structure of the $5d^2$ Re-based double perovskites Ba_2ScReO_6 and Ba_2YReO_6 through powder neutron diffraction. Our inelastic neutron scattering experiments reveal phonon excitations that are well reproduced by the density function calculations and indicate the presence of weak magnetic excitations.

Abstract ID: 147 **M1**

Spin dynamics in the trimer-host compound $Dy_3Ru_4Al_{12}$

Presenter: Han Wang (University of Science and Technology of China, China)

Keywords: spin trimers, diffuse and inelastic neutron scattering, spin dynamics, breathing kagome-lattice, unconventional geometrical Hall effect

In the breathing kagome-lattice compound $Dy_3Ru_4Al_{12}$, spin trimers with a nonzero scalar spin chirality have been proposed as the origin of an unconventional geometrical Hall effect, yet a microscopic model explaining the emergent spin trimers is still missing. Here we combine diffuse and inelastic neutron scattering experiments to study the spin dynamics in $Dy_3Ru_4Al_{12}$. Through molecular dynamics and self-consistent Gaussian approximation calculations, we determine the spin Hamiltonian underlying the breathing kagome lattice formed by the Dy^{3+} spins, which paves the way for the understanding of the ordering phenomena of spin trimers in $Dy_3Ru_4Al_{12}$.

Abstract ID: 224 **M1**

Inelastic neutron scattering and muon spin relaxation investigations of the deuterated Kondo lattices $CeNiSnD_x$

Presenter: Xiaoying Zheng (Zhejiang university)

Keywords: Inelastic neutron scattering, CEF excitation, Kondo lattice, CeNiSnDx

CeNiSn is a Kondo semimetal where a gap opens at low temperatures due to hybridization between 4f and conduction electrons, but a full insulating state fails to develop. Upon the insertion of hydrogen, long range magnetic order is induced. Here we report zero field muon spin relaxation (μSR) and inelastic neutron scattering (INS) measurements of polycrystalline samples of the deuterides $CeNiSnD_x$ (x = 1.0, 1.8). The μSR results confirm magnetic ordering in the whole sample of CeNiSnD below around 4.7 K, while INS reveals two well-defined CEF excitations at around 13 meV and 34 meV in CeNiSnD, and 5 meV and 27 meV for $CeNiSnD_{1.8}$. These results suggest that hydrogenation leads to the localization of the Ce-4*f* electrons, giving rise to long-range magnetic order, and we propose CEF level schemes for both systems that account for the observed magnetic properties.

Abstract ID: 236 **M1**

Chromates: crystal growth, magnetism, and ferroelectricity

Presenter: Haifeng Li (University of Macau), Kaitong Sun (University of Macau)

Keywords: Chromates, Crystal growth, Magnetism, Ferroelectricity

Multiferroics represent a class of advanced materials for promising applications and stand at the forefront of modern science for the special feature possessing both charge polar and magnetic order. Previous studies indicate that the family of *RE*CrO_3 (*RE* = rare earth) compounds is likely another rare candidate system holding both ferroelectricity and magnetism. However, many issues remain unsolved, casting hot disputes about whether *RE*CrO_3 is multiferroic or not. For example, an incompatibility exists between reported structural models and observed ferroelectric behaviors, and it is not easy to determine the spin canting degree. To address these questions, one key step is to grow single crystals because they can provide more reliable information than other forms of matter do. Here, we present the single crystal growth, magnetic properties, and ferroelectricity of orthochromates.

References:

[1] Y. Zhu, S. Wu, Z. Tang, H.-F. Li, A method of centimeter-sized single crystal growth of chromate compounds and related storage device, China Patent No. ZL 2019 1 1281088.8 (2021).

[2] Y. Zhu, J. Xia, S. Wu, K. Sun, Y. Yang, Y. Zhao, H. W. Kan, Y. Zhang, L. Wang, H. Wang, et al., Crystal growth engineering and origin of the weak ferromagnetism in antiferromagnetic matrix of orthochromates from te orbital hybridization, iScience 25 (4) (2022) 104111.

[3] Y. Zhu, K. Sun, S. Wu, P. Zhou, Y. Fu, J. Xia, H.-F. Li, A comprehensive review on the ferroelectric orthochromates: Synthesis, property, and application, Coordination Chemistry Reviews 475 (2023) 214873.

Scientific Poster Session M2. Materials Science and Chemistry

Abstract ID: 23

M2

Phase Transition of $AgTaO_3$ using High-Resolution Neutron Diffraction

Presenter: Junwei Li (the Institute of High Energy Physics, CAS)

Keywords: Phase transition

$AgTaO_3$ is a perovskite that can become piezoelectric by sodium/potassium doping [1]. Understanding its structure is important towards unlocking new materials for lead-free piezoelectric. However, the phase transition of $AgTaO_3$ is difficult to characterise [2, 3]. The phase transition of $AgTaO_3$ was previously studied by Synchrotron X-Ray Diffraction (SXRD) using the Powder Diffraction beamline (BL10) at the Australian Synchrotron. SXRD patterns of $AgTaO_3$ was recorded during heating, with diffraction patterns taken at 10 °C intervals [3]. Rietveld refinement of the SXRD patterns shows the phase transition of $AgTaO_3$ to be

$$R3c \rightarrow Cmcm \rightarrow P4/mbm \rightarrow Pm\bar{3}m$$

This presentation revisits the phase transition of $AgTaO_3$, by studying the same sample with Powder Neutron Diffraction (PND) using the Super High-Resolution Powder Diffractometer instrument at J-PARC. Two grams of polycrystalline sample was brought up to 700 °C, and cooled. PND patterns were collected during cooling, between 700-300 °C (inclusive), with a step size of 10 °C. Rietveld refinement of the PND patterns, using the GSAS II software [5], reveals the phase transition to be

$$R3c \rightarrow Cmcm \rightarrow Pm\bar{3}m$$

with the pseudocubic volume of the sample vs sample temperature revealing an almost linear trend, similar to that found in the SXRD study [4]. A notable difference can be seen between PND and SXRD, in which P4/mbm phase was missing from the PND study. The Splitting of 002 $Pm\bar{3}m$ peak into the 220 and 002 $P4/mbm$ peak, which is apparent in the SXRD study, is missing in the PND patterns.

References:

[1] Y. Wang, L. Qibin, F. Zhao. (2009) J. Alloys Compd. 489 175-178.

[2] H.P. Soon, H. Taniguchi, M. Itoh. (2010) Phys. Rev. B 81 104105.

[3] M.H. Francombe, B. Lewis. (1958) Acta Crystallogr. 11 175–178

[4] U. Farid, H. U. Khan, M. Avdeev, S. Injac, B. J. Kennedy. (2018). JSSC. 258 859-864.

[5] B. H. Toby, R. B. Von Dreele, (2013). J Appl Crystallogr. 46 (2) 544-549.

Abstract ID: 67

M2

Influence of process parameters on microstructure and residual stress in alloys produced by additive manufacturing

Presenter: Erik Walz (STRESS-SPEC Group, Research Reactor FRM-2 Munich, Germany)

Keywords: Additive Manufacturing, Residual Stress, Tensile Test, LPBF

Metal Additive manufacturing (AM) allows printing structures of almost any complexity. Therefore, it is an uprising technique in various industrial sectors like automotive and aerospace [1]. Nevertheless, in the manufacturing method of laser powder bed fusion (LPBF) the used process parameters have a high influence on the final part. They impact texture, residual stress and also the tensile properties [2]. To achieve consistent material characteristics, a pro-found understanding of the process parameter influence is needed [3].

In the current presentation, we investigate the evolution of residual stress, texture and the tensile properties of additively manufactured samples as a function of build direction and diameter. Two different alloys, 316L and $AlSi_{11}Mg_{0.5}$, are used as sample material. They are both widely utilized in AM and form a fcc structure. But 316L has only one phase and is highly anisotropic, whereas $AlSi_{11}Mg_{0.5}$ is a nearly isotropic two-phase metal [4,5].

This study uses high energy synchrotron X-rays to assess the residual stress and the texture of the different samples. Furthermore, *in-situ* tensile tests were conducted to study the elastoplastic behaviour and the dislocation densities. The results are evaluated with respect to the different process parameters. In addition, a comparison between the two alloys is conducted to determine how much the material-specific properties affect the finished component.

References:

[1] Dirk Herzog et al. “Additive manufacturing of metals”. In: Acta Materialia 117 (2016), pp. 371–392.

[2] Jakob Schröder et al. “Diffraction-Based Residual Stress Characterization in Laser Additive Manufacturing of Metals”. In: Metals 11.11 (2021), p. 1830.

[3] E. O. Olakanmi, R. F. Cochrane, and K. W. Dalgarno. “A review on selective laser sintering/melting (SLS/SLM) of aluminium alloy powders: Processing, microstructure, and properties”. In: Progress in Materials Science 74 (2015), pp. 401–477.

[4] Shu Yan Zhang et al. “Investigation of Martensite Transformation in 316L Stainless Steel”. In: Materials Today: Proceedings 2 (2015), pp. 251–260.

[5] Idan Rosenthal, Adin Stern, and Nachum Frage. “Microstructure and Mechanical Properties of AlSi10Mg Parts Produced by the Laser Beam Additive Manufacturing (AM) Technology”. In: Metallography, Microstructure, and Analysis 3.6 (2014), pp. 448–453.

Abstract ID: 116 **M2**

Enhanced Oxygen Ion Conductivity and Mechanistic visualization in $Pr_{1-x}Sr_xVO_{4-0.5x}$

Presenter: Gaoqing Hang (MOE Key Laboratory of New Processing Technology for Nonferrous Metal and Materials, Guangxi Key Laboratory of Optical and Electronic Materials and Devices, College of Materials Science and Engineering, Guilin University of Technology)

Keywords: $PrVO_4$; doping strategy; oxygen vacancy defects; oxygen migration mechanism

$PrVO_4$ has been attracted great interest due to their electronic properties, luminescence, and photocatalyst. In 2018，it was reported that the effect on structure and electrical property of $PrVO_4$ through Mg^{2+} doping, indicated no significant change with introducing of magnesium. So far, no further electrical performance and conduction mechanism analyses were investigated for acceptor doping $PrVO_4$. Herein, the polycrystalline ceramics of $Pr_{1-x}Sr_xVO_{4-0.5x}$ samples were synthesized by conventional high temperature solid-state method. Then the structure, solid solution and electrical conductivities as well as the ionic conduction mechanism were investigated. The structure of Sr^{2+}-doping compound was obtained from the Rietveld refinement carried out over the laboratory XRD and NPD data (Figure 1). The electrical performance results shown an enhancement of about one order of magnitude the oxygen ion conductivity through Sr^{2+}-substitution on Pr^{3+} site in $PrVO_4$. The oxygen vacancy defects stabilization and long-range migration mechanism are being studied by comprehensive characterizations. This study will provide a useful guide for designing new oxygen ion conductors and understanding oxygen ion conduction mechanisms.

Abstract ID: 118 **M2**

Magnetic Structure and Thermal Dynamic Analysis in Water-Coordinated Coordination Polymers

Presenter: YOUNGHU SON (Kyungpook National University)

Keywords: Coordination Polymers, Magnetic Structure

Coordination polymers (CPs) comprised of the linkage of metal ions with ligands, offering intriguing potential as distinctive magnetic systems. They can create multi-dimensional paramagnetic metal chains, especially when using transition metal ions with unpaired electrons like Cr, Mn, Co, and Ni. This arrangement leads to aligned electron spins within CPs, resulting in magnetic interactions that can either enhance or cancel out the magnetic moment. Consequently, CPs characterized by well-defined crystalline structures can be valuable materials for delving into magnetic properties through structural analysis. In this study, we present an analysis of the magnetic properties of water-coordinated CPs, specifically $M(HCO_2)_2(H_2O)_2$, where M can be either Co(II) or Ni(II), using neutron experiments. Interestingly, exposure to high humidity triggered a remarkable structural transformation of non-hydrated metal-organic frameworks, leading to their irreversible conversion into hydrated CPs. We successfully determined the crystal structures of metal-formates non-hydrated and hydrated forms. In our pursuit of understanding the magnetic properties of these coordination polymers (CPs) in their hydrated and non-hydrated forms, we conducted a series of neutron diffraction experiments at different temperatures. These experiments yielded intriguing results, including observing an unusual peak associated with a hydrated form of the Ni-formate and the emergence of a unique unit-cell change as the temperature increased in the case of Ni-formate. We delved into the magnetic structure of metal-formate, aiming to uncover how adsorbed or coordinated water molecules within the CPs influence the alignment of spins within the CPs. To further investigate the unusual contraction along the c-axis that occurs as temperature rises, we have plans to acquire and compare crystal structures through single crystal analysis at both low and high temperatures. We will conduct the detailed Rietveld refinement with magnetic structure to better understand this intriguing topic.

Abstract ID: 146

M2

Translational Diffusion of Water Molecule in Aqueous Alkali Metal Chloride Solutions under Pressure by Quasielastic Neutron Scattering

Presenter: Zhuanfang Jing (Qinghai Institute of Salt Lakes, Chinese Academy of Sciences)

Keywords: Alkali metal ions, water diffusion, ion hydration, high pressure, quasielastic neutron scattering

The dynamics study of water and aqueous solutions under pressure is important in geosciences, planetary modelling, environmental sciences, and biological system, etc. [1,2] However, the information on dynamics of water and aqueous solutions under high pressure at the molecular level is limited because of the difficult acquisition of reliable scattering data at high pressures and the difficulty in distinguishing between water molecules in the ion hydration shell and the bulk. In this work, we performed Quasielastic Neutron Scattering (QENS) experiments at 298 K on pure water and 3 mol/kg alkaline metal chloride solutions (LiCl, NaCl, KCl, RbCl, and CsCl) at 0.1 MPa and 0.7 GPa to compare the translational diffusion of free water and bound water in the salt solutions and the effects of salt and pressure on the diffusion of water molecules.

The QENS experiments were performed using a time-of-flight near-backscattering spectrometer DNA at BL02, J-PARC MLF. The energy resolution was 20 μeV for Si(311), estimated from a width of the QENS profile of vanadium foil. The energy transfer ranged from −0.5 to 1.5 meV. The amplitude of the scattering vector, Q, was in the range of 0.125 to 1.774 $Å^{-1}$. Each sample solution was inserted into a double-cylindrical cell and a hybrid piston cylinder high-pressure cell for measurements at 0.1 MPa and 0.7 GPa, respectively. The double-cylindrical cell was made of aluminum with an outer diameter of an inner cylinder 12 mm, and an inner diameter of an outer cylinder 14 mm, and a thickness of a sample was 1 mm. The high-pressure cell consists of a fretted cylinder made of the high tensile steel (SNCM439) liner with an inner diameter of 8 mm and the Al alloy (NA700) jacket with an outer diameter 30 mm. Each sample was inserted into a gap between a sample cylinder and a rod 0.4 mm thinner than the inner diameter of the cylinder [3]. The QENS data were analyzed using a model function of a delta function, one or two Lorentzian functions, and a constant background with the QENSFit program. Water molecule's diffusion coefficients (D) were obtained from a linear fitting at half-width half-maximum (HWHM) vs Q2 plot in the *Q*-range below 1.0 $Å^{-1}$ with a OriginPro software.

Figure 1(a) depicts the scheme of an ion coordination shell showing the bound water to an ion in the first coordination shell and free water. Figure 1(b) gives the diffusion coefficients of pure water, bound water (Dbound), and free water (Dfree) for all alkali metal chloride solutions at 0.1 MPa and 0.7 GPa. At 0.1 MPa, the Dfree for Li^+ and Na^+ are smaller than that of pure water, while the Dfree for K^+, Rb^+, and Cs^+ are larger than that of pure water; the Dbound for Li^+ and Na^+ are much smaller than that of pure water, the Dbound for K^+ is almost equal to that of pure water, while those for Rb^+ and Cs^+ are larger than that of pure water. These results generally agree with the structure-making/breaking concept of alkali metal ions [4,5]. When the solutions are compressed to 0.7 GPa, both Dbound and Dfree for all alkali metal ions and pure water are smaller than those at 0.1 MPa. This is attributed to the increase in pressure causing the outer water to collapse onto the first shell [6], resulting in a decrease in the diffusion ability of both bound and free water. We observe a very important phenomenon in the present work, i.e., the Dbound for Rb^+ and Cs^+ becomes smaller than that of pure water at 0.7 GPa, meaning that the water molecules around Rb^+ and Cs^+ become less fluidic than that of pure water, and Rb^+ and Cs^+ have the characteristic of the structure-making ions like Li^+ and Na^+. This result is probably because the tetrahedral-network structure transforms to dense random packing structure, such as simple liquids, at 0.7 GPa, and non-hydrogen bonded water molecules tend to surround Rb^+ and Cs^+ [1,7]. This finding agrees with the formation of extended solvation shells of Rb^+ at 1 GPa found in the previous neutron scattering study[7].

Reference:

[1] T. Yamaguchi, N. Fukuyama, K. Yoshida, et al, J. Phys. Chem. Lett., 2021, 12, 250.
[2] S. Klotz, L. Bove, T. Strässle, et al, Nat. Comm., 2009, 8, 405.
[3] T. Hattori, S. Ohira-Kawamura, T. Kawasaki, High Press. Res. 2022, 42, 226.
[4] Y. Marcus, J. Solution Chem., 1994, 23, 831.
[5] Y. Marcus, Chem. Rev., 2009, 109, 1346.
[6] S. Lenton, N. Rhys, J. Towey, et al, Nat. Comm., 2017, 8, 919.
[7] W. Zhang, T. Yamaguchi, C. Fang, et al. J. Mol. Liq., 2022, 348, 118080.

Abstract ID: 148 **M2**

Structure of Ethaline by X-ray and Neutron Scattering with Isotopic Substitution

Presenter: Keke chai (Qinghai Institute of Salt Lakes, Chinese Academy of Sciences)

Keywords: X-Ray/Neutron scattering, DFT calculations, Ethaline structure

Ethaline (choline chloride (ChCl) / ethylene glycol (EG) with a molar ratio of 1:2) is a deep eutectic solvent (DES) that has broad applications in electrochemistry, biomass conversion, and CO_2 capture. The local structure of ethaline is highly needed for understanding its stability, functions, and the underlying mechanisms in various applications. In the present study, we perform X-ray and neutron scattering experiments on isotopically substituted ethaline. The scattering data are analyzed by empirical potential structure refinement modeling to reveal the 3D structure of ethaline. Molecular dynamics simulations and density functional theory calculations will also be performed. These methods have been proved to be successful in elucidating the local structure of some DESs systems [1,2].

The X-ray scattering data for ethaline were collected on BL04B2 at SPring-8. The X-ray wavelength was 0.20095 Å. A sample solution was sealed in a glass capillary with a diameter 2 mm. Isotopically substituted ethaline (ChCl-d9: $C_5H_5D_9ClNO$/EG-d6) was measured on a total scattering spectrometer NOVA at J-PARC MLF. A sample was sealed in a vanadium flat cell of a sample thickness 2 mm. The neutron scattering data were seriously affected by the inelastic scattering effect due to the hydrogen atom. We made the inelastic scattering corrections using two different methods [3,4] and discussed both results. Figure 1 shows the structure functions F(Q)s and the corresponding radial distribution functions G(r)s of ethaline finally obtained by X-ray and neutron scattering experiments.

Abstract ID: 168 **M2**

KWS-X: A Powerful SAXS/WAXS Facility at JCNS-MLZ

Presenter: Baohu Wu (Forschungszentrum Juelich, Juelich Centre for Neutron Science (JCNS))

Keywords: KWS-X, SAXS, WAXS, USAXS, SANS

The new customized SAXS/WAXS instrument from XENOCS was installed in the JCNS X-ray laboratory at the end of 2021. As a young member of our small-angle scattering instrument, which utilizes X-rays as the primary beam, the new instrument is equipped with a high-flux Metal-Jet source and a movable Eiger 2R 4M SAXS detector. Additionally, it features a 4-axis motorized WAXS detector and a Bonse-Hart USAXS, allowing for a wide range of scattering vector q, covering values from 0.0002 to 7 $Å^{-1}$. This corresponds to the ability to investigate structures ranging from a few Angstroms to micrometers. In comparison to other instruments, it also incorporates a spacious sample environment station that can operate under ambient pressure conditions. This versatile sample position can accommodate various sample environment platforms, such as Rheometers, electromagnets, stopped-flow devices, and FT-IR spectrometers, commonly used in SANS experiments. The multitude of sample environmental accessories allows for experiments to be conducted at temperatures ranging from -150 °C to 1000 °C, under various conditions, including shear, tensile, and SEC-SAXS, among others. The instrument's design and the extensive selection of sample environments make it a powerful research tool for investigating nanostructures, including their size and shape, nanoparticle formation mechanisms, and particle-particle interactions in solution.

This instrument will greatly assist users of our neutron scattering instruments, such as SANS and reflectometers, in obtaining valuable complementary X-ray structural information. It will also streamline the process of selecting samples appropriate for neutron equipment, thereby enhancing the efficiency of our neutron scattering instruments, particularly SANS.

Abstract ID: 179 **M2**

Zero Thermal Expansion in $NdBaCo_2O_{5.5+x}$

Presenter: Dong Zhang (IHEP)

Keywords: cobaltite perovskites, neutron power diffraction, magnetovolume effect, zero thermal expansion

Most materials expand with increasing temperatures. However, some materials exhibit anomalous thermal expansion (ATE), including zero thermal expansion (ZTE) and negative thermal expansion (NTE). ZTE materials which are invariable in their dimensions over a certain temperature range are widely concerned because of their potential applications in precision devices, optics, and electronics. They have been found in some magnetic functional materials due to the magnetovolume effect (MVE), which is intimately associated with spontaneous magnetic ordering. In this study, we synthesize a novel MVE material, $NdBaCo_2O_{5.5+x}$, which exhibits nearly ZTE at temperatures between 15 and 170 K. With the help of high-resolution neutron powder diffraction (NPD), the underling mechanism of MVE in $NdBaCo_2O_{5.5+x}$ is attributed to an isostructural phase transition from a large-volume (LV) phase to a small-volume (SV) phase upon heating. The magnetic ground state of the LV phase is antiferromagnetic with a G-type magnetic structure determined by NPD, while that of the SV phase is ferromagnetic based on the magnetization properties. This discovery further enhances the understanding of the anomalous thermal expansion in cobaltite perovskites

Abstract ID: 207 **M2**

Neutron diffraction texture analysis in studies of elastic anisotropy of rocks

Presenter: Roman Vasin (Joint Institute for Nuclear Research)

Keywords: Neutron diffraction, crystallographic texture, elastic anisotropy

It is well established that large regions of the Earth's crust and upper mantle are anisotropic with respect to the propagation of seismic waves. Consideration of the seismic anisotropy is therefore important for thorough understanding the internal structure and evolution of the lithosphere, and has possible implications for structural geology, rock mechanics, earthquake physics, geophysical prospecting, etc. In laboratory, the structural origin of the rock anisotropy is often assessed by measuring elastic P- and S-wave velocities in multiple directions and comparing measurements with microstructure-based modeling of rock elastic properties [1].

In this contribution, the application of time-of-flight neutron diffraction at the specialized SKAT texture diffractometer in FLNP JINR (Dubna) [2] for studies of mineral compositions and crystallographic preferred orientations of minerals are reviewed. Studied rocks include Westerly granite [3], which is often described as an intrinsically elastically isotropic, or very weakly anisotropic rock, and gneisses from different Alpine nappes, where significant elastic anisotropy is observed at ambient conditions [4, 5].

Data, provided by neutron diffraction experiments, are combined with information on crack and pore systems quantified using optical and electron microscopy, X-ray and neutron tomography, to model anisotropic elastic properties of rocks using the modified self-consistent Geo-Mix-Self algorithm, which considers preferred orientations of non-spherical grains, pores and cracks [6]. Modelling results are compared to ultrasonic wave velocities measured in rock samples at increased confining pressures to highlight the influence of crack and pore closure with pressure on elastic properties of rocks. Based on obtained microstructural information, an attempt was made to create an effective large-scale rock massif model with anisotropic elastic properties varying with overburden depth, which may be further compared with seismic data.

References:

[1] Petružálek, M., Lokajíček, T., Přikryl, R., Vavryčuk, V. (2023). Journal of Geodynamics, 158, 102002. https://doi.org/10.1016/j.jog.2023.102002
[2] Keppler, R., Ullemeyer, K., Behrmann, J.H., Stipp, M. (2014). Journal of Applied Crystallography, 47, 1520-1534. https://doi.org/10.1107/S1600576714015830
[3] Lokajíček T., Vasin R., Svitek T., Petružálek M., Kotrlý M., Turková I., Onysko R., Wenk H.R. (2021). Journal of Geophysical Research Solid Earth, 126, e2020JB020878. https://doi.org/10.1029/2020JB020878
[4] Vasin, R.N., Kern, H., Lokajicek, T., Svitek, T., Lehmann, E., Mannes, D.C., Chaouche, M., Wenk, H.R. (2017). Geophysical Journal International, 209(1), 1-20. https://doi.org/10.1093/gji/ggw487
[5] Keppler, R., Vasin, R., Stripp, M., Lokajíček, T., Petružálek, M., Froitzheim, N. (2021). Solid Earth, 2303-2326. https://doi.org/10.5194/se-12-2303-2021
[6] Matthies, S. (2012). Journal of Applied Crystallography, 45, 1-16. https://doi.org/10.1107/S002188981104338X

Abstract ID: 216 **M2**

Polarized neutron reflectometry study on the modulation of resistance and magnetism in resistive switching cobalt ferrite thin films

Presenter: Sheng Cheng (CSNS)

Keywords: Polarized neutron reflectometry, Resistive switching, Oxygen vacancies

In this work, the resistive switching and electrical-control of magnetization in Pt/$CoFe_2O_4$/Nb:$SrTiO_3$ heterostructures have been investigated. The films exhibit classic bipolar resistive switching effect with a maximum switch ratio of about 5×10^3 and good anti-fatigue performance. Associated with resistive switching, the saturated magnetization of the thin film at high resistance state is found to be larger than that at low resistance state. Meanwhile, polarized neutron reflectivity of the thin film under different resistance state were *in-situ* measured. The results reveal that the interfacial migration of oxygen vacancies driven by applied electric field play an important role in the modulation of resistive and magnetism of $CoFe_2O_4$ resistive switching devices.

The 4th Asia-Oceania Conference on Neutron Scattering

Scientific Poster Session M3. Soft Matter and Life Science

Abstract ID: 13 **M3**

A SANS study on the complex structure of CdSe QDs–block copolymers with emission energy manipulation

Presenter: Jong Dae Jang (Korea Atomic Energy Research Institute)

Keywords: Quantum dots, Self-assembly, Stokes shift, Polymer phase behavior, Small angle neutron scattering

The optical property control technology is issued in the recent study to apply the tracking and sensing material for the biology, and a catalyst for the various applications using the multicomponent as the quantum dot (QD)–polymer complex. In recent, the polymeric materials are used a capping material of the QD nanoparticles, and can control the optical properties of QDs with energy level changes. The CdSe QD nanoparticle is the typical research material that can easily extend the optical property. We report the successful application of a QDs–polymer structure type energy transfer that depends on the phase behaviors of the QDs–polymer complex. To the best of our knowledge, this study provides the first demonstration of the optical property control of QDs using by the change of the polymer form factor with the dimensional organization of the QDs–polymer complex.

Abstract ID: 69 **M3**

KWS-3 very small-angle neutron scattering focusing diffractometer at MLZ

Presenter: Baohu Wu (Forschungszentrum Juelich, Juelich Centre for Neutron Science (JCNS))

Keywords: KWS-3, VSANS

KWS-3 is a very small angle neutron scattering diffractometer operated by JCNS at Heinz Maier-Leibnitz Zentrum (MLZ) in Garching, Germany. The principle of this instrument is one-to-one imaging of an entrance aperture onto a 2D position sensitive detector by neutron reflection from a double-focusing toroidal mirror. In current state, KWS-3 is covering Q-range between $3 \cdot 10^{-5}$ and $2 \cdot 10^{-2}$ $Å^{-1}$ and used for the analysis of structures between 30 nm and 20 µm for numerous materials from physics, chemistry, materials science and life science, such as alloys, diluted chemical solutions, hydrogels and membrane systems. Within the last few years we have finalized several big “evolutionary” projects; we have completely re-designed and commissioned the main components of the instrument: selector area, mirror positioning system, main sample station at 10m, beam-stop system; implemented new sample stations at 3.5 and 1.3 m, second (very-high resolution) detector, polarization and polarization analysis systems; adapted the instrument to almost any existing/requested sample environment like 6-position Peltier furnace (-25 °C to 140 °C), high-temperature furnace (< 1600 °C), cryostats/inserts (>20 mK), liquid pressure cell (<5 kBar/10-80 °C), CO2/CD4 gas pressure cell (<0.5 kBar/10-80 °C), humidity cell/generator (5-95%/10-90 °C), magnets (horizontal < 3 T, vertical < 2.2 T), Bio-logic® multimixer stopped flow (5-80 °C), rheometer Anton paar (tangential/radial) etc.

Abstract ID: 117 **M3**

Direct observation of mutual coupling effect in protein-water-glycerol mixture by combining neutron scattering and selective deuteration

Presenter: Yongfeng Ye (Shanghai Jiaotong University)

Keywords: elastic incoherent neutron scattering, selective deuteration, mutual coupling effect, hydrogen bond relaxation, energy barrier

Adding cosolvents in aqueous protein solution can remarkably change the stability and activity of proteins. In particular, the formulation of effective cosolvents, such as glycerol and trehalose, holds paramount importance in preserving proteins, tissues, and organs at low temperatures. Extensive studies have been conducted on the impact of cosolvents on the structure, dynamics, stability, and function of proteins. However, the dynamics of cosolvents in the ternary system is largely unexplored in experiment due to technical difficulty. Specifically, it is quite difficult to experimentally distinguish the dynamics of water and cosolvents in a ternary mixture. Consequently, the interplay between protein, water, and cosolvents is still not fully understood, and a comprehensive interpretation of protein stabilization or denaturation by cosolvents has so far remained elusive.

Here, by combining selective deuteration and neutron scattering techniques, we have characterized the individual motions of each component in the protein-water-glycerol system at varying temperatures. Our results demonstrated that all components exhibited the similar dynamical onset temperature at a fixed time resolution, highlighting the mutual coupling effect between protein, water, and glycerol in the ternary system. Furthermore, we probed the dynamical behavior of the ternary system at different timescales using neutron instruments with different energy resolutions. Interestingly, we observed a shift in the dynamical onset temperature from ~205 K to ~235 K when reducing the time resolution from ~1 ns to ~60 ps, implying an energy barrier of ~43 kJ/mol for system activation. For comparison, the corresponding energy barrier in the binary system of CYP and water was ~35 kJ/mol. Complementary molecular dynamics (MD) simulations corroborated these experimental findings, and revealed that the energy barrier of ~43 kJ/mol in the ternary system could be attributed to the switching of hydrogen bonds between protein, water, and glycerol. Notably, the energy barriers for water-water and protein-water hydrogen bond relaxations in the ternary system were higher than those in the protein-water system. Based on these observations, we propose that the addition of glycerol to aqueous protein solutions can enhance hydrogen bond interactions in the ternary system through the mutual coupling effect, representing one of the protective mechanisms of protein preservation by glycerol.

Our work is unique from previous work as we applied selective deuteration and neutron scattering techniques to characterize a more complicated ternary system rather than a binary system. Meanwhile, the dynamics of all components were independently observed by designing three distinct deuterated samples. The coupling effect in this ternary system is then evidenced by both neutron scattering experiments and MD simulations. Furthermore, the MD-derived hydrogen bond analysis elucidates that glycerol not only suppress the dynamics of protein and water but also raise the relaxation energy barrier, which enriches our understanding of how cosolvents stabilize biomacromolecules.

Abstract ID: 164 **M3**

Structure and dynamics of supercooled water in the hydration layer of poly(ethylene glycol)

Presenter: Yuqing Li (IHEP)

Keywords: quasi-elastic neutron scattering, polymer, molecular simulations, hydration water

The statics and dynamics of supercooled water in the hydration layer of poly(ethylene glycol) (PEG) were studied by a combination of quasi-elastic neutron scattering (QENS) and molecular dynamics (MD) simulations. Two samples, that is, hydrogenated PEG/deuterated water (h-PEG/D_2O) and fully deuterated PEG/hydrogenated water (d-PEG/H_2O) with the same molar ratio of ethylene glycol (EG) monomer to water, 1:1, are compared. The QENS data of h-PEG/D_2O show the dynamics of PEG, and that of d-PEG/H_2O reveals the motion of water. Then temperature-dependent elastic scattering intensity of both samples has shown transitions at supercooled temperature, and these transition temperatures depend on the energy resolution of the instruments. Therefore, neither one is a phase transition, but undergoes dynamic process. The dynamic of water can be described as an Arrhenius to super-Arrhenius transition, and it reveals the hydrogen bonding network relaxation of hydration water around PEG at supercooled temperature. Since the PEG-water hydrogen bond structural relaxation time from MD is in good agreement with the average relaxation time from QENS (d-PEG/H_2O), MD may further reveal the atomic pictures of the supercooled hydration water. It shows that hydration water molecules form a series of pools around the hydrophilic oxygen atom of PEG. At supercooled temperature, they have a more bond ordered structure than bulk water, proceed a trapping sites diffusion on the PEG surface, and facilitate the structural relaxation of PEG backbone.

Abstract ID: 186 **M3**

The multilevel structure of block copolymer self-assembly is studied using SANS

Presenter: Jun Wang (IHEP)

Keywords: SANS, self-assembly, block copolymer, polypeptiod

Solution self-assembly of coil-crystalline diblock copolypeptoids has attracted increasing attention due to its capability to form hierarchical nanostructures with tailorable morphologies and functionalities. While the N-substituent (or side chain) structures are known to affect the crystallization of polypeptoids, their roles in dictating the hierarchical solution self-assembly of diblock copolypeptoids are not fully understood. Herein, we designed and synthesized two types of diblock copolypeptoids, i.e., poly(N-methylglycine)-b-poly(N-octylglycine) (PNMG-b-PNOG) and poly-(N-methylglycine)-b-poly(N-2-ethyl-1-hexylglycine) (PNMG-bPNEHG), to investigate the influence of N-substituent structure on the crystalline packing and hierarchical self-assembly of diblock copolypeptoids in methanol. With a linear aliphatic N-substituent, the PNOG blocks pack into a highly ordered crystalline structure with a board-like molecular geometry, resulting in the self-assembly of PNMG-b-PNOG molecules into a hierarchical microflower morphology composed of radially arranged nanoribbon subunits. By contrast, the PNEHG blocks bearing bulky branched aliphatic N-substituents are rod-like and prefer to stack into a columnar hexagonal liquid crystalline mesophase, which drives PNMG-b-PNEHG molecules to self-assemble into symmetrical hexagonal nanosheets in solution. A combination of time-dependent small/ wide-angle X-ray scattering and microscopic imaging analysis further revealed the self-assembly mechanisms for the formation of these microflowers and hexagonal nanosheets. These results highlight the significant impact of the N-substituent architecture (i.e., linear versus branched) on the supramolecular self-assembly of diblock copolypeptoids in solution, which can serve as an effective strategy to tune the geometry and hierarchical structure of polypeptoid-based nanomaterials.

Abstract ID: 201 **M3**

Application of Neutron Spectroscopy and Imaging to Reveal Drying Behaviour and Preservation of Australian Native Fruits

Presenter: Paul Michalski (Monash University)

Keywords: Food, Australian Native Food, Food Engineering, Neutron Imaging, Neutron Scattering, Process Engineering, Food Preservation, Food Moisture

Food production is being challenged by population growth and increased drought. One way to manage these challenges is with Australian native food crops, which have unique sensory and nutritional properties, while being inherently well-adapted to Australian climate and in which there is emerging a local industry and global interest [1, 2]. A barrier to the industry's growth, however, is understanding how to maximise the retention of quality attributes over the course of preservative processes. This is particularly true for those processes which manipulate food moisture, prompting the need to also understand the behaviour of water in these fruits as they are processed. Measuring the drying kinetics and water sorption isotherms and how these change with processing and temperature has revealed bound water physics in these fruits different to what has been observed for commonly known foods. The extent to which hydrogen (and thus water) scatters neutrons makes them ideal to study moisture in food. By subjecting Australian native fruits, processed in different ways, to neutron backscattering spectroscopy by using Emu in ANSTO, the dynamics of bound water in these unique foods has been characterised. The use of neutron tomography with Dingo in ANSTO has also revealed the local moisture transport and structural changes in these fruits as they are processed under different conditions. The combination of these techniques has given more rigorous insight into the water transport mechanisms in Australian native fruits and allowed for improved understanding of how their preservation can be optimised for longer shelf-life and nutritional/quality retention.

References:

[1] Orians, G.H. and A.V. Milewski, Ecology of Australia: the effects of nutrient-poor soils and intense fires. (1464-7931 (Print)).

[2] S. Laurie, "Australian native foods and botanicals - 2019/20 market study," ANFAB, 2020.

The 4th Asia-Oceania Conference on Neutron Scattering

Scientific Poster Session M4. Engineering and Industrial Applications

Abstract ID: 14 **M4**

Recent results of department for neutron radiation detector development of National research center "Kurchatov Institute" - Petersburg Nuclear Physics Institute named by B.P. Konstantinov

Presenter: Sophia Mokhova (National research center "Kurchatov institute" - Petersburg Nuclear Physics Institute)

Keywords: multiwire proportional thermal neutron chambers, linear position-sensitive neutron detector, the prototype for a 32-channel counter

The department for neutron radiation detectors is directly involved in the design of various detector systems and appropriate electronic software. The latest developments of the department are:

- creation the data acquisition system for the position-sensitive neutron detector;
- development of linear position-sensitive neutron detector;
- development of multiwire proportional thermal neutron chambers with different types of sensitive area and spatial resolution;
- creation the prototype for a 32-channel counter with a network interface for time-of-flight measurements.

The data acquisition system for the position-sensitive proportional neutron detector has a two-dimensional readout and a four-channel time to digital converter (TDC). As a result of the 3He(n, p)T reaction, the signals from the delay line connected to the strips of cathodes X and Y appear. These signals translate to the preamplifiers, which provide the logical pulses with a time reference. The software visualizes data by plotting X and Y coordinates.

The development of linear position-sensitive neutron detector performed within the creation a new thermal neutron powder multi-detector diffractometer for researches at the field of condensed matter under high pressures. An assembly of 126 (6x21 detection units) linear position-sensitive helium detectors is proposed on the basis of the charge-division method of coordinate registration and the detectors are produced.

The development of multiwire proportional thermal neutron chambers (MWPC) is designed to detect scattered neutron radiation with high resolution. The method of channel-by-channel signal acquisition is used to determine coordinates with highest count rate. This simultaneously provides both, required spatial resolution and reduction of the electronics dead time.

The creation of the prototype for a 32-channel proportional counter with a network

interface for time-of-flight measurements is an embedded system. This system unites field programmable gate array (FPGA) and an ARM processor on a single chip. The developed prototype consists of independent parts. The functionality of each part could be changed in order to adopt the device without the necessity of the entire system development. Application software for Windows and GNU / Linux systems, which is used to manage counters, acts as a client, communicates with a server on a single-board computer and receives data from counters.

Water/ice identification in a model PEFC using energy-selective high-resolution neutron imaging

Presenter: Fangzhou Song (Japan Atomic Energy Agency)

Keywords: High-resolution neutron imaging, Energy-selected pulsed neutron imaging, Time-of-flight analysis, Water/ice differentiation

Polymer electrolyte fuel cell (PEFC) is a promising green energy system that has the potential in realizing carbon neutrality for our society. One of the greatest challenges faced by the PEFCs for automobiles is the freezing of water under sub-zero environments, which will block gas channels and thereby lead to cell failure and damage to the cell component. Therefore, it is crucial to understand the freezing and thawing behavior of ice in PEFCs, especially along the cross-sectional direction, such that effective measures can be taken to enhance cold start-up performance of PEFCs. Neutron radiography is a powerful non-destructive method in visualizing the water distribution within PEFCs due to the large neutron cross section of the hydrogen atom in comparison to other high-Z atoms. Beyond water distribution observation, researches have also demonstrated the viability of identifying ice from water by utilizing different neutron total cross sections between ice and liquid water dependent on the neutron wavelengths, which is hereby referred to as water/ice identification [1]. Our past works have conducted water/ice identification in aluminum channels at actual fuel cell scale by means of the energy-selective neutron imaging where the Time of Flight of the pulsed neutron beam was selected [2]. In this work, we have applied the same methodology to visualize the freezing and thawing of water in different cavity layers of a fuel cell by taking cross-sectional neutron transmission images, as a preliminary experiment for further *operando* water/ice identification observations on PEFCs along the cross-section of the PEFC.

A miniature size of a fuel cell, which consisted of gas diffusion layers (GDLs) and aluminum frames with gas channels produced by 3D printing technique, was prepared as a model cell sample. This model fuel cell was filled with water and cooled by a Peltier cooler down to -10 ℃. Consecutive high-resolution energy-selective neutron imaging was conducted throughout the freezing process at the RADEN instrument in J-PARC MLF. By taking the ratio of logarithms of neutron transmission between long and short wavelength neutrons, we defined a ‘water/ice identification parameter’ to confirm freezing of water within the cell. This parameter was spatially resolved on the neutron transmission images to map the water/ice distribution in each layer of the model fuel cell as it was cooled to sub-zero temperatures.

In the presentation, we will discuss the spatial and temporal resolution capacities of the high-resolution energy-selective neutron imaging at the RADEN instrument, and show results of the water/ice identification experiments on the cross-sectional observation of the PEFC.

Reference:

[1] Y. Higuchi, et al., *Phys. Chem. Chem. Phys*. **23**, 1062 (2021).
[2] K. Isegawa, et al., *Nucl. Instrum. Meth. Phys. Res. A*, **1040**, 167260 (2022).

Abstract ID: 34 **M4**

Competitive behavior between TWIP and TRIP in 17Mn-0.5C steel under cyclic loads

Presenter: Hobyung Chae (Korea Atomic Energy Research Institute)

Keywords: Mn steel, TWIP, TRIP, Neutron diffraction, Cyclic load

Due to the growth and expansion of companies operating in difficult settings like offshore, wind turbines, and seismic areas, the behavior of structural materials when subjected to repetitive stresses has gained major importance. Due to its deformation properties, high Mn steel has emerged as one of these materials that holds promise for scenarios requiring cyclic deformation. It is crucial to first understand how high Mn steel reacts and the underlying mechanisms that operate when subjected to cyclic stresses in order to properly regulate its fatigue performance. The behavior of austenite-stabilized 17Mn-0.5C steel under cyclic deformation at both +1 percent and -1 percent strain levels was examined in this study using *in-situ* neutron diffraction. The study will examine how cycle count and loading direction affect stacking faults, twinning, and transformation behaviors.

Abstract ID: 62 **M4**

Pulsed neutron diffractometer for engineering materials studies in J-PARC

Presenter: Stefanus Harjo (Japan Atomic Energy Agency)

Keywords: Diffractometer, Materials engineering, Sample environments

Neutrons are used to investigate stresses and crystallographic microstructures inside engineering materials, taking advantage of their large penetrating power and the ability to see the arrangement of atoms by diffraction methods. Pulsed neutron diffraction with the time-of-flight method is suitable for microscopic structural observation as a bulk average behavior because of the simultaneous measurement of multiple Bragg peaks. Careful analysis of the Bragg peaks in a neutron diffraction pattern can reveal important structural details of a sample material such as internal stresses, phase conditions, dislocations, texture etc. Such information is often crucial in engineering applications and the ability to carry out either *ex-situ* or *in-situ* measurements makes neutron diffraction particularly useful in this respect. The large penetrating power of neutrons also allows *in-situ* investigation of crystallographic information on engineering materials under various environments, including *operando* monitoring during deformation at a wide temperature range from cryogenic to high temperatures, thermo-mechanical processes, and so on. A pulsed neutron diffractometer has been developed in J-PARC and operated for more a decade. The present status of the diffractometer and some highlights will be introduced.

Abstract ID: 95 **M4**

Design of high-precision four-blade slit device under strong magnetic environment

Presenter: Jiajie Li (IHEP)

Keywords: beam size control, four-blade slits, piezoelectric motor, Macro-micro dual-driven

The four-blade slit device is one of the key devices to change the beam size, which is widely used for beam spot size control in the Spallation Neutron Source. Due to the magnetic leakage phenomenon in the strong magnetic sample environment, the motion accuracy of the four-blade slit device will be affected and then it will not be able to meet the normal operation requirements. Therefore, it is necessary to develop a high-precision four-blade slit device under strong magnetic conditions.

In this paper, we analyze the design of the four-blade slit system of the high-energy inelastic scattering spectrometer in the spallation neutron source, and explore the general design method of the high-precision four-blade slit drive device under the strong magnetic environment.

Firstly, the Macro-micro dual-driven method is proposed by utilizing the feature of piezoelectric motor that is not subject to electromagnetic interference. Then, the main components of the drive system are analyzed and selected, and the strength of the key components is verified by finite element analysis. Finally, according to the control requirements of the four-blade slit, the design of the control software of the drive mechanism is completed. The analysis results show that the design is able to realize the driving of the four-blade slit under high irradiation conditions and provides a reference for the design of the four-blade slit device in the synchrotron radiation light source.

Abstract ID: 99 **M4**

Analysis of *in-situ* neutron diffraction data for laminate LIB by iMATERIA

Presenter: Toru Ishigaki (CROSS, NIAPC)

Keywords: LIB, *in-situ* neutron diffraction, Rietveld Analysis

iMATERIA at J-PARC MLF is a general-purpose neutron diffractometer for industrial use. This time, we carried out charging/discharging *in-situ* neutron diffraction measurements using a stacked LIB. We report the results of continuous analysis of time-division data using the multi-point, multi-phase automatic continuous analysis function of the Rietveld analysis program Z-Rietveld.

Abstract ID: 121 **M4**

In Situ Characterization of 17-4PH Stainless Steel by Small-Angle Neutron Scattering

Presenter: Shibo Yan (China Institute of Atomic Energy)

Keywords: 17-4PH; martensitic stainless steel; *in-situ* SANS; precipitation

17-4PH martensitic steel is usually used as valve stems in nuclear power plants and it suffers from thermal aging embrittlement due to long-time service in a high-temperature and high-pressure environment. Here, we characterized the evolution of microstructures at the nano-scale in 17-4PH steel by *in-situ* small-angle neutron scattering (SANS) with a thermo-mechanically coupled loading device. The device could set different temperatures and tensile so that an *in-situ* SANS experiment could dynamically characterize the process of nanoscale structural changes. The results showed that with increasing thermal aging time, the ε-Cu phase precipitates and grows as the temperature is 475 °C and 590 °C, and the ε-Cu phase is spherical at 475 °C but became elongated cylinders at 590 °C. Moreover, the loading stress could aid in the growth of the ε-Cu phase at 475 °C.

The 4th Asia-Oceania Conference on Neutron Scattering

Scientific Poster Session M5. Fundamental Physics, Sources, Methods and Techniques

Abstract ID: 28 **M5**

The VSANS instrument in CSNS – current situation and future development

Presenter: Zehua Han (Institute of High Energy Physics, CAS)

Keywords: Very-Small Angle Neutron Scattering, Small Angle Neutron Scattering, SANS instrument, data reduction

The Very-Small Angle Neutron Scattering (VSANS) instrument successfully completed its acceptance in July 2023. After nearly seven months of tuning and adjustments, we are proud to announce that we have achieved our objective.

The VSANS instrument is a 35 m long instrument with both SANS mode and VSANS mode. Its design is optimized for structural studies of materials with large length scales up to 1 μm, while retaining reasonable structural information down to about 5 Å. This capability is achieved through three main detector banks covering a wide range of scattering angles, along with the VSANS mode which enables reaching smaller minimum scattering vectors.

In the SANS mode, we offer four collimation lengths, 2.49 m, 5.15 m, 9.92 m, and 12.75 m, allowing users to select the most suitable option based on their needs. With a scattering angle range from 0.15 to 30 degrees and available wavelength range from 2.5 to 11 Å, the SANS mode can cover a q range from 0.0018 to 2 $Å^{-1}$. Moreover, the highest flux provided can reach 2.3×10^7 $n/s/cm^2$, making it a world-class instrument. As for the VSANS mode, it can further extend the minimum q to 0.00028 $Å^{-1}$.

We have successfully calibrated the SANS mode with the 12.75 m collimation length using standard samples such as Polystyrene sphere solution with different radii, silver behenate, and silicon. The scattering curves obtained from different detector banks and wavelengths overlap excellently, and the experimental results match well with the theoretical ones. Regarding the VSANS mode, although we haven't achieved a perfect match between the experimental data and theoretical results, we have managed to obtain reasonably scaled results of PS sphere solutions with diameters of 200 nm, 500 nm, and 1000 nm after smearing.

Our future work will primarily focus on the further calibration. For the SANS mode, we need to verify if the current calibration method is applicable to other collimation lengths. In the case of the VSANS mode, we aim to find a better way to perform calibration and evaluate the smear function to ensure better agreement between experimental and theoretical results.

Additionally, the VSANS instrument offers various sample environments, including temperature control, magnetic field, rheology, stop-flow, SAXS and so on. I will provide a brief introduction to these sample environments during this oral presentation/poster.

We have already served several users and obtained promising results actually. Through this presentation/poster, we hope to familiarize colleagues and potential users in the field of SANS with our advanced instrument, gathering valuable suggestions, and attracting more users to utilize our facility.

Abstract ID: 53 **M5**

Surface and Interface Science at the ACNS

Presenter: Stephen Holt (Australian Nuclear Science and Technology Organisation)

Keywords: Neutron Reflectometry, Surface, Interfacial Structure

The suite of instrumentation suitable for studying surfaces and interfaces at the Australian Centre for Neutron Scattering is centered around the two neutron reflectometers, Platypus and Spatz. Supporting the neutron scattering program, in addition to general laboratory facilities are a Rigaku SmartLab x-ray reflectometer, a spectroscopic imaging ellipsometer and a Quartz Crystal Microbalance with Dissipation. These supporting instruments are all available to the user community in association with an approved neutron scattering proposal.

PLATYPUS is the initial neutron reflectometer at the Australian Centre for Neutron Scattering with a capability to study surfaces and interface systems with applications from biomolecules, soft matter through to magnetic thin films [1-3]. There have been a number of significant improvements to both the instrument and data reduction and treatment software [4] over the last two years. On the hardware front the original detector has been replaced [5] enabling higher count rate capabilities, greater detection efficiency at shorter wavelengths and significantly lower background. The slits which define the neutron beam have been replaced with upgraded positioning mechanisms enabling greater flexibility in experimental setup. Most recently new slit blades have been installed resulting in a substantial reduction in instrument background. These changes have significantly enhanced the instrument performance with improved reproducibility.

References:

[1] M. James et al., J. Neutron Research 14, 91 - 108 (2006)

[2] M. James et al., Nuclear Inst. and Methods in Physics Research A, 632, 112 - 123 (2011)

[3] T. Saerbeck et al., Rev. Sci. Instrum. 83, 081301 (2012)

[4] A. Nelson et al., J. Appl. Crystallography, 52, 193 - 200 (2019)

[5] L. Abuel et al., Journal of Neutron Research, 23(1), 53 – 67, (2021).

Abstract ID: 54

M5

The status of neutron imaging instruments at HANARO

Presenter: Jongyul Kim (Korea Atomic Energy Research Institute)

Keywords: neutron imaging instrument

There are two neutron imaging instruments at HANARO, Neutron Radiography Facility (NRF), and Ex-core Neutron irradiation Facility (ENF). Various neutron imaging experiments have been performed using these instruments. Since the NRF has a large beam size(350 × 450 mm) and low neutron flux(2×10^6 n/cm^{2}sec), it is suitable for non-destructive testing of large industrial samples. Especially, a hydrogen fuel cell test station was installed in the NRF and has been mainly conducting experiments with Hyundai Motor's research team to improve the performance by visualizing the water distribution inside the hydrogen fuel cell. However, because the ENF has higher neutron flux than the NRF, we have been measuring relatively small samples with high spatial resolution. The pores and its distributions inside the 3D metal printed sample were confirmed, and the corrosion layer of the metal artifact was visualized. In order to improve the performance of neutron imaging at HANARO, a scientific CMOS camera with 62 Mega pixels (9576 × 6388) and neutron scintillators were prepared. New camera and neutron scintillators are planned to be applied soon and will be tested.

Abstract ID: 94

M5

Electron Dynamics in Neutron Scattering with Hydrogen Atom

Presenter: Mingzhao Xing (Graduate School of China Academy of Engineering Physics)

Keywords: neutron scattering, three-body system, TDSE, momentum spectrum, ionized electron

By measuring the neutron scattering cross-section in neutron-proton (n-p) scattering experiments, numerous models of n-p interactions have been developed. However, the change in the electronic state is not considered during the scattering process. In this study, we introduce a novel theoretical approach to obtain parameters of nuclear interactions from the momentum spectrum of ionized electrons. Modeling the Yukawa potential as the nuclear interaction, the approach based on a three-body system involves the neutron scattering with the hydrogen atom. By employing a semi-classical methodology and solving the Time-Dependent Schrodinger Equation (TDSE), we explore the momentum spectrum of ionized electrons. The electron dynamics processes exhibit significant distinctions at different force ranges. Moreover, this approach offers insights into detecting ultrafast scattering processes.

Abstract ID: 110

M5

Sensitivity Study of NRTA in Spent Fuel Transmutation Detecting

Presenter: Yaoxuan Cui (Institute of Modern Physics, Chinese Academy of Sciences)

Keywords: NRTA, Spent Fuel Transmutation ， Neutron Resonance

The Accelerator Driven Subcritical System (ADS) offers an exceptional solution to the challenge of spent fuel disposal. After transmuting the spent fuel, the content of Minor Actinides (MA) and Long-Lived Fission Products (LLFP) were reduced in the spent fuel. It will significantly decrease the risk of spent fuel to the environment. We must determine the content of MA and LLFP in the spent fuel of transmutation to guarantee that they remain below the safety threshold.

This study will employ Neutron Resonance Transmission Analysis (NRTA) technology, in conjunction with machine learning and Monte Carlo methods, to detect the content of MA and LLFP in spent fuel after transformation, and evaluate the sensitivity of this technology for detecting the content of MA and LLFP.

Abstract ID: 137

M5

REF-V - Cold Neutron Reflectometer at HANARO

Presenter: June Hyuk Lee (Korea Atomic Energy Research Institute)

Keywords: neutron reflectivity, thin film, depth profile, HANARO, reflectometer

Nanoscale surface and interface plays an important role in controlling the chemical and physical properties of materials. Neutron reflectivity is a powerful and nondestructive characterization tool for these nanoscale structures in polymers, biomolecules, metals, and oxides. The low energy (~meV) and high penetration depth (~cm) of neutron enables the structure and composition analysis in sensitive biological membrane and polymer without degradation. In addition, the large difference in neutron scattering length between hydrogen and deuterium allows contrast variation experiments in multi-component samples.

Vertical neutron reflectometer REF-V at HANARO (High-flux Advanced Neutron Application Reactor) facility in Republic of Korea, has been contributing to the research of surface and interface science since 2012. Recent reflectivity studies include the interface structure and its effect on electrical transport in organic semiconductor blends, the vertical structure of Fe-based permanent magnet thin films, ultrathin two-dimensional materials, and more. Reflectometer user can access molecular beam epitaxy system for thin film deposition, X-ray diffractometer, vacuum furnace, and *in-situ* electrochemical/liquid cell. In this presentation, the current status of REF-V instrument and reflectivity research will be discussed.

Abstract ID: 176 **M5**

Reproduction of Neutron Scattering Experiments by Monte Carlo Simulations

Presenter: Ni Yang (University of Chinese Academy of Sciences; Institute of High Energy Physics, Chinese Academy of Sciences; Spallation Neutron Source Science Center, Dong Guan, China)

Keywords: Monte Carlo simulation; Thermal neutron scattering; Open-source software

Simulations of neutron scattering experiments are of importance to optimize instruments and develop data analysis algorithms. In this talk, a new open-source thermal neutron scattering simulation system, the **Pr**obability-c**o**nserved cross section biasing **M**onte Carlo **P**article **T**ransport System (***Prompt***), will be introduced. Supported by its accurate backend scattering physics engine and strong ability in geometric construction, it is capable of simulating the realistic scattering and capturing processes in the sample, detectors and other components of an instrument. Therefore, experiment raw data can be reproduced realistically.

In this talk, we take neutron total scattering experiments of heavy water and light water as examples to demonstrate the performance of ***Prompt***. Simulation procedure and physics models are introduced. We show that the detector responses of simulations have good agreements with the results of experiments.

Abstract ID: 183 **M5**

Mechanical design and construction of the very small angle neutron scattering instrument in CSNS

Presenter: Songwen Xiao (Institute of High Energy Physics, CAS)

Keywords: VSANS; Collimation System; Vacuum Scattering Chamber

It took us four years from January 2019 to January 2023 to complete the mechanical design and construction of the Very Small Angle Neutron Scattering Instrument (VSANS) in China Spallation Neutron Source (CSNS). The acceptance test of VSANS has been completed, and it is the first VSANS instrument based on a spallation neutron source. the collimation system in front of the sample needs to be able to automatically switch four modes (VSANS mode, Traditional SANS mode, Polarized SANS mode, GSANS mode) according to the physical design. three sets of horizontal exchange chambers, five sets of rotary drums, five sets of rotary apertures and two sets of four-blade vacuum slits have been designed and manufactured in the collimation system, the multi-station switching of these device are realized by high-precision horizontal movement, rotation and vertical lifting, and all the devices are connected by front and rear bellows to maintain the overall vacuum environment in the collimation system (the total length is about 13m). A heavy-load sample stage with the capacity of 1 ton and a light-load sample stage with the capacity of 200kg were designed and manufactured for different sample experiments in the sample room. The vacuum scattering chamber with an inner diameter of 2.6 m and a length of 12m is installed after the sample. A sapphire window with the diameter of 380 mm and thickness of 10mm is installed at the front of the scattering chamber, and an aluminum window with the diameter of 400 mm and thickness of 1mm is installed at the end of the scattering chamber. Three 3He detectors which can be moved forward and backward are installed inside the scattering chamber (normally arranged 1m, 4m and 11.5m away from the sample center). The GEM detector for VSANS mode is fixed behind the aluminum window (12.75 m away from the sample). The mechanical structure of VSANS is very complicated with more than 54 axes of high precision motion control in vacuum environment, and we have completed this work well, and the repeated positioning accuracy of all equipment meets the experimental requirements.

Abstract ID: 194

M5

Monte Carlo simulations of TOF SANS instruments at DARIA CANS and IBR-2M reactor

Presenter: Konstantin Pavlov (NRC "KI" - PNPI)

Keywords: compact neutron source, small-angle neutron scattering, Monte Carlo simulations

The work was carried out as part of the development of the instrument set for the compact neutron source Dedicated for Academic Research and Industrial Applications (DARIA), carried out by a large team [1]. DARIA is now being developed as a university-class CANS (Be (p, n), 13MeV, < 100mA) intended for neutron scattering techniques.

The highest priority instruments at the pilot source of the DARIA project include the small-angle neutron scattering (SANS) instrument named as MURENA [2]. The SANS technique, which is in high demand in structural studies, has not yet been implemented in user mode on any of the compact sources in the world, and the fundamental possibility of such implementation is an urgent scientific problem. The purpose of this work is to compare the calculated operating modes of the developed MURENA@DARIA instrument and the existing time-of-flight small-angle instrument YuMO, which has been successfully operating for about 40 years at the IBR-2 pulsed reactor at JINR (Dubna) [3,4].

Complete mathematical models of both instruments have been developed in the McStas software package [5]. For MURENA, the calculated spectrum of the cold moderator of DARIA source and the design parameters of the instrument, described in detail in [2], were used as input data. For YuMO, the spectrum of channel 4 of the IBR-2 reactor and the real parameters of the device were used. The results obtained make it possible to compare the measuring range achievable at the instrument and the average neutron flux density at the sample position, which directly determines the rate of statistics acquisition. It is shown that the expected experimental capabilities of the MURENA are inferior to YuMO both in terms of aperture and range, however, MURENA is capable of acting as a tool for solving a number of problems in a narrower range of transmitted momentum. The difference in capabilities is not as great as the difference in the power of neutron sources such as CANS DARIA and IBR-2. It is also worth noting that McStas and similar functional modeling tools do not provide any ability to calculate the background, and the YuMO model is developed in an idealistic approximation. However, the limit of measurement capabilities due to the background is known from the experience of experimental work at the instrument, and we estimate the background at MURENA@DARIA as being three orders of magnitude lower than that at YuMO at IBR-2.

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References:

[1] K.A. Pavlov, P.I. Konik, N.A. Kovalenko, T.V. Kulevoy, D.A. Serebrennikov, V.V. Subbotina, A.E. Pavlova, S.V. Grigoriev. Crystallography V. 67. No. 1, p. 5-20 (2022).

[2] K.A. Pavlov, N.A. Kovalenko, L.A. Azarova, E.A Kravtsov, T.V. Kulevoy, S.V. Grigoriev. J. Surf. Inv. No. 7. p. 84-92 (2023).

[3] V.A. Vagov, A.B. Kunchenko, Yu. M. Ostanevich, I.M. Salamatin. JINR reports, P.14-83-898, Dubna (1983).

[4] A. Kh. Islamov et al. Crystallography. V. 66. No. 2. P. 230-241 (2021).

[5] P.K. Willendrup, K. Lefmann, Journal of Neutron Research. V. 22. No. 1.P. 1-16 (2020).

Abstract ID: 208 **M5**

Theoretical Investigation of Magnetic Structures in Iron Oxide Nanoparticles Using SANS with ^{3}He Polarization Analysis

Presenter: Yifeng Xiang (Chinese Academy of Engineering Physics)

Keywords: magnetic nanoparticles; small-angle neutron scattering; polarized ^{3}He analyzation

Magnetic nanoparticles have a wide range of applications in areas such as biology, medicine, and pollution control. Understanding the magnetic structure of magnetic nanoparticles is of significant importance for maximizing their applications.

Small-angle neutron scattering techniques are widely used in the study of magnetic nanoparticles. This is because there is often a significant difference in the nuclear and magnetic scattering cross-sections of the samples, making traditional neutron scattering techniques less effective in distinguishing between nuclear and magnetic scattering. However, by employing ^{3}He polarization analysis techniques and introducing nuclear magnetic coupling terms, it is possible to effectively distinguish between the nuclear and magnetic scattering components, thus allowing for a more accurate study of the magnetic behavior of magnetic nanoparticles. ^{3}He polarization analysis leverages the spin properties of neutrons and provides information about the magnetic structure by measuring changes in the neutron spin states during scattering. An experimental method for measuring the nuclear and magnetic scattering cross-sections of magnetic iron oxide particles, as well as a data processing procedure to effectively distinguish between the two, have been designed through simulated experiments, improving accuracy when compared to traditional angle-averaging methods.

Abstract ID: 223 **M5**

Development of a Universal User Service System for Neutron Scattering

Presenter: Jiangshu Hong (IHEP)

Keywords: User Service System, Web System, Neutron Scattering, System Design

In 2018, the China Spallation Neutron Source (CSNS) officially opened its neutron beamline to the public, inviting high-quality proposal applications each year. The User Services System of CSNS, responsible for providing technical support for proposal application and evaluation, was designed and developed in the same year. The system facing to CSNS operational requirements and offers functionalities including proposal application, safety training, news announcements, visit requests, and experiment report feedback. In alignment with the collaborative objectives of the scientific research information system of the Institute of High Energy Physics, Chinese Academy of Sciences, the system integrates the IHEP unified authentication system, experiment system, accommodation system, and card issuing system, streamlining workflows across various departments to enhance management efficiency. Furthermore, with an international outlook, the system achieves internationalization by improving its English portal and offering international user guidance and information retrieval capabilities.

As CSNS-II spectrometer begins pre-research, as well as expanded beamline applications like white neutron sources and accompanying proton beams put into use, the CSNS User Services System is confronted with the need for more extensive and intricate application forms, review processes, and beamline reservation requirements. Additionally, the development of High Energy Photon source and the completion of the Southern Advanced Light Source Pre-Research Platform introduce heightened organizational and management demands for the user service system. The existing system exhibits limitations in scalability, performance bottlenecks, and maintainability issues. In response, we have undertaken a comprehensive redesign and adjusted the system architecture, utilizing the low-code platform 'cordwood,' to develop a versatile user service system for neutron scattering instruments and other facilities.

The new user service system, empowered by cordwood's FormMaking form engine and Flowable 6 process engine, offers flexibility in configuring parameters for various experimental devices and supports diverse user scenarios and interface designs, as well as approval workflows. Additionally, it provides open standard APIs and documentation, self-service registration, and data integration capabilities. Presently, the new user service system is in its final stage of operational testing, with the successful migration and testing of historical data, and it is set to open to the public shortly

Abstract ID: 241 **M5**

Current performance of *in-situ* experimental conditions for CSNS

Presenter: Mengjia (Dou)

Keywords: Sample environment

The sample environment is a crucial auxiliary apparatus for neutron scattering instruments, facilitating the provision of diverse experimental settings to augment the research capabilities of these instruments. The sample environment group of the Chinese Spallation Neutron Source (CSNS) has developed more than 25 sets of *in-situ* experimental services since the instrument's commissioning in 2018. The sample environment group developed a broad range of sample conditions to meet the needs of many users, such as low temperature, high temperature, high pressure, magnetic field, and soft matter. This poster showcases the most current improvements and modifications made to the sample environment. Furthermore, a few test applications created in conjunction with users are also presented.

Abstract ID: 243 **M5**

Sample environment of neutron scattering for *in-situ* catalysis study

Presenter: Chengyang Wang (CSNS)

Keywords: Sample environment; *in-situ* catalysis; neutron scattering

Knowledge and understanding of the fundamentals of catalysis, establishing the relationship between catalyst structure and performance, and explaining the mechanism of action in real catalytic processes are the keys to realizing the development of high-performance catalysts and promoting the green, low-carbon, and sustainable development of the industry. In contrast to X-ray techniques, neutron scattering techniques have a variety of selectivity for the light elements involved in catalytic reactions, such as carbon and hydrogen, as well as for the light species interacting with the catalyst surface. At the same time, the strong penetrability of neutrons makes them very suitable for probing the evolution of key active sites in catalysts under *in-situ* conditions. Here, we have designed three types of sample environment devices (gas-solid reactor, gas-liquid-solid reactor, and ammonia reactors) applied to *in-situ* catalytic studies of neutron scattering. The simulation results show that these devices can realize *in-situ* catalytic reactions with neutron scattering at temperatures ranging from room temperature to 800 °C and pressures ranging from 0.1 MPa to 5 MPa. These sample environment devices provide technical support for the study of catalytic constitutive relationships using neutron scattering techniques.

Abstract ID: 245 **M5**

The scintillator neutron detectors for neutron scattering instruments in CSNS

Presenter: Tang Bin (IHEP)

Keywords: Scintillator neutron detector; 6LiF/ZnS (Ag); Wave-Length Shifting Fiber; SiPM; Detection efficiency; Position resolution

Chinese Spallation Neutron Source (CSNS) is an accelerator based multidiscipline user facility constructed in Dongguan, China. It has been running steadily with three established instruments from March 2018. According to the construction plan of the CSNS, twenty neutron instruments will be built at last as multidisciplinary platforms for scientific research. Huge number of neutron detectors are needed for the program. Due to the shortage of ^{3}He gas and the rapidly increasing price, the larger area scintillator neutron detectors as the alternative of 3He tubes are under development since 2011 in CSNS. 6LiF/ZnS (Ag) combining with Wave-Length Shifting Fibers (WLSFs) detectors had been installed in several established spectrometers for the scattering neutron detect. The detail performers of these scintillator detectors are reviewed here. And the future development of the new type of scintillator neutron detector in CSNS is discussed.

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