American Conference on Neutron Scattering

Advances in Neutron Facilities, Instrumentation and Software

* Invited Paper

SESSION A02.01: Neutron Source and Facilities I

A02.01.01*
Neutron Scattering Facilities at the McMaster Nuclear Reactor
Patrick Clancy; McMaster University, Canada

The McMaster Nuclear Reactor (MNR) is a 5 MW open-pool reactor located on the campus of McMaster University in Hamilton, Ontario. Following the closure of the NRU Reactor at Chalk River in March 2018, MNR is the only facility in Canada with neutron scattering capabilities. At present, MNR is home to two neutron scattering instruments: the McMaster Alignment Diffractometer (MAD), a general purpose triple-axis spectrometer, and the McMaster Small Angle Neutron Scattering beamline (MacSANS). In this talk I will describe the current status of the neutron scattering facilities at MNR, present several recent scientific highlights, and discuss our plans for future upgrades and expansion.

A02.01.02
Present Status of LAHN, the Argentine Neutron Beam Laboratory
Javier R. Santisteban, Karina Pierpauli and Gabriela Aurelio; Comisión Nacional de Energía Atómica, Argentina

The Argentine Neutron Beam Laboratory (LAHN) will be a large-scale facility available to users worldwide, equipped with state-of-the-art instrumentation to fully exploit the neutron beams produced by the RA-10 reactor in the area of science and technology. The neutrons of a thermal D_2O source (~$4x10^{14}$ n/cm^2.s) and from a cold D_2 source (~$1x10^{14}$ n/cm^2.s) will illuminate instruments located at a large neutron guide hall (~70x50m^2), and at a hall directly adjacent to the reactor face. LAHN is conceived as a national laboratory which should become the leading institution in neutron science in Latin America. Main challenges of the LAHN project are (i) to implement a suite of state-of-the-art neutron scattering instruments, (ii) to build a solid neutron scattering user community, (iii) to form the human resources necessary for defining, implementing, operating and using the instruments.
In this work we present the strategies and activities developed to achieve these goals, and the current state of the project. This includes a description of the suite of eight instruments defined for the first stage of the laboratory, together with their scientific cases and the different strategies adopted for their provision. We also describe a comprehensive program developed to foster the user community, train LAHN human resources and increase LAHN visibility in order to reach a wider group of stakeholders.

A02.01.03
Neutron Scattering at Missouri—Current Status and Future Prospects
Helmut Kaiser; University of Missouri, United States

The 10 MW nuclear research reactor (MURR) has been in operation at the University of Missouri for more than 50 years and the facility has a long history in neutron scattering research. Currently, we have four neutron scattering instruments in service: a triple-axis spectrometer (TRIAX), an unpolarized neutron reflectometer (GANS), and two double-axis diffractometers (2XC and PSD). This presentation will provide an overview of the layout and performance of the instruments and of ongoing research projects. The PSD neutron powder diffractometer has recently been upgraded with new electronics and software and with an expansion from 5 to 15 linear position sensitive He-3 detector tubes. Some features have been left unchanged, however, specifically its neutron optics with a double focusing bent perfect Si(511) crystal monochromator (λ = 1.48 Å) and a solid angle per detector setting of 20° horizontal. The most significant improvements are higher counting rates, lower background, and a userfriendly interface. I will highlight the new capabilities and ongoing research projects with the upgraded PSD diffractometer. Future plans to expand our suite of neutron instruments include the addition of a thermal neutron beam imaging station. I present a conceptual design and Monte Carlo calculations. The science case concerning Plant Imaging and Tomography will be discussed. Supported by MURR and NSF Grant No. DGE-1069091.

A02.01.05

Playing with Neutrons at the MIT Nuclear Reactor Lab

Boris Khaykovich[1] and Muhammad Abir[2,1]; [1]Massachusetts Institute of Technology, United States; [2]Phoenix LLC, United States

MIT operates a 6 MW nuclear reactor, which hosts several research programs ranging from in-core irradiation to medical isotopes production to neutron imaging and neutron instrumentation development. As such, this reactor is one of a handful of active neutron-research centers outside of the national user facilities at Oak Ridge and NIST. We are involved especially in the development of neutron instrumentation, such as focusing mirrors (Wolter mirrors) and focusing multiplexing analyzers for diffractometers. Besides, we conduct early-stage imaging and diffraction experiments in collaboration with MIT faculty members. These activities not only train students, but they also allow for high-risk initial research, measurements of highly radioactive samples, or other measurements that are not easily done at national user facilities. Here we will report on recent examples of such measurements at the MIT Nuclear Reactor. We also present a case for continuing support of university-based neutron sources.

A02.01.06

Neutron Delivery System Upgrade at the NCNR

Daniel Adler; National Institute of Standards and Technology, United States

The NIST Center for Neutron Research (NCNR) is preparing for an extended shutdown in 2023 in order to upgrade its cold source, when it will move from a liquid hydrogen (LH2) moderator to a liquid deuterium (LD2) moderator. This cold source upgrade will offset neutron flux losses caused by the potential fuel change from high to low enriched uranium. To make room for the removal of the LH2 cold source and for the installation of the LD2 cold source, a large portion of the neutron guide system and about ½ million pounds of shielding will need to be disassembled due to the current horizontal orientation of the assembly. This creates an opportunity to upgrade the oldest neutron guidelines in the facility (NG 5-7). NG 5 will be replaced with ballistic guides designed to optimize neutron flux at the sample position, while NG 6 and NG 7 will be replaced with guides coated with higher m values. This extended shutdown also provides an opportunity for a major upgrade of the NG A Spin Echo instrument with the installation of a new velocity selector and new superconducting precession coils. Every aspect of this project will need meticulous management to achieve the goal of a safe assembly while minimizing the length of the reactor shutdown. Shutdown preparations are underway while also maintaining an operational facility. Preparations include the design, manufacturing, and delivery of the new guideline components. Challenges during the shutdown include the logistics of the installation and ensuring safety when working in high radiation areas. Extensive planning and rehearsals of major elements involving potential radiation exposure will ensure any exposure levels are consistent with ALARA (As Low As Reasonably Achievable). The NCNR is on course for a successful facility upgrade thanks to the diligent efforts of the engineering and project management team.

A02.01.07

Cross-Section Libraries for Moderator and Reflector Materials Used in Cold and Thermal Neutron Sources

Jose R. Granada; Argentine Atomic Energy Commission, Argentina

Neutron scattering techniques and neutron applications in general are powerful and well-established tools for research in science and technology. On one side, the nuclear industry demands more accurate data and procedures for the design and optimization of advanced fission reactors, especially for the treatment of fuel and moderator materials. On the other hand, the newer neutron scattering applications are highly intensity-limited techniques that demand reducing the neutron losses between source and detectors. The Neutron Physics Department at Centro Atomico Bariloche (CNEA, Argentina) has been developing new models for the interaction of slow neutrons with materials, particularly those of interest for thermal and cold neutron sources. Our aim is to produce scattering kernels and cross section data for the corresponding energy range. The approach involved the determination of the excitation frequency spectra for liquid and solid materials, employing Molecular Dynamics and *ab initio* calculations, in combination with processing codes (NJOY, NCrystal). In the case of quantum liquids, we used experimentally determined frequency spectra, bearing in mind that calculations involving quantum treatments are still producing disparate results. Whenever necessary, specific modifications were introduced in the standard codes, to account for coherent effects (Sköld approximation). During the last few years, we studied thermal moderators like light and heavy water [1], cold moderators like liquid para- and ortho-hydrogen [2], a 'cool' moderator like liquid ethane over the temperature range where that phase exists [3], and also neutron reflectors like diamond nanopowder and magnesium hydride [4]. The generated cross-section libraries for those materials were validated against experimental data, in most cases from transmission and scattering measurements performed by us.

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[4] J.R. Granada, J.I. Márquez Damián, C. Helman. Studies on Reflector Materials for Cold Neutrons. UCANS-VIII - 8th International Meeting of Union for Compact Accelerator-Driven Neutron Sources (2019). Paris, France.

SESSION A02.02: Instrument Development and Optimization I

A02.02.01
Upgrade of the Neutron Spin Echo Spectrometer at the NIST Center for Neutron Research
Norman Wagner[1], Michihiro Nagao[2,3], Antonio Faraone[2], Christoph Brocker[2,4], Stefano Pasini[5], Olaf Holderer[5], Christoph Tiemann[5], Richard Achten[5], Tadeusz Kozielewski[5], Michael Monkenbusch[5] and Dan A. Neumann[2];[1]University of Delaware, United States; [2]National Institute of Standards and Technology, United States; [3]Indiana University, United States; [4]University of Maryland, United States; [5]Forschungszentrum Jülich GmbH, Germany

Neutron Spin Echo (NSE) spectroscopy measures the dynamics of materials on longer time scales than any other neutron scattering method. Currently instruments in the US routinely reach Fourier times of 100 ns. However, recent advances in the optimization of the precession field significantly increase the field integral homogeneity and therefore the maximum Fourier time, as already implemented on IN-15 [1] at ILL and J-NSE-Phoenix [2] at the MLZ. The University of Delaware, in collaboration with NCNR, has received funding from the NSF through the Mid-scale RI-1 program to acquire, assemble and commission a new NSE spectrometer employing optimally designed superconducting precession coils developed for the J-NSE-Phoenix, increasing the maximum Fourier time 2.5x. The installation of the new instrument is planned for 2023 during an outage of the NCNR to install a new D_2 cold source. Taking advantage of the new design, the increased flux provided by the new cold source, and a number of instrument elements optimized for long wavelength operation, a Fourier time of 300 ns should be achieved routinely, with the possibility of reaching 700 ns for strongly scattering samples.

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[2] S Pasini, O Holderer, T Kozielewski, D Richter, M Monkenbusch, J-NSE-Phoenix, a neutron spin-echo spectrometer with optimized superconducting precession coils at the MLZ in Garching, Review of Scientific Instruments. 2019;90(4):043107.

A02.02.02
Time-of-Flight Neutron Spin Echo Data Reduction and Analysis
Piotr Zolnierczuk[1], Olaf Holderer[1], Stefano Pasini[1], Laura Stingaciu[2] and Michael Monkenbusch[1]; [1]Forschungszentrum Jülich GmbH, Germany; [2]Oak Ridge National Laboratory, United States

Neutron spin echo (NSE) spectroscopy is one of the most powerful techniques to study the dynamics of soft matter [1]. The SNS-NSE instrument [2] at the ORNL Spallation Neutron Source is the first, and to date the only one, instrument for high resolution NSE spectroscopy installed at a pulsed neutron source. The main advantage of the pulsed source NSE is the ability to resolve the neutron wavelength and collect neutrons over a wider bandwidth. This allows one to determine S(Q,t) on a flexibly chosen quasi continuous (Q,t) grid that can be selected a posteriori, trading statistical error with grid resolution. DrSPINE [3] is capable to reduce the data from a pulsed-source SNS-NSE spectrometer as well as from a reactor-based J-NSE [4] spectrometer. We will describe the algorithms and present examples of the data reduced with the aid of DrSPINE

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A02.02.03
Development of Superconducting RF Neutron Spin Flippers and Application to the MIEZE Technique at Oak Ridge National Laboratory
James R. Dadisman and Fankang Li; Oak Ridge National Laboratory, United States

Neutron Resonance Spin Echo (NRSE) was proposed as an alternative to the Neutron Spin Echo (NSE) technique which could potentially achieve higher energy resolutions, though technical limitations have prevented NRSE from surpassing NSE. A promising variation of NRSE, Modulated Intensity from Zero Effort (MIEZE), shows great promise as a method of probing dynamics in magnetic structures or protonated samples. In the simplest form of MIEZE, all spin manipulation is performed before the sample, which is what enables the measurement of depolarizing samples or sample environments. MIEZE requires RF spin flippers which are compact, with minimal phase aberrations and high spin flipping efficiency. The application of High Temperature Superconductor (HTS) technology is beneficial for achieving these characteristics, which has led to the development of RF adiabatic neutron spin flippers using HTS technology at Oak Ridge National Laboratory. These RF flippers have been applied to MIEZE measurements of standard samples to study the feasibility of a dedicated MIEZE beamline or as additional capability to existing Small Angle Neutron Scattering (SANS) instruments. An overview of the RF flipper design and test results will be presented.

A02.02.04
KWS-3 Very Small Angle Neutron Scattering (Focusing) Diffractometer—New Opportunities for Users
Vitaliy Pipich; Forschungszentrum Jülich GmbH, Germany

KWS-3 is a very small angle neutron scattering diffractometer operated by Jülich Centre for Neutron Science (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 3×10^{-5} and 2×10^{-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 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 1.3m, 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 (<1900°C), cryostats/inserts (>20mK), liquid pressure cell (<5kBar/10-80°C), CO_2/CD_4gas pressure cell (<0.5kBar/10-80°C), humidity cell/generator (5-95%/10-90°C), magnets (horizontal <3T, vertical <2.2T), Bio-logic® multimixer stopped flow (5-80°C), rheometer RSA II (tangential/radial) etc.

A02.02.06
Dynamic Nuclear Polarization Enhanced Neutron Protein Crystallography
Dean Myles[1], Josh Pierce[1], Matt Cuneo[2], Ken Herwig[1], Flora Meilleur[1,3] and Jinkui Zhao[4]; [1]Oak Ridge National Laboratory, United States; [2]St. Jude Children’s Research Hospital, United States; [3]North Carolina State University, United States; [4]Institute of Physics, China

Harnessing the spin dependence of the neutron scattering cross section for hydrogen, Dynamic Nuclear Polarization (DNP) is a potentially powerful technique for neutron diffraction measurements, especially for biological systems. Polarizing the neutron beam and aligning the proton spins in a polarized sample modulates and tunes the coherent and incoherent neutron scattering cross-sections of hydrogen, in ideal cases maximizing the scattering from - and visibility of - hydrogen atoms in the sample while simultaneously minimizing the incoherent background to zero. We have developed a prototype system for the purpose of performing proof-of-concept Neutron Macromolecular Crystallography measurements which highlight the potential of DNP. We will describe DNP concepts, experimental design, labelling strategies and the most recent results, as well as considering future prospects for data collection and analysis that these techniques enable.

SESSION A02.03: Neutron Source and Facilities II

A02.03.01*

Compact Accelerator Neutron Sources—A New Paradigm for Innovation and Education

David V. Baxter; Indiana University, United States

The term Compact Accelerator-driven Neutron Sources (CANS) refers to an emerging class of neutron sources based on accelerators running at low enough energies prevent spallation reactions in the target. A few facilities based on such accelerators have been centers of innovation and education in the neutron scattering field for several decades, but recently organizations have been starting to consider this class of source at considerably larger scales as well. In this overview, I will summarize the current state of the art for CANS-style facilities and review a few recent examples of significant technology/technique development that demonstrate the importance of CANS facilities to the future of the world's neutron ecosystem.

A02.03.03

Structural Response of a Slit-Shaped Graphene Nanopore to Adsorption—Observation by *In Situ* Neutron Diffraction

Joseph Schaeperkoetter[1], Haskell Taub[1], Helmut Kaiser[1], Zachary Buck, Matthew Connolly[2] and Carlos Wexler[1]; [1]University of Missouri, United States; [2]National Institute of Standards and Technology, United States

We have investigated adsorption-induced deformation in graphene oxide framework materials (GOFs) using neutron diffraction at sample pressures up to 140 bar. GOFs, made by solvothermal reaction of graphite oxide (GO) and benzene-1,4- diboronic acid (DBA), are a suitable candidate for deformation studies due to their narrow (~1 nm), monodispersed, slit-shaped pores whose width can be measured by diffraction techniques. We have observed, in situ, a monotonic expansion of the slit width with increasing pressure upon adsorption of xenon, methane, and hydrogen under supercritical conditions [1]. We find that the expansion of the three gases can be mapped onto a common curve based solely on their Lennard-Jones parameters, in a manner similar to a law of corresponding states. All scattering measurements were performed on the 2-axis powder diffractometer at the Missouri University Research Reactor (MURR). [1]. Schaeperkoetter, J. C. *et al.* Adsorption-Induced Expansion of Graphene Oxide Frameworks: Observation by in Situ Neutron Diffraction. *ACS Omega* (2019) doi:10.1021/acsomega.9b02589.

Funding Acknowledgement: This work was supported by the National Science Foundation Grant No. DGE-1069091.

A02.03.04

Development of ^{3}He Polarization Capabilities at the China Spallation Neutron Source

Zachary Buck[1,2], Tianhao Wang[1], Wolfgang Kreuzpaintner[1], Syed Mohd Amir[1], Junpei Zhang[1] and Xin Tong[1]; [1]Institute of High Energy Physics, Chinese Academy of Sciences (CAS), China; [2]University of Missouri, United States

Neutron polarization techniques have been used in various instrumentation at neutron sources around the world to study a wide range of materials and their magnetic properties. At the China Spallation Neutron Source (CSNS), the polarized neutron and sample environment groups are developing a complete system of *in-situ* and *ex-situ* ^{3}He neutron spin filters (NSF) to support ongoing beamline design/construction efforts and improve user satisfaction. In this talk, we will discuss the current status and future developments of polarized ^{3}He systems using Spin Exchange Optical Pumping (SEOP) at the CSNS. Initial performance tests on polarized ^{3}He NSFs fabricated at CSNS reveal ^{3}He polarization lifetimes of up to 240 hours. Further development of these NSF systems will provide a reliable source of polarized neutrons for the current beamlines at CSNS, which include small angle neutron scattering (SANS), neutron reflectometry and powder diffraction, in addition to those instruments approved for the next phase of construction.

SESSION A03.01: Instrument Development and Optimization II

A03.01.01*

First Measurements at the CANDOR Polychromatic Reflectometer

David P. Hoogerheide, Alexander J. Grutter, Brian Maranville and Charles F. Majkrzak; National Institute of Standards and Technology, United States

The CANDOR reflectometer at the NIST Center for Neutron Research marries the advantages of time-of-flight polychromatic reflectometers, such as those commonly employed at pulsed neutron sources, to the high time-averaged flux of a reactor neutron source. CANDOR's unique energy dispersive detector, currently comprising 108 individual wavelength-sensitive neutron detectors operating at over 90% efficiency, allows simultaneous detection of cold neutrons in the 4 Å to 6 Å wavelength range. In this talk, I will describe instrument design, detector operation and performance, and data reduction considerations. Reflectivity curves measured by CANDOR using polychromatic detection will be compared to standard curves measured at NIST's monochromatic reflectometers, and the performance of CANDOR's full polarization capabilities will be discussed.

A03.01.02
The CAMEA and BiFrost Massively Multiplexed Crystal Analyzer Sectrometers
Henrik M. Ronnow; EPFL, Switzerland

The CAMEA principle of Continuous Angle Multiple Energy Analysers is being implemented at multiple neutron sources. Compared to direct time of flight spectrometers, CAMEA-type spectrometer offer higher count rates, are better suited to complicated sample environment, and can measure smaller samples. I will present the design and first performance results from the recently commissioned CAMEA spectrometer at the Swiss neutron Source at PSI, which operates with a crystal monochromator. Next I will present design and performance predictions for the BiFrost instrument, which is being constructed as an indirect time-of-flight spectrometer at the European Spallation Source.

A03.01.03
Update on the NG-5 Cold Neutron Quantum Materials Spectrometer at the NCNR
Leland W. Harriger, Jeffrey Lynn and Dan A. Neumann; National Institute of Standards and Technology, United States

A summary of the NCNR project to replace the SPINS cold triple axis at NG-5 with a modern, state-of-the-art high wave vector and energy resolution cold spectrometer will be presented. The new primary spectrometer has now seen multiple design iterations with the final design fully analyzed by Monte-Carlo. The new front end will upgrade the existing rectangular Ni-58 guide to an elliptical supermirror guide with a change from a vertically focusing to double focusing monochromator. As well, the scientific community has identified versatile resolution tailoring, in both Q and energy, as a key feature required to probe the wide variety of energy scales, correlations, and orders studied. Often these states must be resolved on increasingly small samples, thereby requiring the additional ability to balance resolution and intensity. To this end, the virtual source has been optimized in conjunction with a series of masks such that the front end Q and energy resolution can independently controlled with exceptionally high efficiency. With the beam characteristics at the sample now fully optimized, modeling of different analyzer designs is underway, with emphasis given to multiplexed geometries and resolution matching of the front end. Results for a RITA-II or UFO like analyzer will be presented. Taken together, these upgrades will improve the throughput by two orders of magnitude while also substantially improving both the flexibility and maximum accessible Q and energy resolution.

A03.01.04
A Multi-Analyzer Triple Axis (MANTA) Spectrometer for the HFIR at ORNL
Marcus Daum[1], Gabriele Sala[2], Adam Aczel[2], Garrett E. Granroth[2], Lee Robertson[2], Tao Hong[2], Jaime Fernandez-Baca[2], Martin Mourigal[1], Mark L. Lumsden[2] and Barry Winn[2]; [1]Georgia Institute of Technology, United States; [2]Oak Ridge National Laboratory, United States

A new cold triple axis spectrometer is under development for the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory (ORNL). The instrument will use a curved and focusing guide to provide a virtual source that feeds a double focusing monochromator. A 1.4 m focal distance will provide a spot size as small as 2cm x 2cm at the sample position. The instrument is optimized to operate with an incident energy between 2.3 and 25 meV. To efficiently use the neutrons scattered off the sample, a multi-analyzer backend is planned. Such an analyzer consists of several crystals placed in series so neutrons with multiple final energies can be scattered simultaneously into different locations on a position sensitive detector. Multiple analyzer channels will be used to cover an extended angular range. This anticipated configuration closely follows the CAMEA design of PSI. A full description of the planned instrument and standard metrics of instrument performance will be discussed. Furthermore, to illustrate how the instrument will perform, Monte Carlo Ray tracing simulations of typical inelastic samples will be presented.

A03.01.05
Implementation of Polarized Neutron Spectroscopy on TOF Spectrometer NEAT at Helmholtz Zentrum Berlin
Gerrit Guenther[1], Veronika Grzimek[1], Ramil Gainov[1,2], Ferenc Mezei[3,4], Janos Füzi[4], Earl Babcock[5], Zahir Salhi[5], Alexander Ioffe[5], Klaus Kiefer[1], Hanjo Ryll[1] and Margarita Russina[1,5]; [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany; [2]RWTH Aachen University, Germany; [3]ESS ERIC, Sweden; [4]Wigner Research Center, Hungary; [5]JCNS, Germany

Time-of-flight spectroscopy with polarized neutrons is still not very common today, mostly because of the large reduction in flux caused by polarization of incoming beam. The utilization of polarization analyzers often lead to additional transmission losses and limitation in detector solid angle, which further decrease the count rate. A decisive increase of the neutron efficiency has been achieved at the time-of-flight (TOF) cold neutron spectrometer NEAT at Helmholtz Zentrum Berlin as the result of a large scale technical upgrade [1]. Using modern technology and innovative instrument design the upgrade resulted in 300 fold count rate increase placing NEAT on similar level of performance as the world leader spectrometer IN5 at ILL, despite of the order of magnitude lower cold neutron flux at the reactor in Berlin [1]. This large gain made possible the implementation of polarized neutron spectroscopy as one of the novel features of new instrument. In the implemented setup the polarization of the incoming neutrons is realized using specially designed transmission polarizer with eight “V cavity” channels [2],[3]. The channels have non-polarizing supermirror-coated, opaque side walls and neutron-transparent Si cavity polarizing plates, coated by m=3 polarizing supermirror on both sides. The nominal operational wavelength band width of the polarizer is 2.5 – 8 Å, with measured polarization efficiency between 92 and 96 % for well collimated beam [2]. The incoming neutron flux is about 32 % of the non-polarized incoming beam. The neutron beam polarizer is placed inside a 3.8 m long evacuated neutron “guide changer”. The design of the hardware allows us to switch between polarized and un-polarized incoming beam options in less than 30 sec [2]. Polarization analysis is realized using a 3He gas analyzer toroidal cell, that covers about 130° in the horizontal plane of the detection angle. The neutron polarization is guided by a PASTIS like setup developed at MLZ [4]. Despite of the combined neutron intensity decrease due to beam polarization and analysis, the count rate is about an order magnitude higher than in un-polarized neutron experiments before the upgrade. The setup has been successfully tested and applied for the identification and spectroscopic analysis of coherent and incoherent scattering in hydrogen rich samples. Illustrative examples will be discussed.

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A03.01.06

Methods for Handling Aberation in Spherical Neutron Polarimetry

Jacob A. Tosado[1,2], Wangchun Chen[2] and Efrain Rodriguez[1,2]; [1]University of Maryland, United States; [2]National Institute of Standards and Technology, United States

Spherical Neutron Polarimetry is a three-dimensional measurement technique used to determine the polarization property tensor of a material. This property tensor is dependent on the neutron scattering angle 2θ and any magnetic interaction with that material. The 2θ dependence requires a rotation of the polarimeter's measurement axes through the horizontal scattering plane about an axis vertical to it. The presence of magnetic interaction requires an isotropic transport of the scattered neutron beam polarization. Consequently, a complete calibration of a spherical neutron polarimeter involves the characterization of two fields, the measurement axis field and the incident polarization field. Here, we present the latest characterization of these two fields using the Small Angle Neutron Polarimetry Apparatus (SANPA) recently developed at the NIST Center for Neutron Research. We describe our methods for identifying, compensating and eliminating aberration in these fields including modifications to the hardware and software made in this effort.

A03.01.07

Wide Angle Spherical Neutron Polarimetry at Oak Ridge National Laboratory

Nicolas Silva[1], Tianhao Wang[2], Chenyang Jiang[3], Fankang Li[3], Masaaki Matsuda[3], Jillian Ruff[1], Roger Pynn[4], Xin Tong[2], Barry Winn[3] and Lisa DeBeer-Schemitt[3]; [1]Oak Ridge Associated Universities, United States; [2]Institute of High Energy Physics, China; [3]Oak Ridge National Laboratory, United States; [4]Indiana University, United States

Polarized neutron scattering has been widely used to study magnetism in materials. Traditional neutron polarization techniques can only measure the scattered neutron polarization parallel or antiparallel to the incident neutron polarization. This leaves the polarization components perpendicular to the incident neutron polarization inaccessible. Whereas, spherical neutron polarimetry (SNP) measures all the components in the polarization matrix in which the off-diagonal terms contain the information of chirality and nuclear-magnetic interference. Thus, SNP is a powerful tool to study certain complex magnetic structures in materials. Wide-angle SNP is being realized at Oak Ridge National Laboratory

(ORNL) for multiple beamlines including: the polarized triple-axis spectrometer (HB-1) and general-purpose small angle neutron scattering instrument (CG-2) at the High Flux Isotope Reactor (HFIR), as well as the hybrid spectrometer (HYSPEC) at the Spallation Neutron Source (SNS). The SNP device consists of three units: incoming/outgoing neutron polarization manipulation regions, sample environment and a zero-field chamber.
The incoming and outgoing neutron polarization control regions are composed of magnetic guide fields, combined with high temperature superconducting YBCO films that can align the neutron polarization into any desired direction. The zero-field chamber is made from mu-metal to create a region of near zero magnetic field along the neutron path and for the sample to reside in. The sample environment is a custom dilution refrigerator (orange cryostat). Initial testing was performed at the University of Missouri Research Reactor (MURR) that showed functionality of all the components. Using the results from MURR modifications were made and the device was then run and tested at HYSPEC.

SESSION A03.02: Software I—Analysis, Modeling and Machine Learning

A03.02.01*
Application of Machine Learning in Condensed Matter Physics
Anjana M. Samarakoon and Alan Tennant; Oak Ridge National Laboratory, United States

Realistic modeling and realization of complex phases are the key challenges to understand the underlying physics in materials. Conventional simulation approaches struggle to deal with the need to account for multiple and competing interactions, as well as relate models and data together. Exploration of high-dimensional parameter spaces for exotic phases such as spin liquids or spin glasses using high-performance computing (HPC) and collection of high-quality experimental data are the essential components to deal with these challenges. Experimental techniques such as Neutron Scattering and computer resources such as GPU-based supercomputers are now advanced enough to address these developments. Traditional condensed matter problems become big data-mining challenges where machine-learning treatments prove essential. By training neural networks over large numbers of models, machine learning techniques discriminate between different models and identify different physical regimes including the formation of spin liquids and unusual broken symmetries. Moreover, these trained networks allow us to extract the most relevant information out of experimental data by denoising and removing irrelevant information such as background and experimental artifacts. A few examples of machine-learning assisted modeling on neutron scattering data including single-crystal and powder spectroscopy are shown.

A03.02.02
Using Machine Learning to Understand Disorder in Materials from Diffuse Scattering
Thomas Proffen; Oak Ridge National Laboratory, United States

Advances in machine learning (ML) and artificial intelligence (AI) are already having a revolutionizing impact in many areas such as image, speech recognition or advancing self-driving cars. These techniques are starting to have impact on materials science and the focus of this contribution is accelerating neutron and X-ray scattering science using data analytics and machine learning approaches using the example of diffuse scattering analysis. Great experimental advances haven been made and modern neutron and x-ray diffractometers allow researchers to collect large volumes of neutron and x-ray diffraction data containing strong Bragg intensities as well as weak extended diffuse scattering features holding the key to understanding the complex structure and disorder in materials. Researcher's ability to visualize, analyze and model such data has not kept up and is becoming the bottle neck to progress. Data analytics capabilities can accelerate discovery by enabling rapid, quasi-real-time data reconstruction and analysis; by permitting rapid, convenient, and secure data sharing; and by providing access to sophisticated software for advanced feature detection and mapping. Traditional analysis of diffuse scattering combines chemical knowledge and intuition to build a model and to extract scientific knowledge from the diffuse scattering data. In fact the idea presented was inspired by the Atlas of Optical Transforms [1] used to understand diffuse scattering on x-ray films by comparing it to the optical transforms o various disordered patterns in the book. In this presentation, results from a demonstration project using feature extraction and machine learning to analyze materials with stacking faults will be presented. These concepts can be generalized to include all types of disorder and present a path to more comprehensive diffuse scattering analysis in the future.
[1] G. Harburn, Charles Alfred Taylor, T. R. Welberry (1975), Cornell University Press

A03.02.03

A Reverse Monte Carlo Refinement Python Program for Analyzing the Diffuse Neutron Scattering of Single Crystals

Zachary Morgan[1] and Feng Ye[2]; [1]Michigan Technological University, United States; [2]Oak Ridge National Laboratory, United States

A program written in Python for the analysis of diffuse neutron scattering data using Reverse Monte Carlo is showcased. The program allows for the refinement of magnetic, occupational, and displacive disorder to obtain spin- composition-, and displacement-pair correlations, respectively. Each disorder module is parallelized for performance and optimized for memory efficiency. Illustrations of extracting short range correlations are shown using the geometrically frustrated pyrochlore lattice composed of corner-sharing tetrahedra. In addition, demonstrative examples of refinements of single crystal data collected from CORELLI, a Spallation Neutron Source diffuse scattering spectrometer at Oak Ridge National Laboratory, are also shown. These examples include magnetic disorder in Bixbyite, a manganese iron oxide mineral, and combined occupational displacive disorder of carbonate in a triangular lattice system Ba3Co2O6(CO3)0.7. The program provides a simple, yet effective utility for characterizing the disorder in single crystals from neutron scattering experiments.

A03.02.04

Structure-Mining—An Automated Tool to Find Candidate Structures from Neutron and X-Ray Diffraction Data

Long Yang[1,2], Pavol Juhas[3], Maxwell Terban[4], Matthew Tucker[2] and Simon Billinge[1,3]; [1]Columbia University, United States; [2]Oak Ridge National Laboratory, United States; [3]Brookhaven National Laboratory, United States; [4]Max Planck Institute for Solid State Research, Germany

Here we present a new approach to obtain candidate structures from neutron and x-ray atomic pair distribution function (PDF) data in a highly automated way. It pulls, from structural databases, all the structures meeting the search criteria and performs structure refinements on them without human intervention. Tests on various material systems show the effectiveness and robustness of the algorithm in finding the correct atomic crystal structure. It works on crystalline and nanocrystalline materials including complex oxide nanoparticles and nanowires, low-symmetry and locally distorted structures, and complicated doped and magnetic materials. The approach has been tested on x-ray data, but also the testing cases include the neutron PDF data collected at the NOMAD beamline of the SNS. This approach could greatly reduce the traditional structure searching work and enable the possibility of high-throughput real-time automated analysis of PDF experiments in the future. Structure-mining will become available on a cloud-based PDF analysis platform, PDFitc (PDF in the cloud), at https://pdfitc.org. L.Y. and M.G.T. acknowledge support from the ORNL Graduate Opportunity (GO) program. S.J.L.B. acknowledges support from NSF through grant DMREF-1534910. P.J. was supported by the New York State BNL Big Data Science Capital Project under the U.S. DOE Contract No. DE-SC0012704. M.W.T. gratefully acknowledges support from BASF.

A03.02.05

ICE-MAN—The Integrated Computational Environment-Modeling and Analysis for Neutrons at ORNL

Timmy Ramirez-Cuesta; Oak Ridge National Laboratory, United States

ICE-MAN is a modeling and analysis workbench for multi-modal studies, designed with neutron science in mind. The integrated and extensible environment provides scientists with a common interface to a suite of tools, and developers with a common API to seamlessly add new functionality. This project aims to reduce the barrier to analyze and interpret neutron scattering experiments in combination with other multi-technique research studies. It streamlines the workflow between different experimental techniques, computer modeling, and databases and reduces the time and learning curve needed to access them thus making a holistic approach to data interpretation more amenable and efficient.

1) ICE-MAN overcomes the limitation of an individual's expertise to utilize different atomistic modeling techniques and to quickly compare simulated and experimental data.
2) At ORNL, ICE-MAN provides tools that can be used in 10 instruments.
3) ICEMAN can be used in many ways: a) as a virtual machine in VirtualBox, b) as Docker containers and c) as a web application hosted by CADES (https://iceman.ornl.gov/ui/ICEMAN), in this form it is available to any user with an ORNL account. At present, it has two main modules, **OClimax** and **QClimax**. Also. there are several small modules to generate input files, read output files and convert formats.
OClimax can model phonon and vibrational spectra for comparison with inelastic neutron scattering instruments and can be used to rigorously model both polycrystalline and single-crystal spectra, including resolution considerations. Currently, OClimax is principally used on VISION (BL-16B) but can also be used to analyze phonon data from ARCS, CNCS,

HySPEC, SEQUOIA, triple axes spectrometers (ORNL), LET, MAPS, MERLIN, TOSCA, (ISIS), DCS (NIST), etc. A necessary step in analyzing data with OClimax is performing DFT calculations. The ICEMAN project aims to simplify this step in the analysis procedure, allowing for fast setup of initial files and running scripts for different DFT packages. The focused resources applied to data analysis on VISION (BL-16B) have contributed to it being the world leader in neutron vibrational spectroscopy measurements. The scientific output of the spectrometer is roughly 80% dependent on these analysis capabilities and has significantly improved the scientific impact of the instrument.
QClimax, on the other hand, provides users with a flexible, straightforward environment to enable fitting to complex user-defined functions. It allows fits to be performed to data from multiple Q values simultaneously and provides global fitting parameters. QClimax can be used to analyze QENS data from any quasielastic spectrometer, including BASIS, CNCS (ORNL), DCS, HFBS (NIST), IRIS, OSIRIS (ISIS), TOFTOF (FRM II), etc. The ICEMAN project is still under active development, and the QENS analysis capabilities of QClimax are being refined with feedback from instrument staff and users.

A03.02.06
Rapid Analysis of Neutron Scattering Time-of-Flight Data Using Phonon Explorer Software Package
Dmitry Reznik; University of Colorado Boulder, United States

Recently built time-of-flight (TOF) spectrometers, the most powerful of which are at the Spallation Neutron Source (SNS) at ORNL, enable comprehensive investigations of phonon dispersions and other lattice dynamical effects. However, their full potential has not yet been realized, because there are no effective software tools available that allow rapid comprehensive exploration of the 100+ Gb single crystal datasets that the instruments generate. A typical dataset contains maps of the scattering function S(**Q**,w) covering hundreds, often thousands Brillouin zones. We developed a software package called Phonon Explorer (https://github.com/dmitryr1234/Phonon-Explorer) and successfully demonstrated its capabilities on three completed research projects spanning a variety of experimental conditions. Its main features are efficient browsing of S(**Q**,w), background subtraction, and multizone fitting. The package enables rapid sophisticated real time data analysis during phonon measurements on TOF spectrometers, which makes it possible to adjust experimental conditions and strategy during experiments. The talk will demonstrate main features of the software on an example of our recent investigation of optic phonons in a high temperature superconductor $HgBa_2CuO_{4+\delta}$. This work was supported by the DOE, Office of Basic Energy Sciences, Office of Science, under Contract No. DE-SC0006939

SESSION A04.01: Sample Environment Development

A04.01.01*
An Overview over High Pressure Development and High Pressure Neutron Studies at Oak Ridge National Laboratory
Yan Wu and Bianca Haberl; Oak Ridge National Laboratory, United States

Pressure is a powerful and frequently used tool across a variety of fields. It is used for material synthesis, since it allows for the creation of exotic materials with unusual structures that brings novel physics properties. Similarly, it is used to study phase transformations of materials and illustrate underlying interactions behind materials properties. This enables new physics and helps to understand the intrinsic mechanisms in materials. When pressure is used *in situ* during neutron scattering studies, new possibilities becomes available. The pressure cell is the key component for any high pressure study. In order to boost pressure studies and extend the high pressure capability for neutron scattering, the Neutron Scattering Division at Oak Ridge National Laboratory (ORNL) has devoted considerable efforts to the development of different pressure cells. Beyond several 'standard' purchased pressure cells like the Paris-Edinburg press or various types of gas pressure cells, many different models of pressure cells suitable for neutron scattering have been developed internally and through various collaborations. These include neutron diamond anvil cells, large volume and low neutron background clamp cells, and a mini McWhan cell. Those pressure tools allow us the capability of material science with neutron scattering under pressure from a few hundred bars to 400 kbar and above. With the continuous efforts of ORNL scientists, various new and improved pressure cells are gradually employed across different neutron beamlines to enable magnetic phase and structure transitions investigations, studies of lattice dynamics changes, the direct monitoring of material synthesis processes and much more. Those high pressure cells are also becoming available to use for in various scientific disciplines in the neutron scattering user program. *This study used resources at SNS and HFIR, the DOE Office of Science User Facilities operated by the ORNL and was supported by U.S.*

DOE, Office of Science.

A04.01.02

4D Rheo-SANS Sample Environment for Soft Matter, Biology and Materials Processing

Norman Wagner[1,2], Richard Dombrowski[2], John Lim[2] and Yu-Jiun Lin[1]; [1]University of Delaware, United States; [2]STF Technologies LLC, United States

Under the auspices of the DOE SBIR/STTR program, we have developed a new sample environment for neutron scattering applicable to a broad range of soft matter and biological materials under shear fields and processing conditions. This sample environment directly addresses the unmet need for simultaneous measurement of stresses and microstructure in all three planes of shear flow across a broad range of material properties, and conditions (T, P) with ~10 millisecond time resolution. The need for this sample environment has been identified by the broad soft-matter and biological, neutron scattering user community and is equally critical for research in materials processing, with broad, industrial R&D use. The new sample environment works on a commercial stress controlled rheometer that is capable of both stress and rate control. Rheological and SANS performance are demonstrated using an aqueous complex fluid comprised of a wormlike surfactant. Stress-SANS rules are identified showing how the instrument can elucidate rheological material properties that are difficult or impossible to access otherwise. Future improvements and applications will be discussed.

A04.01.03

Ultra-High Field Magnets for Neutron Scattering

Mark Bird; Florida State University, United States

For many years various research groups around the world have been developing magnets based on High Temperature Superconducting (HTS) materials. The National High Magnetic Field Lab in Tallahassee Florida has been a leader in this field for many years having completed the first 25 T test coil in 2003, the first 27 T test coil in 2007, the first demonstration of a quench protection system in 2011, the first 45 T test coil in 2017, the first 32 T all-superconducting magnet in 2017, etc. Presently we are developing a 40 T superconducting solenoid for condensed matter physics experiments. The status of magnet technology for ultra-high field solenoids is presented along with a route forward for developing split HTS magnets with a vertical field at 25 T or more, well beyond the 15 T presently available from magnets of this configuration employing Low Temperature Superconductors.

A04.01.05

Ultra-High Temperature Neutron Scattering at Oak Ridge National Laboratory

Dante Quirinale; Oak Ridge National Laboratory, United States

The Neutron Sciences Directorate at ORNL maintains and develops a large suite of high temperature sample environments. This includes conventional furnace systems for temperatures up to 1600 °C as well as a range of complementary levitation systems, enabling neutron scattering and thermophysical measurements at temperatures up to 3000 °C for a wide range of materials. Presented will be an overview of the current capabilities of the levitation program, including aerodynamic and electrostatic levitators, several recent scientific successes, and the unique furnaces currently in development for use at both SNS and HFIR, including a beamline aero-acoustic levitator and a novel electrostatic levitation furnace for ultra-high temperature in-situ residual stress measurements.

A04.01.06

Microwave Stimulated Inelastic Neutron Scattering in Cr8

Timothy R. Reeder[1], Jonas Kindervater[1], Veronica Stewart[1], Yishu Wang[1], Qiang Ye[2], Jose A. Rodriguez-Rivera[2,3], Yiming Qiu[2,3], Nicholas Maliszewskyj[2], Yamali Hernandez[2], Tyrel McQueen[1] and Collin Broholm[1]; [1]Johns Hopkins University, United States; [2]National Institute of Standards and Technology, United States; [3]University of Maryland, United States

The physical properties of magnetic condensed matter systems are typically measured while the sample is in thermal equilibrium with its surroundings. We describe the commissioning of a high power, high frequency microwave spectrometer designed to drive magnetic systems out of equilibrium while measuring the inelastic neutron scattering spectrum as a function of time. A 105 (210) GHz signal is generated at 1 (0.3) W, and directed through a compact, 3D quasi-optical bridge to the sample. With a DC magnetic field, we can tune the system to a magnetic resonance which effectively gives us some excitation selectivity. Reflected microwaves are detected by a phase and polarization sensitive superheterodyne mixing schema. This design allows for compatibility with different low-temperature magnets, the power necessary to induce a statistically significant population inversion required for neutron scattering, and the ability to do Pulsed Electron Spin Resonance experiments as a standalone unit. Using this instrument, we have shown that we can pump a molecular magnet in resonance at 4.6 T out of equilibrium at T=1.5 K using microwaves at 105 GHz, and with event mode neutron detection, we have measured the momentum and energy dependent dynamical structure factor as a

function of time after a saturation pulse finding relaxation timescales on the order of seconds.

SESSION A04.02: Instrument Development and Optimization III

A04.02.02

50 Years of Highly Oriented Pyrolytic Graphite Applied to Neutron Scattering Instrumentation

Hao Qu[1], Xiang Liu[1], Michael Crosby[1], Brian Kozak[1] and Andreas K. Freund[2]; [1]Momentive, United States; [2]Self Employed, France

About 50 years ago, following earlier developments by A.W. Moore *et al.* [1], *Highly Oriented Pyrolytic Graphite* (HOPG) was introduced as thermal neutron monochromator and filter material [2, 3]. Since then, Momentive and its predecessor have been supplying in excess of 70,000 HOPG parts not only for neutron scattering applications, but also as x-ray monochromators in materials research. The HOPG products are fabricated by hot-pressing pyrolytic graphite raw material grown by chemical vapor deposition. High-quality crystals of various grades are available for different applications. These crystals can be customized with excellent precision to different sizes, flat or curved shapes, to meet specific requirements. Being a central component of a great variety of instruments, HOPG has served the neutron scattering community over half a century to collect an immense amount of data. Still today its outstanding performance as optical element for neutron beam conditioning is unequalled by any other crystalline material. This superiority stems from the favorable nuclear properties of carbon (small absorption and incoherent scattering cross-sections, big coherent scattering length) and the specific crystalline structure (small thermal diffuse scattering cross-section, layered crystal structure). We take this opportunity to review the neutron diffraction properties and applications of HOPG as well as fabrication issues. The real crystal defect structure revealed by imaging techniques is correlated with the parameters used in the mosaic model (mosaic spread, mosaic block size, uniformity). The diffraction properties (rocking curve width as determined by both the intrinsic mosaic spread and the diffraction process, peak and integrated reflectivities, filter transmission) as a function of neutron wavelength or energy can be predicted with high accuracy and reliability by diffraction theory using empirical primary extinction coefficients extracted from a great amount of existing experimental data. The results of these calculations are given as graphs and tables permitting to optimize HOPG monochromator characteristics for any given experimental situation. We also address mechanical issues such as stress resistance, mounting and bonding HOPG on focusing devices and assembling crystals to achieve sizes that exceed presently available dimensions. Finally, we outline possible future developments.

[1] A.W. Moore, A.R. Ubbelohde and D.A. Young, "*Annealing of pyrolytic graphite under pressure"*, Nature, Volume 198 (1963), pp. 1192-1193.
[2] T. Riste and K. Otnes, "*Oriented graphite as a neutron monochromator"*, Nuclear Instruments and Methods, Volume 75 (1969), Issue 2, pp. 197-202.
[3] J. Bergsma and C. Van Dijk, "*Pyrolytic graphite as a second order neutron filter"*, Nuclear Instruments and Methods, Volume 51 (1967), Issue 1, pp. 121-124.

A04.02.03

A First Demonstration of the Use of Gas Cluster Ion Beams (GCIB)—An Innovative Surface-Modification Nanotechnology for Improving the Performance of Neutron Supermirror Optics

David R. Swenson; American Physics and Technology llc, United States

Gas Cluster Ion Beams (GCIB) and Accelerated Neutral Atom Beams (ANAB) are emerging technologies that are used to modify the structure and composition of surfaces at the nanoscale. The technique is based on the emission of a compressed gas through a small orifice into a region of high vacuum. The gas cools and condenses as it expands inside a specially shaped nozzle that facilitates the formation of a jet of clusters. The clusters are ionized by electron impact and then are accelerated electrostatically as a charged particle beam. The technique is analogous to "sand blasting" but the particles are nanosized and can have velocities high enough to break chemical bonds. We have used lower-energy beams of Argon clusters to smooth the surface of substrates and thin-films for the manufacture of neutron supermirrors. These techniques allow new freedom in the choice of materials and geometries as they are capable of producing atomic-level smoothness on planar and curved surfaces and on conductive and insulating materials. Our studies have included a variety of metallic and non-metallic substrate materials and various combination of dose and energy of GCIB/ANAB processing. The smoothness has been evaluated mainly using Atomic Force Microscopy (AFM). The performance of Ni-Ti, m=3, supermirrors manufactured using borosilicate-glass substrates have been evaluated using neutron reflectometry at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory. The experiment compared supermirrors made using untreated and treated substrates.

A04.02.04
Development Beamlines at the High Flux Isotope Reactor
Lowell Crow; Oak Ridge National Laboratory, United States

As a part of its development work Neutron Optics and Polarization team at ORNL runs neutron instrument development beamlines at the High Flux Isotope Reactor (HFIR). These beamlines enable measurements for new neutron techniques, component development, and continuing improvements to instrumentation at the HFIR and the Spallation Neutron Source (SNS). The Polarized Cold Neutron Development Beamline, at the CG4B position in the HFIR cold guide hall, entered commissioning operation in 2018. The CG4B instrument provides a stable cold neutron test bed for full scale tests of Larmor techniques for future neutron instruments. The new instrument is installed along the CG4 cold neutron guide. It uses two plastically deformed Si (111) crystals at a deflection angle of 122 degrees to form a 5.45 Å wavelength beam. The beam path allows about 7 m of space for optical components, which are supported by variable height lift tables. The usual polarizing element is a supermirror S-bender, while V-cavity supermirrors and ^{3}He cells are also available for polarization analysis. The first experiment involved imaging of neutron capture induced He fluorescence for studies of turbulence. The most recent experiments include a demonstration of neutron flippers using radio frequency superconducting flippers set up in a geometry for MIEZE (modulated intensity with zero effort) operation, and a quantum entanglement measurement using Wollaston prisms. Small angle scattering with dynamical nuclear polarization of hydrogenous samples is planned within the next few HFIR cycles. The team also operates the Polarized Neutron Development beamline on the HB-2D thermal beam position at HFIR. HB-2D provides a tool for development and testing of polarizers, polarized neutron devices, and polarized neutron techniques. This beamline typically uses a pyrolytic graphite monochromator, producing a 4.25 Å wavelength, and may use crystal, supermirror, or He-3 polarizers and analyzers in various configurations. The emphasis on this instrument is on component characterization, and on preparing polarized configurations for use on the user instruments. Between now (2020) and 2024, the HFIR will require replacement of its permanent beryllium reflector, which will in turn lead to a reinstallation of the beam instrumentation at HFIR. The development beamlines will play a role in preparation for this work, and will eventually reappear in a different configuration

A04.02.05
The Effects of Microstructure in Neutron Beam Window Materials on Neutron Beam Properties
Kyle Grammer, Erik B. Iverson and Franz X. Gallmeier; Oak Ridge National Laboratory, United States

The selection of window materials along the neutron path from the source to the sample position is a complex problem with a number of considerations dependent on the requirements of the instrument end-station. Beam windows should be comparably thin in order to reduce attenuation of the neutron beam as well as minimize the introduction of noise in the scattering signal in order to maximize performance of the instrument, and windows should be thick enough to be structurally sound for use as a vacuum window. The microstructure of the material may produce scattering artifacts that are undesirable for a particular instrument configuration. An example of this is the grain structure of a polycrystalline alloy introducing noise due to small-angle neutron scattering as well as affecting the shape of the neutron spectrum due to Bragg scattering. Measurements and simulations that illustrate the effects of various types of beam window materials on the properties of the neutron beam will be discussed.

A04.02.06
Neutron Instruments Using HiTc Superconductors (1) Wide Angle Spin Echo, (2) Wollaston Prisms Combined with RF Flippers, Multiplexing Focusing Analyzer for Efficient Stress-Strain Measurements, Plant Roots/Soil Imaging with Grating Optics Combined with Compact Thermal Neutron Source and Magnetic Compound Refractive Lenses for Neutron Microscopy
Jay T. Cremer; Adelphi Technology, Inc., United States

Presented is neutron Spin Echo (NSE) instrument, using a pair of high temperature superconducting (HiTc) Wollaston prisms, combined with a HiTc RF flipper, enabling simultaneous measurements of spatial and time dependence of density fluctuations in a wide range of hierarchical and disordered meso-scale materials. Early initial progress of an inexpensive HiTc-based Wide Angle Spin Echo (WASP) instrument is also presented. The WASP instrument would increase the range of neutron scattering angles measured simultaneously, thereby accessing a larger range of Q and enabling an increased data collection rate. And presented is multiplexing, focusing analyzer for efficient, fast stress-strain measurements, employing a multi-foil analyzer. Each foil is constructed of focusing bent single crystals of Si, enabling polychromatic residual stress neutron diffraction to determine residual stress tensors, raster large samples, or screen multiple samples. Also presented is a thermal neutron radiographic/tomographic imaging system, using a portable, moderated, DD neutron generator, combined with an inexpensive, large area, grating-based, imaging-scattering optic for imaging plant/soil systems with 1-micron resolution. Finally, presented are focusing and imaging results of magnetic compound refractive lenses at ILL pf2-VCN and D33 beamlines, used to construct simple and compound neutron microscopes.

SESSION A04.03: Software II—Analysis, Modeling and Resolution

A04.03.01*
Challenges for Grazing Incidence Neutron Scattering at Pulsed Sources—Beyond Basic Experiments and Data Analysis
Valeria Lauter, Andrei T. Savici, Steven Hahn, Rajeev Kumar and Joti P. Mahalik; Oak Ridge National Laboratory, United States

Conventional analysis of reflectometry data provides *only* structural parameters via fitting model to the data. Can we obtain access to the interaction parameters causing this structure? To realize this one needs a different approach to the data analysis, that includes development of computational workflow capable of generating theoretical models in quantitative agreement with the data. Grazing Incidence Neutron Scattering experiments simultaneously measure specular reflection, off-specular scattering (OSS) and grazing incidence small angle scattering (GISANS) and deliver the most exhaustive and detailed information on the 3-dimensional structure of thin films and hidden interfaces on enormous length scale. At present, most of published data in reflectometry are obtained with specular reflectivity, from which the structural information perpendicular to the sample surface is obtained along the Q_z component of the wave vector transfer. However, functionality often arises at the mesoscale, where defects, interfaces, and non-equilibrium structures are formed [1], which cannot be resolved only by specular reflectivity alone. Spallation neutron sources deliver outstanding experimental conditions to perform *simultaneously* a combined measurement of specular reflection, OSS and GISANS using time-of-flight (TOF) [2]. GINS pilot experiments performed at the SNS on the Magnetism Reflectometer [2] on a multilayer heterostructure of magnetic nanoparticles self-assembled in a block-copolymer matrix will be presented. Thus, a combination of GINS experiments with the computational workflow capable of generating theoretical models in quantitative agreement with experimental data establishes a direct and precise correlation between local interfacial characteristics and global physical properties. The first results on the implementation of a computational workflow integrating high performance computing (HPC) with GINS experiment via an intuitive, cross-platform user interface is being developed at SNS/ORNL and will be presented [3]. Work supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, and the US Department of Energy, by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory.

[1] From Quanta to the Continuum: Opportunities for Mesoscale Science, a report from the Basic Energy Sciences Advisory Committee (2012) http://science.energy.gov/~/media/bes/pdf/reports/files/From_Quanta_to_the_Continuum_rpt.pdf
[2] V. Lauter, H.J.C. Lauter, A. Glavic, B. Toperverg, book chapter in Reference Module Material Science Elsevier, 2016
[3] Mahalik J.P., Dugger J.W., Sides S.W., Sumpter B.G., Lauter V.V., Kumar R., "Interpreting Neutron Reflectivity Profiles of Diblock Copolymer Nanocomposite Thin Films Using Hybrid Particle-Field Simulations", *Macromolecules,* **51,** 8, 3116–3125 (2018)

A04.03.03
Super-Resolution in Real and Reciprocal Spaces
Jiao Y. Lin[1,2], Garrett E. Granroth[2], Fahima Islam[2], Richard Archibald[2], Gabriele Sala[2], Douglas L. Abernathy[2], Matthew Stone[2], Iyad Al-Qasir[2] and Anne Campbell[2]; [1]Satelytics Inc, United States; [2]Oak Ridge National Laboratory, United States

Super resolution techniques, popularized as magical through television dramas, are now ubiquitous in modern digital cameras and cell phones. In scientific research, super-resolution (SR) techniques have revolutionized fields such as fluorescence microscopy and biology, and new SR techniques continue to be invented for and applied in real-space imaging instruments. In this talk, recent applications of super-resolution techniques in **reciprocal-space** imaging of quantum excitations by neutron scattering spectrometers will be presented, along with relevant **real-space** SR imaging techniques. Neutron spectroscopy is a tool of choice for studying exotic magnetic and vibrational excitations in solids. Direct Geometry Spectrometers (DGS) at spallation neutron sources allow the collection of massive datasets, but the quantum excitations are obscured by asymmetric instrument broadening that varies in the dynamic range of measurement. Clearly resolving fine features in the excitation spectra of novel materials is a long-standing challenge that pushes the limit of DGS. In this presentation, we will discuss two super-resolution techniques recently in development for DGS spectroscopy. Multi-frame super-resolution imagery principles and techniques were found applicable to DGS data, and 5X resolution enhancements were achieved in measurement of phonon density of states, a reduced representation of vibrational property of condensed matter. The second technique was inspired by image correlation techniques crucial for stereo imaging or 3D reconstruction. It was adapted to tackle the problem of constraining spin-wave models, a routine challenge in understanding neutron scattering data for magnetic materials. These developments may impact designs of future generation of neutron instruments.

A04.03.05
NeXpy—A GUI Toolbox for Analyzing Neutron Scattering Data
Raymond Osborn; Argonne National Laboratory, United States

NeXpy is a GUI application designed to facilitate creating, reading, visualizing, and manipulating neutron and x-ray scattering data stored in NeXus files (https://nexpy.github.io/nexpy/). Files that are loaded into NeXpy can be inspected in a hierarchical tree view and plotted in Matplotlib windows with GUI control of features such as color maps, data smoothing, plot legends, and skewed axes. Arbitrary 1D and 2D slices and projections through multidimensional data sets are easily plotted, with limits that can be synchronized across multiple files for detailed comparisons. Projections can also be made of data stored in multiple files as a function of a parametric variable such as temperature or pressure. An intuitive Python API, accessible from a built-in Jupyter shell, allows the file contents to be accessed, fitted, modified, and saved as NeXus data without a detailed knowledge of the NeXus format. A built-in script editor facilitates both data analysis and algorithm development within an integrated environment, and a plug-in architecture allows new functions to be added to NeXpy menus for specialized applications. The goal of NeXpy is to provide neutron and x-ray scattering scientists with tools that enable new data analysis methods to be explored and implemented rapidly without the learning curve of more elaborate frameworks, such as Mantid. Work supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division

SESSION A05.01: Imaging, Tomography and Residual Stress

A05.01.01
A Multi-Wavelength Neutron Monochromator for Measurements of Stress and Texture
Thomas Gnaupel-Herold[1] and El'ad Caspi[1,2]; [1]National Institute of Standards and Technology, United States; [2]Nuclear Research Centre, Israel

A novel triple-wavelength monochromator is presented. The device consists of stacks of thin silicon wafer blades with orientations [400], [311], and [422]. The horizontal curvature is variable to allow optimization of the figure of merit (FM) at different take-off angles. The vertical curvature is fixed. Furthermore, the crystals have a common [011] zone axis that make double reflections possible which produce wavelength combinations of the type $\text{lamda}_{Si400}+\text{lamda}_{Si311}$, $\text{lamda}_{Si400}+\text{lamda}_{Si422}$ or $\text{lamda}_{Si422}+\text{lamda}_{Si311}$. The purpose of the device is to map several diffraction peaks into a narrow angular window (Delta-2th<15°) without peak overlap. This works particularly well for materials of cubic or hexagonal crystal symmetry that also represent a large majority of samples investigated for stress or texture. The primary benefits are increased sample throughput for texture measurements and smaller uncertainties in stress measurements.

A05.01.04
Neutron Radiography Capabilities at LANSCE
Danielle Schaper, Alexander Long and Sven C. Vogel; Los Alamos National Laboratory, United States

Due to the nature through which neutrons interact with materials, neutron radiography offers a powerful non-destructive probe that often is complementary to similar probes with x-ray and charged particle radiography. In this talk, we will present a broad picture of the current neutron radiography capabilities at the Los Alamos Neutron Science Center (LANSCE), ranging from those measurements done at the Energy Resolved Neutron Imaging (ERNI) beamline to fast-neutron radiography done at the Flight Path 60 Right (FP60R) beamline. Specifically, we will discuss how ERNI measurements can be used to characterize nuclear materials for possible future (Gen. IV) reactor designs and how fast neutrons can be used to test and characterize newly-developed scintillator materials.

A05.01.06
Neutron Dark Field Imaging with a Far Field Interferometer

Daniel S. Hussey, Kathleen M. Weigandt, Paul Kienzle, David Jacobson, Ryan P. Murphy, Jacob M. LaManna, Victoria DiStefano, Peter Bajcsy, Michael G. Huber, Liya Yu and Nikolai Klimov; National Institute of Standards and Technology, United States

Neutron dark field imaging opens the possibility to access structural features in the nanometer range in a neutron image that has spatial resolution of >50 μm. Specifically, dark field images are a measure of the pair correlation function at an autocorrelation length ξ, where $\xi = \lambda z / Pd$, with λ the wavelength, z the sample to detector distance, and Pd the period of the interference pattern. An advantage of the far field interferometer geometry is that Pd is linearly related to the separation of the two phase gratings generating the interference pattern. Thus, it is possible to change Pd by orders of magnitude, and hence scan ξ by order of magnitude while keeping the distance between the detector and sample fixed. Combined with the ability to obtain tomography, dark field imaging with a far field interferometer opens the possibility of three-dimensional, multi-scale data sets, where each voxel of order 50 μm contains a pair correlation function over the range of about 1 nm to 1 μm. For this reason, NIST is developing the far field interferometer as a potential new user instrument. In this presentation, we report on our initial efforts to reduce the data acquisition time and improve the data quality through higher interference pattern visibility produced by newly fabricated phase gratings.

A05.01.07
Algorithms for Neutron Scattering Tomography
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Neutron scattering measurements are sensitive to sample features that are much smaller than the achievable resolution of neutron position sensitive detectors. While scattering experiments typically do not provide a real space picture of the sample, we show that passing neutron diffraction patterns through phase recovery algorithms recovers the real space phase of the neutron wave. This phase is then related to the projection of the neutron ray through the sample, and by measuring diffraction patterns as a function of sample rotation, it is possible to perform computed tomography on the recovered phase sinogram. Demonstrations will be presented for two-dimensional reconstructions of phase and absorption gratings using double crystal diffractometer (USANS) datasets, as well as three dimensional reconstructions of magnetization spin textures using diffraction measured in the far field (SANS). The grating shapes are successfully recovered by the reconstructions, and unique information about the evolution of the spin textures in the sample bulk is decimated. Implementation of physical assumptions about the sample in the reconstruction algorithm, the importance of building validation datasets, and extension of the algorithm class to other sample types will be discussed.

Poster Session: Advances in Neutron Facilities, Instrumentation and Software

PA.01.02
Incident Optics Design for the MANTA Instrument at HFIR
Garrett E. Granroth[1], Marcus Daum[2,1], Barry Winn[1], Lee Robertson[1], Adam Aczel[1], Jaime Fernandez-Baca[1], Martin Mourigal[2] and Mark L. Lumsden[1]; [1]Oak Ridge National Laboratory, United States; [2]Georgia Institute of Technology, United States

A new Multi analyzer triple axis (MANTA) spectrometer is under development for the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory (ORNL). The existing building places tight constraints on the position of the beamline. Which make the optics design a unique and interesting challenge. The instrument specific optics starts once the guides for all of the cold source instrument separate downstream of the cold source. The MANTA guide then curves in the horizontal to thread two openings in the bunker that ensures that instrument will be out of line-of-sight to the core. In the vertical direction the direct beam path is upwards so the guide curves in order to bring the guide to the level. Between the two fixed points in the bunker, an elliptically focusing guide transports the neutrons to a virtual source 1.4m upstream of a double focusing monochromator. The position of the beginning of the elliptic focusing is controlled by ensuring that the cross section of the beam is smaller than a neutron velocity selector that is placed just downstream of the second bunker opening and by the placement of the focal point which is controlled by the space available for the sample table and the multi analyzer backend. In the vertical and after the neutron velocity selector the guide is a diverging guide to provide a less divergent beam incident on the monochromator. The double focusing monochromator is pyrolytic graphite and follows a traditional focusing method in the vertical and uses a Rowland Geometry in the horizontal. The 1.4m focal distance was chosen so that a minimum incident energy of 2.5meV could be accessed. The process of determining this guide configuration and focal distance will be presented and the expected performance of such a configuration will be given. This work was performed at ORNL under contract number DE-AC05-00OR22725 for USDOE. MD acknowledges the support of the USDOE Office of Science Graduate Student Research Fellowship.

PA.01.03
High Temperature Sample Environments for Neutron Scattering at ORNL

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Oak Ridge National Laboratory houses two world-leading neutron scattering facilities which boast many different instrument suites. The sample environment group supports these instruments by providing many different types of equipment, we will overview the high temperature program and capabilities available at these facilities for example: High temperature air and vacuum furnaces, high temperature closed cycle refrigerator systems, and levitator systems that can heat samples up to 2000^{o} C. In addition to existing equipment, the high temperature sample environment is continually developing new capabilities to keep up with the growing scientific needs through new equipment and technique development.

PA.01.06
The Halbach Ring for Alliance of Magnetism and Soft-Matter

Valeria Lauter, Timothy R. Charlton, John Katsaras, Mathieu Doucet, T. N. Lamichhane and Parans Paranthaman; Oak Ridge National Laboratory, United States

Neutron scattering experiments measure structure factor amplitudes in reciprocal space. In reflectometry the inversion of reciprocal space data to a unique real space scattering length density (SLD) profile requires information on the phase of the complex reflection amplitude – a quantity that is lost during scattering. In addition, experimental background may further limit the scope of the data that can be used for analysis. All these factors contribute to a situation where extracting a scattering length density (SLD) profile becomes non-trivial. In particular this problem may be amplified in the case of biological (bio-membranes) and soft-matter (polymer) samples that may possess intrinsically low neutron contrast. For a broad class of non-ferromagnetic materials, this problem can be solved using a direct inversion procedure proposed in Refs. [1,2] that requires a polarized neutron beam and a sample with an additional magnetic reference layer. Thus, using a ferromagnetic reference layer (i.e. Co saturated in-plane) two SLD (for reflectivity with spin-up R+ and spin-down R-) are obtained. A third value that corresponds to the non-magnetic SLD can be obtained from a demagnetized layer (that is difficult to control) or magnetized perpendicular to the plane of the film. To achieve this a magnet capable of saturating the magnetic reference layer, both in and out of the plane of the sample is needed. Moreover, in cases where the confidence interval of the SLD profile is such that a structural feature cannot be resolved, we can obtain a series of different contrast data sets by magnetizing the reference layer at different angles with respect to the sample normal. This way of varying neutron contrast is less complicated than the current state of the art used for bio-membrane and other soft matter studies that make use of different H_2O/ D_2O mixtures, where the exchange of H_2O/D_2O is never perfect and in some cases, may destroy the delicate samples adsorbed to the substrate. Recently we started development of a novel prototype Halbach ring magnet for the Magnetism Reflectometer at the SNS using ORNL's unique ability to additively manufacture permanent magnets. First results are presented. Upon completion of this project the ability to directly invert reciprocal space data into real space structures will become available for practical application in reflectometry experiments. Work supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, and the US Department of Energy, by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory. E-mail of the corresponding author: lauterv@ornl.gov

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PA.01.07
Sample Area Shielding on TAX/HB3 at HFIR
Songxue Chi, Jonathan Smith, Michael Cox, Daniel M. Pajerowski, Travis J. Williams and Jaime Fernandez-Baca; Oak Ridge National Laboratory, United States

HB-3 is a thermal neutron triple-axis spectrometer (TAS) known for its high neutron flux. Unfortunately, this strength also leads to high radiological and neutronic background. To mitigate this situation, we've investigated a few solutions including the sample area shielding, which was recently installed on HB3. It consists of omega-shaped track around the sample position whose open ends extend toward the monochromator drum. Two trains of linked shielding pieces are fixed to a window on the analyzer arm to follow the beam path downstream the sample. I will discuss its design, the shielding materials and the test results.

PA.01.08
Inelastic Neutron Scattering and Ultrasound Studies of Lattice Dynamics in Bismuth-Antimony
James Torres, Victor Fanelli, Andrew May, Michael E. Manley, Barry Winn, Alexander I. Kolesnikov and Raphael P. Hermann; Oak Ridge National Laboratory, United States

Over the last few decades, semimetals such as bismuth, antimony, and their alloys have driven many theoretical and experimental investigations to understand how their electronic properties can be tuned via composition, temperature, pressure, and magnetic field [1]. In particular, $Bi_{1-x}Sb_x$ alloys provide access to the topologically insulating state at ambient conditions [2], and the $Bi_{0.89}Sb_{0.11}$ alloy is a promising candidate to study Weyl fermions experimentally [3]. In this context, we performed inelastic neutron scattering and resonant ultrasound spectroscopy (RUS) measurements to understand how the lattice dynamics of $Bi_{0.89}Sb_{0.11}$ is affected by its topology through electron-phonon coupling. We observe evidence of a phase transition at low temperatures and moderate magnetic field of a few tesla applied along the trigonal direction of the crystal in the ultrasonic response. Future work is planned to integrate RUS – a highly sensitive probe of elastic moduli – into neutron beamlines at Oak Ridge National Laboratory to precisely locate and characterize transitions *in situ* and provide a live and intrinsic state variable for the samples.

Acknowledgements:
This work is sponsored in part by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy. We thank D. Vu, J. Heremans and colleagues at Ohio State University for providing the sample and foundations for this work.

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PA.01.10
3D Scanning and 3D Printing Single Crystal Mounts for Neutron Scattering
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We present methods to quantify sample shapes and generate sample mounts, as motivated by needs of neutron scattering experiments. Sample scanning was performed using photogrammetry and laser scanning. Parts were first prototyped with 3D plastic printers, and then 3D AlSi10Mg prints. The final part holds the sample with more points of contact than is possible with traditional manufacturing, and the goodness of fit between mount and sample was measured with X-ray tomography. We show AlSi10Mg to have favorable properties for many types of neutron mounts.

PA.01.11
Additive Manufactured B_4C Scattered Beam Collimation for Diamond Anvil Pressure Cells
David C. Anderson, Fahima Islam, Corson Cramer, Desarae Goldsby, Derek Siddel, Amy Elliott, James Kiggins, Bianca Haberl, Jamie J. Molaison and Garrett E. Granroth; Oak Ridge National Laboratory, United States

A neutron collimator for use with Diamond Anvil Cells at the SNAP high pressure instrument at Oak Ridge National Laboratory's (ORNL) Spallation

Neutron Source (SNS) was collaboratively designed using material and geometrical optimization techniques by a group of ORNL engineers, scientists and technicians. Material characteristics such as the size and shape of B_4C powder were optimized for the 3D printing process. Geometric effects on manufacturability were studied by iteratively examining the relationship between the ratio of absorber size to opening size. The desired overall size of the collimator was achieved by assembling the collimator from 5 pieces and designing novel ways of minimizing error by including features to desensitize optimal collimating performance of the part against the physical constraints of the printer's available build volume, as well as any possible manufacturing deviations resulting from the behavior of the green part during the powder bed removal process and thermal deformation during binder curing. These potential variations from the nominal design of the collimator were also minimized by tuning the manufacturing parameters of the printer. Furthermore we investigated the benefits of infiltrating the material with Al as compared to superglue. The optimization process included not only finding the best channel width and length to maximize the signal to noise ratio, but also ensuring it still worked with blades removed in downstream and intermediate sections to avoid mismatch at boundaries. This work will describe the details of both the materials optimization and the geometrical optimization. This work is supported by the Laboratory Director's Research and Development Fund of Oak Ridge National Laboratory, An US DOE Laboratory.

PA.01.13

Compact Force-Amplified Pneumatic Remote Pressure Control Mechanism for Neutron High-Pressure Diamond Anvil Cell and Top-Loading Cryostats

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A large number of physical phenomena, such as superconductivity and quantum critical phenomena, often appear only at very low temperatures below 5 K. There is an immense interest to investigate these phenomena at high pressure as a means of tuning interatomic distances, and thus the interaction parameters controlling these phenomena, in a continuous and controlled fashion. The simultaneous generation of high pressure and ultra-low temperatures is highly desirable in neutron scattering, but achieving multi-gigapascal pressures in this regime remains extremely challenging. Generally, the current P-T conditions for neutron scattering experiments are limited to either relatively low pressures of about 2 GPa at temperatures below 5 K, or to relatively high temperatures at pressures of tens of GPa. The ability to reach 10-20 GPa at 1-2K and having the ability to control pressure rapidly and reliably online (i.e. without having to interrupt the experiment and while minimizing setup and sample alignment time) is critical for understanding the behavior of quantum and other multifunctional materials at such extreme conditions. A number of relatively large-volume Diamond Anvil Cells (DACs) for high-pressure neutron scattering have been recently developed at ORNL (Boehler et., 2013; Haberl et al, 2017; Boehler et al., 2017). Moreover these DACs can be combined with pneumatic devices for accurate remote pressure control during the experiments. Nevertheless the existing pneumatic attachments for generating sufficient load of 10-12 tons are massive and very large (> 120 mm OD), which prevents using the DACs with remote pressure control in top loading cryostats which can reach temperatures below 4K and have a bore diameter of 100 mm or smaller. Here we present the novel compact force-amplified pneumatic pressure control mechanism for neutron DACs, which allows accurate remote pressure control in the DACs inside a top-loading cryostat with bore size of 70 mm or larger. The pressurizing device (attachment to DACs) has an outside diameter of less than 69 mm and consists of pneumatic bellows and a lever arm force amplifier. The bellows with 58mm effective diameter can generate the force of 4 tons using standard He tank gas pressure of ~150 bar. The three lever arms further amplify the force by about 3 times resulting in a total generated remotely controllable load of up to 12 tons, which is sufficient to generate pressure in neutron DACs in the order of 20-100 GPa (depending on diamond type and anvil culet size). The new development represents a break-through in remote pressure control in DACs and has very strong potential for expanding experimental capabilities in high-pressure materials sciences, including neutron scattering at extreme conditions.

This development is based upon work supported by the U.S. DoE, Office of Science, SBIR Phase I program under Award Number DE-SC-0019678.

PA.01.17
Predictive Model of Charge Mobilities in Organic Semiconductor Small Molecules with Force-Matched Potentials
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The effects of local dynamic disorder on the ultimate performance limit of organic semiconductors (OSC) is poorly understood. In this regard, the density functional tight binding (DFTB) semi-empirical, quantum mechanical method holds promise as a computationally efficient screening tool for local disorder and charge mobility in candidate OSC materials. Here, we show that force matching a many-body interaction potential to Density Functional Theory (DFT) molecular dynamics data yields highly accurate DFTB models capable of reproducing the low-frequency modes measured by inelastic neutron scattering. Application of this DFTB model, Chebyshev Interaction Model for Efficient Simulations (ChIMES), requires several orders of magnitude fewer computational resources than DFT calculations while largely retaining accuracy, allowing for a broader exploration of materials and conditions than previously possible. We have subsequently determined charge mobilities from our model for a number of previously unstudied OSC molecules using transient localization theory. The approach we establish here could provide synthetic parameters to design the next generation of OSC with tailored properties for industrial applications.

PA.01.19
Status of the ^{3}He NSF Program at the NCNR
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^{3}He neutron spin filters (NSFs) are an integral part of the NIST Center for Neutron Research (NCNR) as the program continues to improve NSF performance on current instruments, such as the Small Angle Neutron Scattering (SANS) and Thermal Axis Spectrometer (TAS) instruments. Due to improvements in polarized neutronic performance, neutron spin transport, and minimization of ^{3}He polarization loss occurred during the adiabatic fast passage (AFP) NMR based ^{3}He polarization inversion, employment of a GE180 toroid cell has led to significant scientific from the Multi-Angle Crystal Spectrometer (MACS). The use of NSFs at the NCNR have already been expanded to the Very Small Angle Neutron Scattering (VSANS) instrument. Implementation of ^{3}He NSFs on the Chromatic Analysis Neutron Diffractometer Or Reflectometer (CANDOR) using a new magnetostatic cavity developed specifically for this instrument will occur in the near future.

PA.01.20
Wavelength Dependent Neutron Transmission of Aluminum Infiltrated Boron Carbide
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We examine a series of additively manufactured boron carbide samples that have been infiltrated with a matrix of aluminum. Samples were produced from aluminum infiltrated additive manufactured boron carbide, (B_4C). Samples were approximately 5 cm by 5 cm in area with thicknesses of 0.5, 1.0, 1.5, 2.0, and 2.5 mm. We examine the transmission and scattering as a function of wavelength and sample thickness. We find that the wavelength dependent neutron transmission for 0.5 mm thick samples compares well to traditional stretched films coated with enriched boron carbide.

PA.01.21
New Dilution Refrigerator Capability for SANS Instruments at NCNR
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Many materials science neutron experiments at NCNR, and other neutron scattering facilities around the world, require ultra-low temperatures. Small Angle Neutron Scattering (SANS) instruments have very rigid requirements for the sample environment. Materials in the neutron beam must be “transparent” to neutrons otherwise they will produce too much background. At NCNR we are developing the sample environment for ultra-low temperature measurements at SANS instruments. 50mK has been reached using the standard dil fridge insert's inner vacuum chamger (IVC) in the SANS orange cryostat (OC). What is left is the testing with the single crystal silicon IVC. We are showing the designs of the orange cryostat's single crystal silicon VTI tail and the IVC for the dilution refrigerator insert. The designs have almost no aluminum (less than a few micron) in the neutron beam and a wide angle for neutron scattering so the scientists can acquire high Q data.

PA.01.22

Experimental Design and Information Content in Neutron Reflectometry

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Access to large-scale neutron scattering facilities is limited and making effective use of the awarded experiment time can be essential for the successful completion of a research project. When designing a neutron scattering experiment one seeks to ensure that the measurement is sensitive to features of interest and that it is carried out in the shortest amount of time needed to reach a desired significance level. Highlighting parts of the structure by isotopic labeling is a common strategy in neutron scattering to achieve this goal, as is embedding elements of known composition and structure within the sample and choosing a suitable instrument configuration and measurement scheme. While there is a great flexibility in designing a neutron scattering experiment, a quantitative measure for assessing which implementation maximizes the gain in information has been lacking and the community largely follows empirical best-practices. We have introduced a quantitative framework to determine the gain in information from neutron reflectometry (NR) experiments using information theory and Bayesian statistics [1]. The information gain is computed as the difference in entropy between the posterior and prior parameter distributions from a model-fit to reflectivity data from virtual experiments. This measure of information gain is used as a tool for experimental optimization. We implemented marginalization of the entropy with respect to a subset of model parameters, which allows to optimize the experimental design with respect to parameters of interest to the experimenter. By describing the entire measurement process as an information theoretical problem, fundamental insights into why certain designs are more effective are accessible. We have first applied this framework to fundamental optimization problems in the design of NR experiments involving test structures and biomimetic model membranes. We determined optimal measurement times and maximum momentum transfer values. We investigated the optimum number and type of bulk solvent contrast when measuring fluid-immersed samples, and the utility of buried (magnetic) substrate layers with high scattering length density for increasing the amplitude of the reflectivity and for direct inversion of the reflectivity data. We have further taken a detailed look at the optimum combination of scattering contrasts within biological surface architectures [2]. While our results in many cases confirm existing best-practices, they also provide surprising insights into when they are ineffective.

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