ORNL Second Target Station Instrument Introduction

The Second Target Station (STS) at Oak Ridge National Laboratory's (ORNL) Spallation Neutron Source (SNS) will provide transformative new capabilities for discovery science, enabling breakthroughs in many areas of materials research and development, including polymers, quantum matter, biotechnologies, structural materials, and energy storage.

The STS Instrument Systems group will construct eight world-class instruments, as listed herein, ready to transition to operations and begin commissioning by the end of the project. STS will provide unique capabilities for experiments that require:

- Time-resolved measurements of kinetic processes and beyond-equilibrium matter
- Simultaneous measurements of hierarchical architectures from the atomic scale to microns and beyond
- Measuring small samples of newly discovered or synthesized materials
- Examining new frontiers in materials at extreme conditions

The STS will have capacity for 22 beamlines that will complement those at the SNS First Target Station (FTS) and the High Flux Isotope Reactor (HFIR). An instrument selection process took place between August 2020 and July 2021 to select the eight instruments that will be constructed as part of the STS project. The user community submitted 12 instrument proposals, which were then evaluated using the process described in the Selection Process for Second Target Station Project Instruments. As part of this process, instrument proposals were evaluated by an external instrument review committee based on defined criteria, including scientific impact, relevance to the user community, compatibility with the STS facility's unique capabilities, as well as quality and feasibility of the instrument concept. The committee then submitted recommendations to the STS project and Neutron Sciences Directorate (NScD) management.

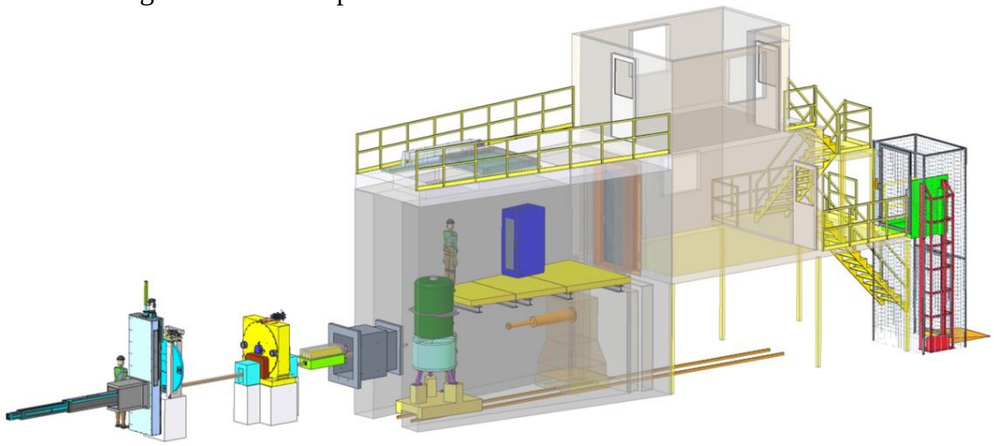
The eight instruments selected to be constructed as part of the STS project are here in alphabetical order.

STS Instrument

BWAVES
CENTAUR
CHESS
CUPI^{2}D
EXPANSE
PIONEER
QIKR
VERDI

BWAVES

Time-of-Flight Broadband Spectrometer



CONTACT

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DESCRIPTION

BWAVES (Broadband Wide-Angle VElocity Selector spectrometer), is a neutron spectrometer that can select the velocity (that is, the wavelength) of detected neutrons after they are scattered by a sample. It is the first inverted geometry spectrometer where the energy of detected neutrons can be chosen mechanically by a wide-angle velocity selector, irrespective of limitations imposed by crystal analyzers or filters.

BWAVES will serve as a gateway (and often as the one-stop) spectrometer for neutron scattering studies of dynamics in a broad range of materials, in the same manner as the SANS and neutron diffraction instruments serve as gateways for structural studies.

BWAVES features and capabilities will include:

- A dynamic range spanning 4.5 decades and covering energy transfers from ~0.010 meV to above 500 meV.
- The capability to characterize relaxational excitations gradually emerging as a function of temperature, or other thermodynamic variables, to efficiently decipher complex dynamic landscapes.
- A small beam size to study very small samples (a few microliters in volume) and facilitate the use of small, advanced sample environment equipment.
- A unique open-tabletop sample geometry to provide easy access to the sample when applying multimodal external stimuli, including default optical access to the sample.
- A novel WAVES rotor and capability to integrate different sets of STS source characteristics, such as frequency, cold neutrons, high brightness, compact moderators.

APPLICATIONS

BWAVES will be optimized for bioscience and chemical science, as well as for studying novel materials such as for energy applications, novel soft matter such as recyclable polymers, and for better understanding the biological processes in emerging biotechnologies and medical technologies. It will also enable measurements of both vibrational and relaxational excitations within the same continuous scattering spectra. The small beam size of 5 mm by 5 mm will enable studies of the samples of only a few microliters in volume, critical for measurements of hard-to-synthesize samples and for the use of advanced sample environment equipment. Further, the open geometry access will allow convenient simultaneous application of multimodal techniques to the sample. With truly outstanding characteristics and no analogues worldwide, BWAVES will serve as the gateway (and oftentimes the final stop) for neutron scattering studies of dynamics in materials over the broadest possible range.

EXPECTED SPECIFICATIONS

Table of standard operation parameters (not using a higher energy resolution booster mode).

Energy resolution at the elastic line	0.020 meV, FWHM
Neutron beam size	~ 5 mm by 5 mm
Maximum energy transfer	~ 1000 meV
Inelastic energy resolution, ΔE/E	2.0-2.5% up to 60 meV, 3.0-4.5% up to 250 meV
Momentum transfer at the elastic line	0.2 $Å^{-1}$ - 0.8 $Å^{-1}$
Maximum momentum transfer	~ 20 $Å^{-1}$
Momentum transfer resolution at the elastic line	~ 0.1 $Å^{-1}$

EXAMPLES FOR BER-RELATED RESEARCH

Supported lipid assemblies: C. L. Armstrong, M. D. Kaye, M. Zamponi, E. Mamontov, M. Tyagi, T. Jenkins, M. C. Rheinstadter, Diffusion in single supported lipid bilayers studied by quasi-elastic neutron scattering, Soft Matter **6**, 5864 (2010).

Lipid vesicles: V. K. Sharma, E. Mamontov, D. B. Anunciado, H. O'Neill, V. Urban, Nanoscopic dynamics of phospholipid in unilamellar vesicles: Effect of gel to fluid phase transition, J. Phys. Chem. B **119**, 4460 (2015).

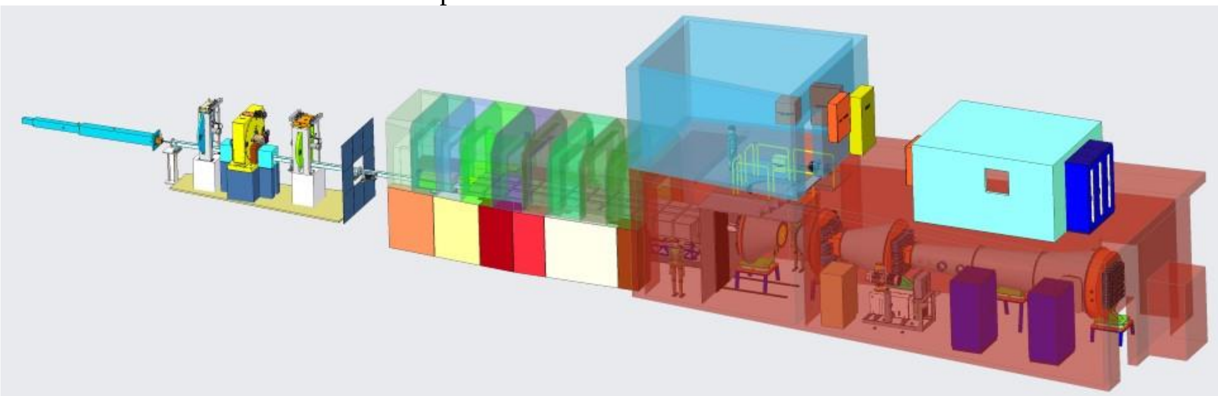
Intracellular protein dynamics: D. B. Anunciado, V. P. Nyugen, G. B. Hurst, M. J. Doktycz, V. Urban, P. Langan, E. Mamontov, H. O'Neill, *In vivo* protein dynamics on the nanometer length scale and nanosecond time scale, J. Phys. Chem. Lett. **8**, 1899 (2017).

Lipoprotein particles: M. Golub, B. Lehofer, N. Martinez, J. Ollivier, J. Kohlbrecher, R. Prassl, J. Peters, High hydrostatic pressure specifically affects molecular dynamics and shape of low-density lipoprotein particles, Sci. Rep. **7**, 46034 (2017).

Molecular-level dynamics in microbes: M. Salvador-Castell, M. Golub, N. Martinez, J. Ollivier, J. Peters, P. Oger, The first study on the impact of osmolytes in whole cells of high temperature-adapted microorganisms, Soft Matter **15**, 8381 (2019).

CENTAUR

SANS / WANS Diffractometer and Spectrometer



CONTACT

Shuo Qian qians@ornl.gov STS Instrument Scientist

DESCRIPTION

CENTAUR will be a small- and wide-angle neutron scattering (SANS/WANS) instrument with diffraction and spectroscopic capabilities to simultaneously probe time-resolved atomic- to meso-scale structures in hierarchical systems under in situ or in operando conditions. Simultaneous WANS and diffraction capabilities will be a unique capability among neutron scattering instruments in the United States.
Its direct geometry spectrometer mode will extend momentum transfer and energy transfer to a lower Q and provide a unique capability for inelastic SANS studies.

- **High-performance, optimized SANS/WANS.** The minimum Q is similar to main-stream SANS instruments ~ 0.001 $Å^{-1}$. The divergence on sample is adjustable for different experiments.
- **Diffraction capability.** Up to 20 $Å^{-1}$ simultaneously with SANS, bridging atomic- to meso-scale structures
- **Direct geometry spectrometer capability.** A removable high-speed monochromatic chopper near the sample position provides a unique inelastic SANS capability for incident energy 0.5- 500 meV
- **Polarization neutron analysis.** Up to 0.3 $Å^{-1}$
- **User-friendly sample environment.** Walk-in sample space, simplified sample environment device change, and a wide range of sample environments: SANS sample cells, automatic sample changers, automatic inline flow cell, liquid handling robot, temperature/pressure/humidity control, flow-through size-exclusion chromatography, stroboscopic sample environment capability, other in situ cells as needed, such as strain and shear; closed-cycle refrigerators, and low-temperature cryostats, such as helium-3 and dilution refrigerators, and magnets

APPLICATIONS

The instrument will provide much needed capabilities in soft matter and polymer sciences, geology, biology, quantum condensed matter, and other materials sciences that need in situ and in operando experiments for kinetic and/or out-of-equilibrium studies. Beam polarization and a high-resolution chopper will enable detailed structural and dynamical investigations of magnetic and quantum materials. The instrument's excellent resolution will make it ideal for low-angle diffraction studies of highly ordered large-scale structures, such as skyrmions, shear-induced ordering in colloids, and biomembranes.

Soft Matter

Examples include polymers, colloids, micelles, complex fluids, gels and blends, and microemulsions

Material Sciences

Additive manufacturing, metallurgical alloys, advanced composites, and porous materials

Geosciences

Soils and Earth formation rocks; planetary and meteorite geoscience

Biological Systems

Biomacromolecules such as proteins, RNA/DNA, lipids and their multi-component complexes; intrinsically disordered proteins (IDPs) and regions (IDRs), liquid-liquid phase separations, and biopharmaceuticals

Quantum Condensed Matter

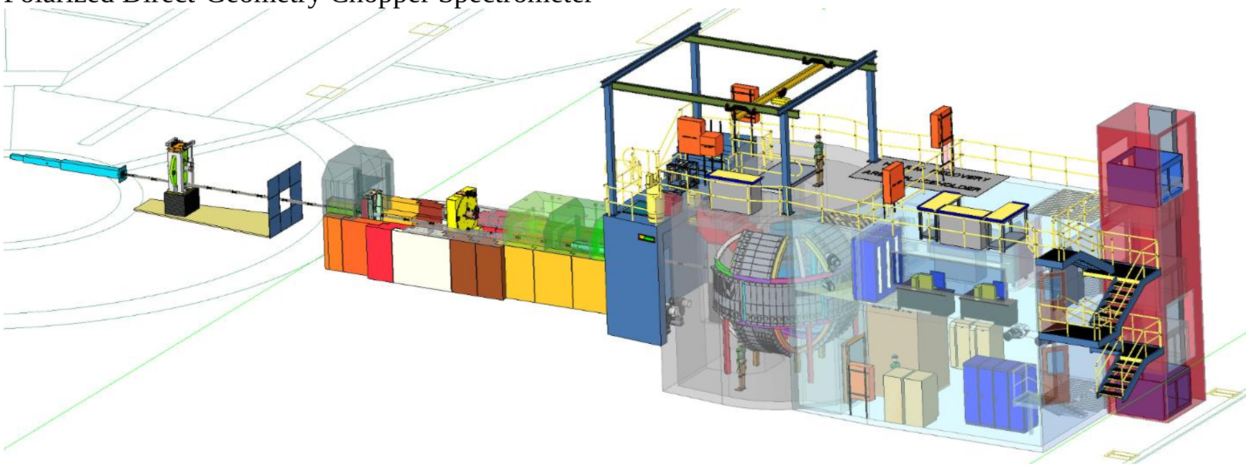
Spin texture, skyrmion, vortex lattices, Brillouin scattering, and magnetic domains

EXPECTED SPECIFICATIONS

Sample size	Typical radius 1–5 mm, other shapes possible with different apertures (e.g., 4×8 mm^2 or smaller); minimum static solution sample in volume ~100 µL;); minimum beam size 1×1 mm^2 for scanning imaging or tomography	
Q range	Maximum dynamic range 0.001–20 $Å^{-1}$ simultaneously. Variable Q range with different flux/divergence settings.	Examples: • Typical solution scattering is 0.002-2.0 $Å^{-1}$ • Typical moderate-ordered sample is 0.001-6 $Å^{-1}$ • Typical diffraction samples is 0.001-20 $Å^{-1}$
Detector coverage	Covers the whole Q range simultaneously without repositioning	
Wavelength bandwidth	7.4 Å (15 Hz), 14.8 Å (7.5 Hz)	
Q resolution ($\Delta Q/Q$)	Forward detectors (small- and wide-angle): < 10% Backscattering detectors (diffraction): < 1%	
Time resolution	>1 second (with moderate scattering samples; integrated flux on sample up to 7.6E8 n/s/cm^2)	
Additional capability	Inelastic SANS spectrometer (incident energy E_i: 0.5-500 meV) Polarized analysis up to 0.3 $Å^{-1}$	

CHESS

Polarized Direct-Geometry Chopper Spectrometer



CONTACT

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DESCRIPTION

CHESS (Complex, Unique and Powerful Imaging Instrument for Dynamics) will be a direct-geometry neutron spectrometer designed to detect and analyze weak signals intrinsic to small cross-sections, such as small mass, small magnetic moments or neutron absorbing materials. The instrument will be optimized to enable studies on quantum materials, spin liquids, thermoelectrics, battery materials, superconductors, and liquids.

Capable of simultaneously measuring dynamic processes over a wide energy range for very small samples, CHESS will be the spectrometer of choice for initial exploration of new materials. Its broad dynamic range will also be well suited for measuring relaxation processes and excitations in soft and biological matter.

The 15 Hz repetition rate of the Second Target Station (STS) will allow using the Repetition Rate Multiplication technique (RRM), which greatly expands the information that can be gained in a single measurement. CHESS will also be designed to employ XYZ polarization analysis.

APPLICATIONS

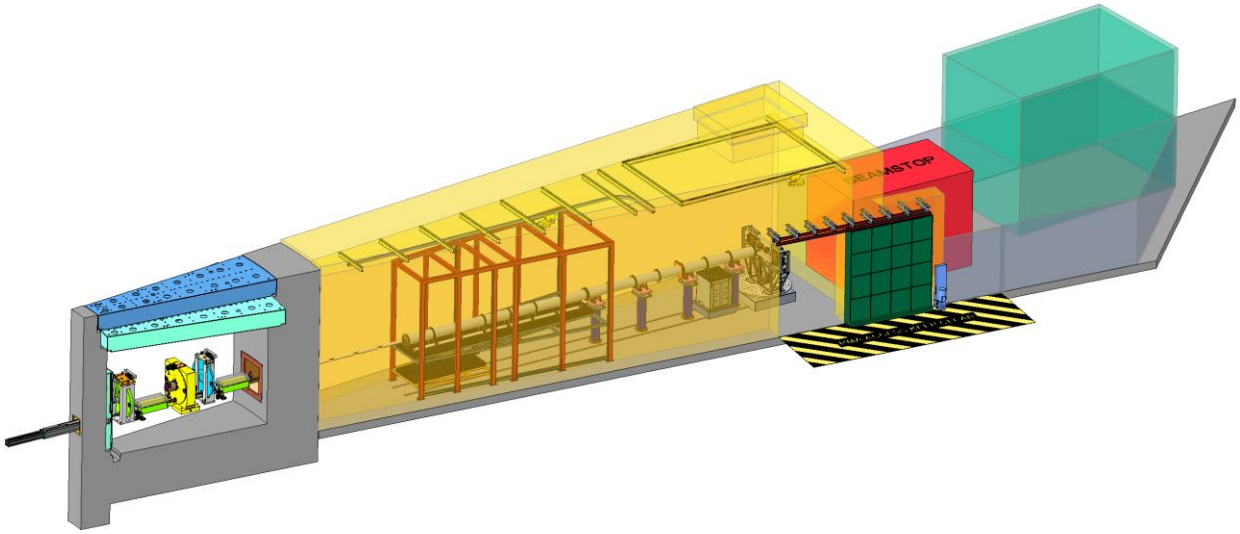
- Collective excitations in single crystals and powder materials such as spin waves, phonons, and unconventional responses
- Exotic ground states in quantum, frustrated, itinerant, and disordered magnets
- Unconventional superconductors, non-Fermi liquids, and quantum criticality
- Molecular magnetism and molecular spin qubits
- Liquids and complex fluids, such as dilute protein solutions, biological gels, and selective absorption of molecules on surfaces
- Dynamics in confined geometries

EXPECTED SPECIFICATIONS

Beam spectrum	Cold neutrons
Moderator	Tube, ST-17
Beam size at sample	Round, variable: ∅ = 0.1-2 cm
Detector solid angle coverage	Ω~2π sr
Incident energy range (ΔE)	$0.2 \leq E_i$/meV ≤ 80 ($1 \leq \lambda$/Å ≤ 20) (RRM capable)
Incident energies per pulse	1 - 8 using RRM mode
Energy transfer resolution at the elastic line ($\delta E/E$)	2%-5% E_i flexible
Total bandwidth ($\Delta\lambda$)	7–8 Å
Q-range (ΔQ)	$0.025 \leq Q$/Å$^{-1} \leq 10$
Q-resolution ($\delta Q/Q$:	2% – 5%
Polarization	Polarized beam and XYZ polarization analysis
Beam divergence at sample	Wavelength independent: FWHM=2.0°
Moderator to M-chopper (L_1)	30 m
M-chopper to sample (L_2)	1.5 m
Sample to detector (L_3)	2.5 m
Detector type	^{3}He tubes, 8-pack

CUPI2D

High-flux, broadband, cold neutron imaging instrument



CONTACT

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DESCRIPTION

CUPI^{2}D (Complex, Unique and Powerful Imaging Instrument for Dynamics) is designed to combine direct and indirect imaging across a broad range of length and time scales. The instrument combines Bragg edge imaging and neutron grating interferometry. CUPI^{2}D is designed for applications that involve length scales from angstroms to micrometers, and time scales from minutes to hours. Leveraging the high flux of cold neutrons from the high-brightness STS cylindrical moderator, CUPI^{2}D permits in situ and in operando experiments.

Samples can be placed at locations from ~18 to ~33 meters from the moderator, with a field of view ranging from ~3x3 cm^2 to ~15x15 cm^2. For measurements at 33 meters, the wavelength bandwidth will be ~8 angstroms, and the wavelength resolution will be ~0.4%.

APPLICATIONS

- Engineering materials
    - Defects in advanced materials, such as additively manufactured alloys
    - Hydrogen embrittlement and crack initiation
    - Degradation and failure mechanisms in critical structures
- Cementitious materials
    - Pore structures
    - Embedded interfaces
    - Phase formation under thermal and mechanical loading
- Nuclear materials
    - Precipitation in light water reactor fuel cladding
    - Microscale and mesoscale defects for advanced reactor materials
- Biology and ecosystems
    - Complex interplay of water, nutrients, and carbon across the rhizosphere
    - Soil aggregation and soil biofilm formation

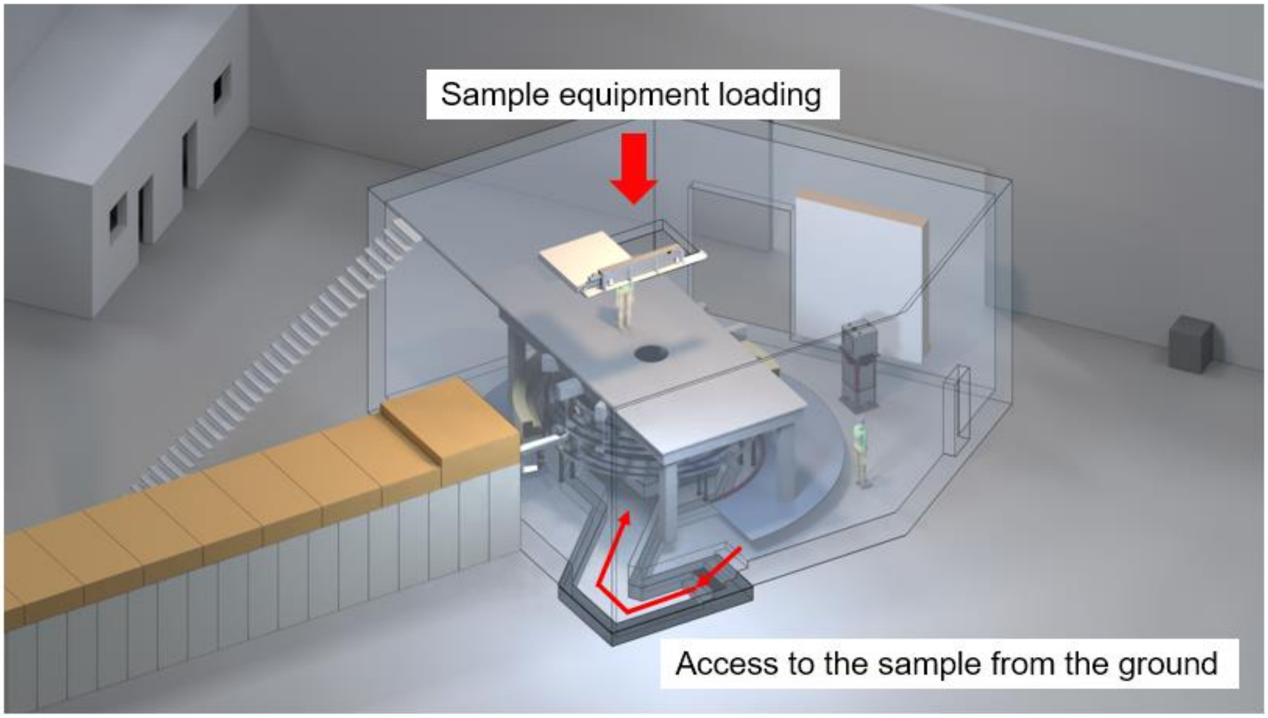
- Medical and dental biomaterials
  - Relationship between bone growth, strain and porosity after restorative surgery
  - Tumor structures, margins, and vascular networks

EXPECTED SPECIFICATIONS

Beam spectrum	Cold, thermal
Moderator	Coupled parahydrogen cylindrical moderator
Wavelength bandwidth	~8Å
Spatial resolution	10 to 100 microns
Resolution Δd/d	~0.4%
Source-to-detector distance	21m to 33m
Sample-to-detector distance	A few mm to tens of cm
Detection system and resolution	Micro-channel plate Timepix4 detectors; cameras (sCMOSs or Timepix camera): down to few microns of spatial resolution
Flux on sample (n/s/cm^2)	1×10^7 to 1×10^9 depending on the L/D setting
Field of View	Up to 15cm × 15cm in 2D imaging

EXPANSE

Neutron Spin Echo with Wide-Angle Coverage



CONTACT

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DESCRIPTION

EXPANSE will incorporate wide-angle detector banks to provide approximately two orders of magnitude in the exchanged wavevector, Q, -range and a wavelength band that can provide about four orders of magnitude in Fourier times. The instrument naturally expands, with good overlap, the dynamic ranges offered by BASIS and NSE at the Spallation Neutron Source (SNS) and CHESS at the Second Target Station (STS) in a wide *Q* range, towards lower energies (slower dynamics). This instrument will provide a unique capability that is not presently available. First, EXPANSE will utilize the wide wavelength bandwidth, $\Delta\lambda \approx 4$ Å, available from STS combined with wide-angle detector modules to enable data collection over a wide momentum transfer range from 0.05 $Å^{-1}$ to 3.14 $Å^{-1}$ and Fourier time range from ~30 ps to ~90 ns in typical operation mode (NSE mode). The wide momentum transfer range (2 orders of magnitude) and Fourier time range (~4 orders of magnitude when two wavelength settings are combined) will enable pair distribution function (PDF) type data analysis by obtaining real space-time correlation function, $G(r, t)$, from Fourier transforming the intermediate scattering function, $I(Q, t)$. The length and time scales covered by EXPANSE are complementary to other QENS techniques. Second, the significantly enhanced source brightness (a factor of ~20 compared to the first target station (FTS)) will enable the possibility of time-resolved spectroscopic experiments or non-equilibrium dynamic studies. The high flux of STS will also enable EXPANSE to measure incoherent dynamics, which is currently challenging because of the inherently low signal to noise ratio in incoherent scattering measurements. Moreover, EXPANSE, with its high detector coverage, will be able to measure efficiently the incoherent scattering signal, which is spread over the whole scattering solid angle.

APPLICATIONS

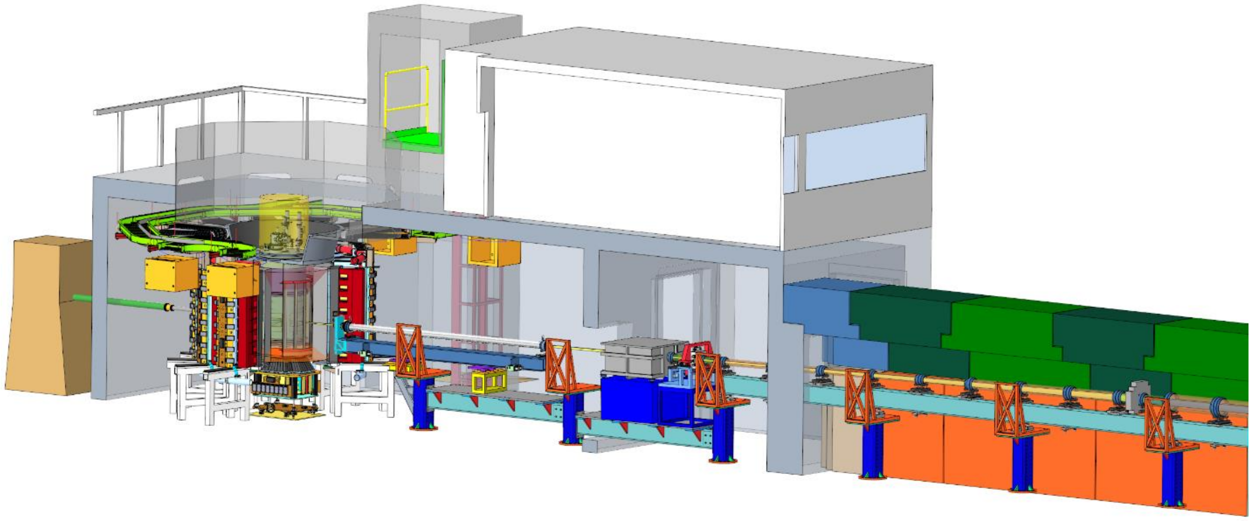
- Membrane, protein dynamics.
- Liquid dynamics
  Example: Luo P., Zhai Y., Falus P., García Sakai V., Hartl M., Kofu M., Nakajima K., Faraone A., Z Y. Q-dependent collective relaxation dynamics of glass-forming liquid Ca0.4K0.6(NO3)1.4 investigated by Nature Communications 13 2092-1-2092-4 2022

EXPECTED SPECIFICATIONS

Property Name	Characteristics
Available wavelength	4 to 16 Å
Wavelength band	~ 4 Å (15 Hz)
Incident beam divergence	< 1.5 º
Maximum field integral	~ 0.27 T·m
Detector solid angle	140º × 2.5º array of ^{3}He tube detectors
Momentum transfer range	0.05 Å^{-1} to 3.14 Å^{-1}
Fourier time range	30 ps to 90 ns (using 4 to 12Å)
Direct geometry mode	Energy resolution 10 μeV to 300 μeV Incident energy range 0.5 meV to 9 meV Corresponds to 0.1 ps to 100 ps

PIONEER

Single-crystal diffractometer with polarization option



CONTACT

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DESCRIPTION

PIONEER is a time-of-flight, single-crystal diffractometer optimized for studying small-volume samples (< 1mm^3) in a range of sample environments, including high/low temperature, magnetic field, and pressure. The instrument will provide world-leading capabilities by reducing sample volume requirements for single-crystal neutron diffraction experiments by more than one order of magnitude, allowing detailed atomic-scale structural characterization of materials at the earliest stages of discovery when large crystals are typically unavailable. PIONEER will be capable of measuring tiny crystals (~ 0.001 mm^3) and ultra-thin epitaxial films (~10 nm thicknesses × 25 mm^2 area). It will also provide a polarized beam option to study weak magnetic scattering signals and support a high-resolution mode to probe large unit cells up to 200 Å. PIONEER will leverage the unique Second Target Station source characteristics of high cold-neutron flux and a small beam footprint with the latest advances in neutron optics, neutron spin manipulation, instrument design, and computational techniques to enable rapid data collection despite small-volume samples and weak signals. Time-of-flight resolution will significantly reduce reflection overlap and lower the background noise. With a 4-Å wavelength band and 4.4-sr detector coverage, PIONEER will measure a broad reciprocal space at a single sample rotation. The 800-mm sample-to-detector distance will provide flexibility in using various sample environments.

APPLICATIONS

- Quantum Materials
  - Unconventional superconductivity
  - 4*d*-5*d* strong spin-orbital coupling systems
  - Topological materials
- Functional materials for energy applications
  - Metal-organic frameworks (MOFs)
  - Polyoxometalates
  - Multiferroic oxides
  - Complex hydrides
  - Thermoelectric materials
- Thin films and artificial heterostructures

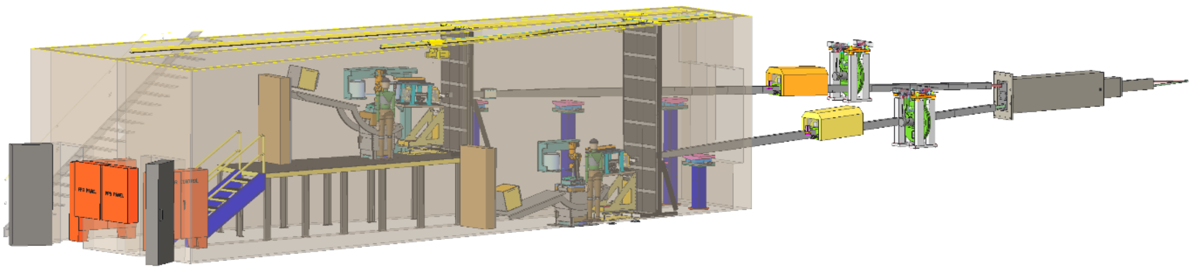
    - Antiferromagnetic spintronics
    - Multiferroics
- Planetary sciences and mineral physics
    - Natural mineral inclusion
- Time-resolved studies
    - Spin relaxation
    - Time-resolved crystallography

EXPECTED SPECIFICATIONS

Moderator	Cylindrical coupled para-H_2 (20 K)
Sample-to-detector distance	0.8 m
Best resolution ΔQ/Q	< 0.3%
Average flux (n cm^{-2} s^{-1}) at 0.7 MW	6.8×10^8 (1.5-5.5 Å, high flux mode)
Beam size (square)	0.5 – 5 mm, variable
Beam divergence (FWHM)	0.2°-0.6°, variable
Sample size (single crystal)	0.001 – 10 mm^3
Sample size (thin film)	thickness > 10 nm area, up to 25 mm^2
Unit cell size	up to 200 Å
Wavelength bandwidth	4.0 Å (15 Hz)
Useful wavelength range	1 – 6 Å
Q range	0.15 - 12 $Å^{-1}$
Detector angular coverage	-159° - 98° (horizontally) -36° - 47° (vertically)
Detector type	SiPM Anger camera
Detector resolution	0.6×0.6 mm^2
Solid angle coverage	4.0 sr (top cylindrical) 0.4 sr (bottom planar)

QIKR

'Cinematic' Imaging Reflectometer for Time-Resolved Measurements



CONTACT

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DESCRIPTION

QIKR will be a general-purpose, horizontal-sample-surface reflectometer consisting of two independently operable end stations – one with the incident beam directed up and one directed down. It will collect specular and off-specular reflectivity data faster than any other such instrument. Using pulse skipping (7.5 Hz), it will often be possible to collect complete specular reflectivity curves using a single instrument setting to provide "cinematic" operation, in which the user "videos" the sample undergoing time-dependent modification.
Samples in time-dependent environments, such as temperature, electrochemical, or when undergoing chemical alteration will be observed in real time with frame rates as fast as 1 Hz in some cases. Cinematic data acquisition promises to make time-dependent measurements routine, with time resolution specified during post-experiment data analysis. QIKR will collect data 25× faster than existing instruments over a sufficient dynamic range *D* to enable cinematic measurements for most samples. Depending on the sample structural parameters of interest, single data set frame rates will range from seconds to minutes.

Cinematic operation will be deployed to observe such processes in real time as *in situ* polymer diffusion and reaction, battery electrode charge-discharge cycles, hysteretic phenomena, membrane protein insertion into lipid layers, and lipid flip-flop.

APPLICATIONS

- Soft matter
  - Polymer diffusion
  - Chemical transformation of reactive films
  - Hydrogels
  - Fouling
  - Structure properties of films under shear
  - Synthetic membranes
  - Responsive films
  - Polymer brushes under shear
  - Surface modification
  - Reactions at oil-water interfaces
- Energy materials

- Biomaterials
  - Model membranes
  - Lipid flip-flop
  - Structure of transmembrane peptides
  - Biocompatible coatings
  - Surfactant and phospholipid monolayers
  - Drug delivery
  - Protein conformation to membranes
  - Influence of synthetic nanoparticles on membrane structure

EXPECTED SPECIFICATIONS

Beam spectrum	Thermal, Cold
Moderator	H_2 coupled
Wavelength bandwidth	2.5 Å < λ < 25 Å (at 7.5 Hz on lower station)
Source-detector distance	20 m (lower station)
24 m (upper station)	
Detector	Pixelated 2D PSD (<2×2 mm^2 resolution)
Beam footprint at sample	Variable from 5×10 to 25×75 mm^2
Q-range (θ-θ geometry)	0.008-0.35 $Å^{-1}$
Q-range (θ-2θ geometry)	0.005-0.50 $Å^{-1}$
Q resolution (δQ/Q)	0.02-0.07
Dynamic range	10

EXAMPLES FOR BER-RELATED RESEARCH

T. Auth, S. Dasgupta, and G. Gompper, "Interaction of Particles and Pathogens with Biological Membranes", in *Physics of Biological Membranes*, edited by P. Bassereau and P. Sens, (Springer International Publishing: Cham, 2018), pp 471-498.

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D.P. Hoogerheide, S.Y. Noskov, D. Jacobs, L. Bergdoll, V. Silin, D.L. Worcester, J. Abramson, H. Nanda, T.K. Rostovtseva, and S.M. Bezrukov, "Structural features and lipid binding domain of tubulin on biomimetic mitochondrial membranes", PNAS 114 (18), E3622 (2017).

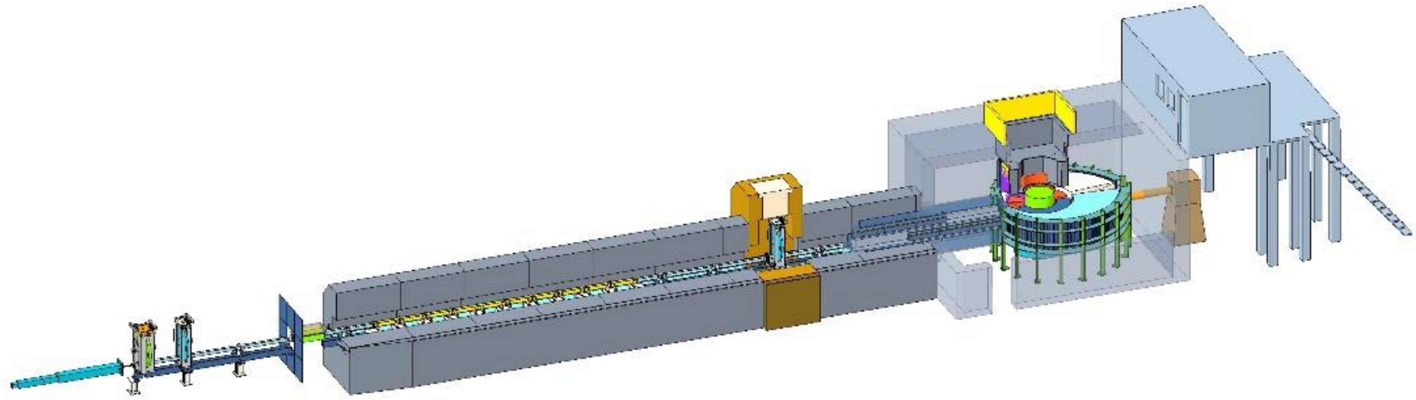
A. Junghans, E.B. Watkins, R.D. Barker, S. Singh, M.J. Waltman, H.L. Smith, L. Pocivavsek, and J. Majewski, "Analysis of biosurfaces by neutron reflectometry: From simple to complex interfaces", Biointerphases 10 (1) 019014 (2015).

M.D. Phan, O. Korotych, N.G. Brady, M.M. Davis, S.K. Satija, J.F. Ankner, and B.D. Bruce, "X-ray and neutron reflectivity studies of styrene-maleic acid copolymer interactions with galactolipid-containing monolayers", Langmuir 36, 3970 (2020).

C.G. Siontorou, G.-P. Nikoleli, D.P. Nikolelis, and S.K. Karapetis, "Artificial Lipid Membranes: Past, Present, and Future", Membranes 7 (3), 38 (2017).

VERDI

Versatile Diffractometer with wide-angle polarization analysis



CONTACT

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Stuart Calder (caldersa@ornl.gov, NScD)

DESCRIPTION

VERDI will excel at diffraction studies of powders and single crystals, allowing routine measurements of milligram-size samples, large unit cell organic compounds, small-magnetic moment compounds, and diffuse signals. The instrument will utilize a large single-frame bandwidth and will offer high-resolution at low momentum transfers and excellent signal-to-noise ratio. A horizontal elliptical mirror concept with interchangeable guide pieces will provide high flexibility in beam divergence to allow for either a high-resolution powder mode, a high-intensity single crystal mode, and a polarized beam option. This diffractometer will be equipped with wide-angle polarization analysis capabilities and will be optimized for studies under extreme conditions of temperature, pressure, and magnetic field. The implementation of polarization allows the isolation of not only magnetic scattering but also incoherent scattering, which offers clear advantages to the study of nonmagnetic hydrogen-based materials.

APPLICATIONS

- Powder and single crystal neutron diffraction studies of large unit cell biological and protein systems
- Spin polarized neutron protein crystallography in high magnetic fields and mK temperatures
- Separation of coherent from nuclear-spin incoherent scattering using polarization analysis

EXPECTED SPECIFICATIONS

Beam size at sample	3 × 3 mm^2 to 10 × 10 mm — variable
Variable beam divergence	0.2° (Horizontal), 1° (Vertical): High resolution 1°(Horizontal), 1° (Vertical): High intensity
Q-range	0.1 $Å^{-1} \leq Q \leq 9$ $Å^{-1}$ (15 Hz)
Q-resolution	$\Delta Q/Q \approx 0.3\%$
Bandwidth ($\Delta\lambda$)	6 Å (15 Hz)
Detector type/ layout / coverage	logarithmic spiral: ^3He tubes from 1.2 to 3.1m 5 -165deg (Horiz.), ± 15° (Vert)- polarized, 34° (Vert) - unpolarized
Polarization	Polarized beam and wide-angle analyzer (2theta =160deg)
Sample environment	mK temperatures, applied field, high-pressure, sample changer