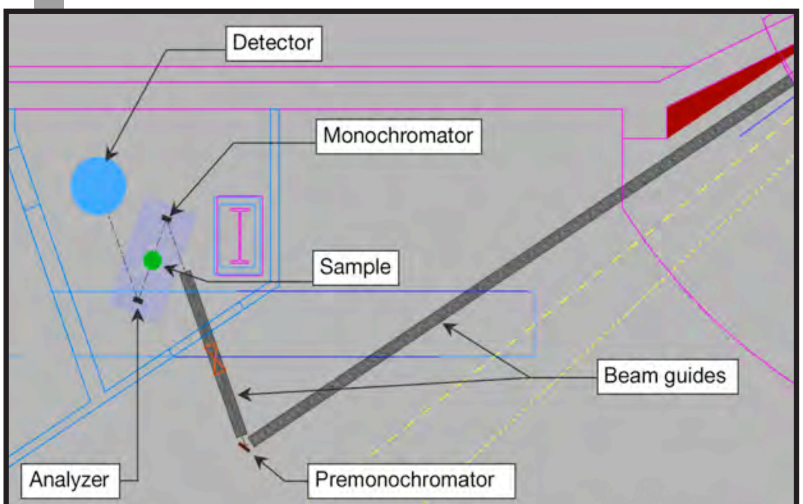
# Instrument Fact Sheet

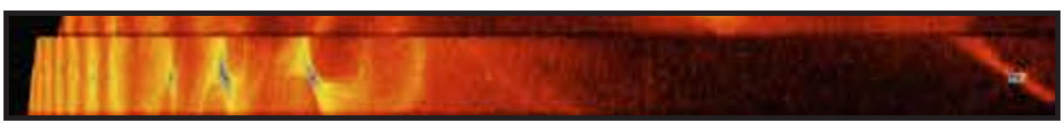
## Beam Line 1A

Spallation Neutron Source

# USANS – Ultra-Small-Angle Neutron Scattering Instrument

The USANS instrument is designed for the study of hierarchical structures in natural and man-made materials. It can be considered an advanced version of the classical Bonse-Hart Double-Crystal Diffractometer (DCD), which, in contrast with its single-wavelength reactor-based analog, will operate with the discrete multiwavelength spectrum of Bragg reflections. The optical scheme of the USANS instrument is similar to that of the conventional Bonse-Hart DCD; however, the pulsed nature of SNS offers an opportunity to separate the orders of Bragg reflection in time space using the time-of-flight technique. Thus, the concept of the USANS technique allows optimization of the neutron flux and the Q resolution, following the principles of dynamical diffraction theory.



*Discrete multiwavelength spectrum created by a family of Bragg reflections.*

## Specifications

| | |
|---|---|
| Moderator | Decoupled poisoned hydrogen |
| Source-detector distance | 30 m |
| Focusing premono-chromator | Cooper mosaic Cu(111) crystals |
| Monochro-mator and analyzer | Si(220) channel-cut, triple-bounce crystals |
| Bragg angle | 70° |
| Wavelength spectrum | 4 Bragg reflections at 3.6, 1.8, 1.2, 0.9 Å |
| Q range | $7 \times 10^{-6}$ Å$^{-1}$ < Q < $5 \times 10^{-3}$ Å$^{-1}$ |

Status: Under construction

## Applications

Ultra-small-angle neutron scattering provides a new way to solve a broad range of scientific problems such as

- Supramolecular structure of polymer blends
- Macroscale self-similarity of rocks
- Structure of colloidal crystals and alloys
- Hydration of cement pastes
- Aggregation in colloidal dispersions
- Self-assembling of polymers
- Mesoscopic structure of natural composites
- Structure of granular powders
- Morphology of colloidal reinforcing fillers
- Structure and morphology of complex fluids
- Rheology and morphology of hydrogels

## For more information, contact

Instrument Scientist: Michael Agamalian, magamalian@ornl.gov, 865.576.0903

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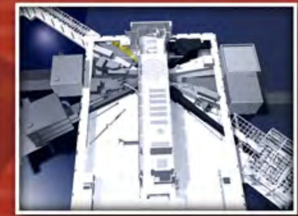
# INSTRUMENT Fact Sheet

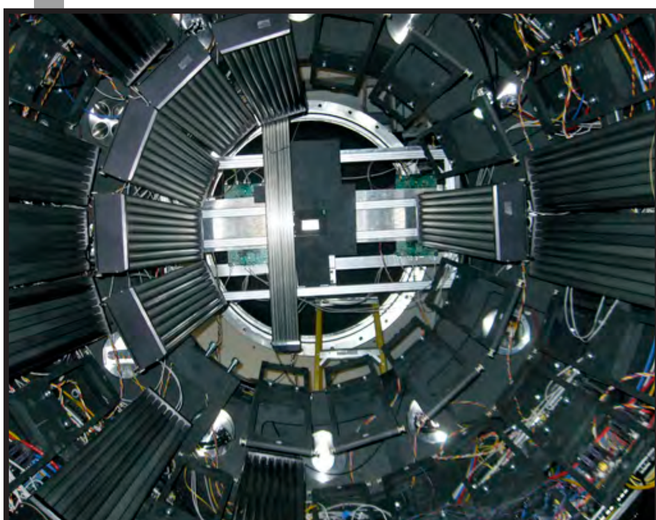
BEAM LINE 1B

SPALLATION NEUTRON SOURCE



## NOMAD – NANOSCALE-ORDERED MATERIALS DIFFRACTOMETER

NOMAD is a high-flux, medium-resolution diffractometer that uses a large bandwidth of neutron energies and extensive detector coverage to carry out structural determinations of local order in crystalline and amorphous materials. The instrument enables studies of a large variety of samples, ranging from liquids and solutions, glasses, and nanocrystalline materials to long-range-ordered crystals. The enhanced neutron flux at SNS, coupled with the advanced neutron optics and detector features, allows for unprecedented access to high-resolution pair distribution functions, small-contrast isotope substitution experiments, small sample sizes, and parametric studies.



### SPECIFICATIONS

| | |
|---|---|
| Moderator | Decoupled poisoned supercritical hydrogen |
| Moderator-to-sample distance | 19.5 m |
| Sample-to-detector distance | 0.5–3 m |
| Wavelength range | 0.1–3 Å |
| Detector angular range | 3–175° scattering angle |
| Initial coverage | 4.0 sr |
| Full detector complement | 8.2 sr |
| Flux on sample | ~$1 \times 10^{8}$ neutrons $cm^{-2}$ $sec^{-1}$ |

Status: Available to users

### APPLICATIONS

- Environmental (e.g., solvent) effects on and direction of nanoscale structure formation
- In situ structural changes in nanoscale oxide catalysts used in automobile catalytic converters
- Structure of hydrogen storage materials under in situ conditions
- Transient structures of materials under extreme conditions (e.g., at high temperature or high pressure under the influence of transient fields or in metastable states)

### FOR MORE INFORMATION, CONTACT

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Instrument Scientist: Mikhail Feygenson, feygensonm@ornl.gov, 865.661.4813

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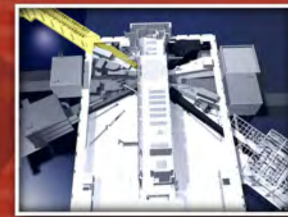
# Instrument Fact Sheet

Beam Line 2

Spallation Neutron Source



## BASIS – Backscattering Spectrometer

BASIS is designed to provide extremely high-energy resolution near the elastic peak, enabling studies of the diffusive dynamics of molecules on the atomic length scale (quasi-elastic neutron scattering). This instrument features very high flux and a dynamic range in energy transfer that is approximately five times greater than what is available on comparable instruments today. In addition, this instrument provides the capability of shifting the incident neutron bandwidth, enabling inelastic scattering with 18 meV energy transfer and a resolution of several microelectronvolts.

### Specifications

| Si 111 | |
|---|---|
| Elastic energy | 2.08 meV |
| Bandwidth | ±250 $\mu$eV |
| Resolution (elastic) | 3.5 $\mu$eV |
| Q range (elastic) | 0.2 Å$^{-1}$ < Q < 2.0 Å$^{-1}$ |
| Solid angle | 1.2 sr<br>2.4 sr<br>(future upgrade) |

| Si 311 (future upgrade) | |
|---|---|
| Elastic energy | 7.64 meV |
| Bandwidth | ±1700 $\mu$eV |
| Resolution (elastic) | 10 $\mu$eV |
| Q range (elastic) | 0.38 Å$^{-1}$ < Q < 3.8 Å$^{-1}$ |
| Solid angle | 1.2 sr |

Status: Available to users

### Applications

BASIS can be used to probe dynamic processes in various systems on the pico- to nanosecond time scale. It is well suited for probing diffusive and relaxational motions but can also be effectively used for studying some types of collective excitations in condensed matter. Applicable fields of study include, but are not limited to, biology, polymers, small molecules, complex fluids, magnetism, materials science, ionic conductors, catalysts, H storage materials (functional energy-related materials), and low-energy spin excitations.

### For more information, contact

Instrument Scientist: Eugene Mamontov, mamontove@ornl.gov, 865.574.5109

Instrument Scientist: Souleymane Omar Diallo, omardiallos@ornl.gov, 865.576.6188

Instrument Scientist: Niina H. Jalarvo, jalarvonh@ornl.gov, 865.360.0304

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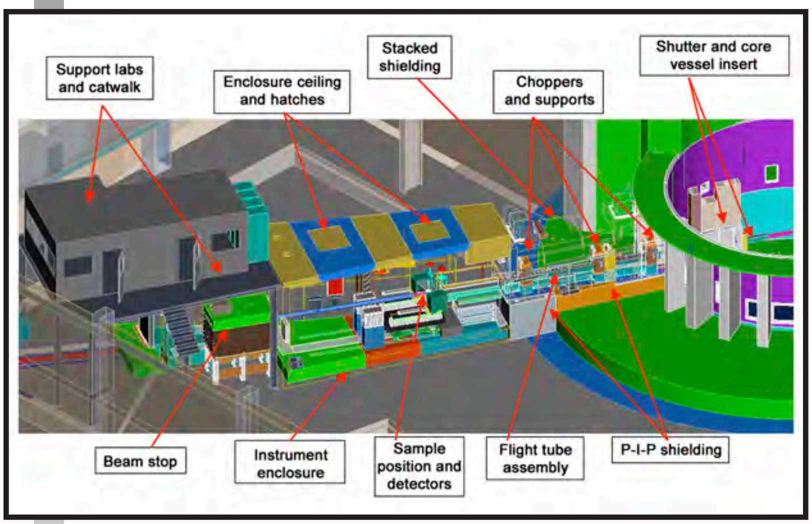
# INSTRUMENT Fact Sheet

BEAM LINE 3

SPALLATION NEUTRON SOURCE

## SNAP – Spallation Neutrons and Pressure Diffractometer

The Spallation Neutrons and Pressure (SNAP) diffractometer, a high-flux, medium-resolution instrument, uses highly integrated advanced area detectors, beam-focusing optics, and pressure chambers to study a variety of powdered, single-crystal, and amorphous materials under extreme pressure and temperature. Traditional Paris-Edinburgh presses are used to reach 25 GPa. The instrument staff and its instrument development team are making progress with "large-volume" diamond anvil cells in hopes of significantly extending the pressure range currently accessible to neutron diffraction. The goal is to routinely achieve pressures of 50 to 100 GPa for samples on the order of 0.1 mm$^3$. Though such high pressures are not yet available to general users, commissioning-type experimental collaborations are welcome.




## Applications

- Hydrogen under extreme conditions
- Real-time in situ monitoring of "real rocks" as an analogue to the down-going slab in the subduction context
- Planetary ices—structure and strength of ices under pressure
- Silicate melts—glasses at high pressure and temperature and the dynamical changes occurring during heating and pressurization
- Strength and rheology of materials and the relationship to brittle and ductile failure, including stress release as a function of time
- Structural changes accompanying transitions in Fullerenes and their derivatives
- Hydrogen bonding in organic and inorganic systems as a function of pressure and temperature, including liquids

## Specifications

| | |
|---|---|
| Moderator | Decoupled poisoned supercritical hydrogen |
| Source-to-sample distance | 15 m |
| Sample-to-detector distance | 50 cm |
| Angular coverage | $26^o > 2\Theta >$ 138° horizontal ±34° vertical |
| Wavelength range (bandwidth) | |
| Pressure range | <25 GPa |
| Temperature range | 100-1500 K (w/ reduced pressure range) |
| Focused beam size | From 1 cm to <100 $\mu$m |
| Liquids and glasses | Q min = 0.7 Å$^{-1}$ Q max = 17 Å$^{-1}$ |
| At $2\Theta = 90^o$ (crystalline powder) $0.5 \le d \le 8.0$ Å$^{-1}$ | |
| At $2\Theta = 35^o$ (glasses & liquids) $0.7 \le d \le 17$ Å$^{-1}$ | |

Status: Available to users


### For more information, contact

Instrument Scientist: Chris Tulk, tulkca@ornl.gov, 865.574.5764

Instrument Scientist: A. Moreira dos Santos, dossantosam@ornl.gov, 865.576.5218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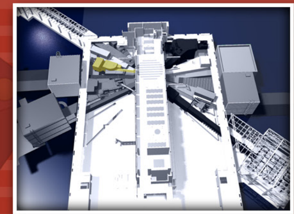
# Instrument Fact Sheet

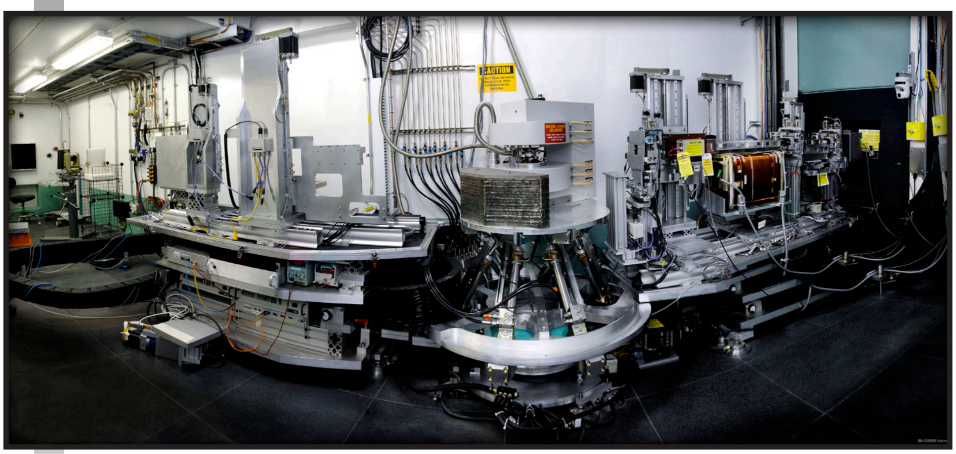
Beam Line 4A

Spallation Neutron Source



## Magnetism Reflectometer

The Magnetism Reflectometer is dedicated to reflectometry studies of magnetic thin films, superlattices, and nanoscale structures. The combination of the high-power SNS and the use of advanced neutron optics allows for off-specular scattering studies of in-plane magnetic and nonmagnetic structures. Wide-angle diffraction geometry is available for experiments on thin films and multilayers. The availability of polarized neutrons and polarization analysis suggests that this instrument can also be used for specific studies of nonmagnetic thin-film samples. Examples of the latter include contrast variation, incoherent background reduction, and phase determination for direct inversion of reflectivity data into real-space scattering-length density profiles.




### Specifications

| | |
|---|---|
| Source-to-sample distance | 18.703 m |
| Sample-to-detector distance | 2.450 - 2.580 m |
| Detector size | 21 x 18 $cm^2$ |
| Detector resolution | 1.5 mm |
| Moderator | Coupled supercritical hydrogen |
| Bandwidth | $\Delta\lambda$ = 2.74 Å |
| Wavelength range | 1.8 Å < $\lambda$ < 14.0 Å |
| Q range | 0 $Å^{-1}$ < Q < 6 $Å^{-1}$ |
| Magnetic field max | 1.2 T with a gap of 50 mm and 3 T with a gap of 10 mm |
| Polarization | 98.5% |
| T range | 5 - 750 K |
| Minimum reflectivity | $10^{-8}$ |

Status: Available to users

### Applications

The Magnetism Reflectometer is applicable primarily to studies with thin magnetic films, an increasingly important area of solid-state physics. Experiments could also benefit engineering, metallurgy, or biological problems. Instrument capabilities allow, for example, studies of magnetic recording media and magnetic sensors, as well as depth-dependent studies of structural/magnetic nanoparticles or domains. The instrument's unique capabilities provide for multilength-scale experiments, and it has sufficient beam intensity for detailed structural/magnetic phase-diagram determinations.

### For more information, contact

Instrument Scientist: Valeria Lauter, lauterv@ornl.gov, 865.387.5389
Instrument Scientist: Artur Glavic, glavicag@ornl.gov, 865.241.1743

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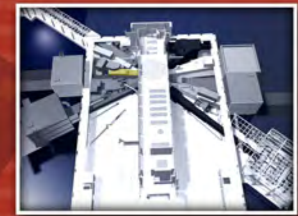
# INSTRUMENT Fact Sheet

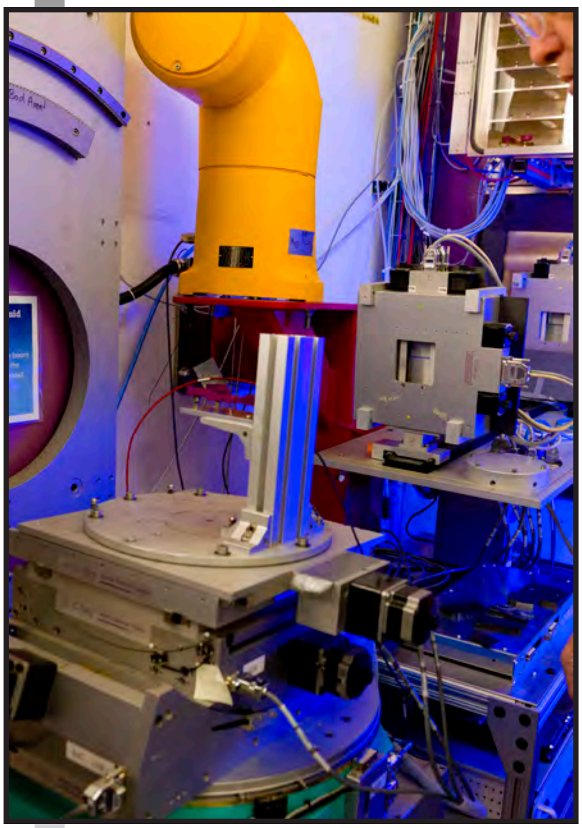
BEAM LINE 4B

SPALLATION NEUTRON SOURCE



## LIQUIDS REFLECTOMETER

The Liquids Reflectometer features a horizontal sample geometry and thus can accommodate air/liquid surfaces in addition to air/solid and liquid/solid interfaces. Active vibration isolation minimizes capillary-wave production by the external environment. Data rates and Q range covered at a single scattering angle setting are sufficiently high to permit “real-time” kinetic studies on many systems. Time-resolved experiments include investigations of chemical kinetics, solid-state reactions, phase transitions, and chemical reactions in general.



### APPLICATIONS

The Liquids Reflectometer is useful for a wide range of science. Current areas of interest include biomaterials, polymers, and chemistry involving thin layers of surfactants or other materials on the surfaces of liquids, such as cell-membrane analogs. These systems provide a flexible platform to study structure-property relationships at the boundary between hard and soft matter, with applications in biomimetics, bio-sensing, and bio-compatible films; hydrogen storage and fuel cells; and polymers.

### SPECIFICATIONS

| | |
|---|---|
| Source-to-sample distance | 13.6 m |
| Sample-to-detector distance | 1.5 m |
| Detector size | 20 x 20 $cm^2$ |
| Detector resolution | 1.3 x 1.3 $mm^2$ |
| Moderator | Coupled supercritical hydrogen |
| Bandwidth | $\Delta\lambda$ = 3.5 Å |
| Wavelength range | 2.5 Å < $\lambda$ < 17.5 Å |
| Q range (air/liquid) | 0 $Å^{-1}$ < Q < 0.3 $Å^{-1}$ |
| Q range (air/solid) | 0 $Å^{-1}$ < Q < 0.3 $Å^{-1}$ |
| Minimum reflectivity | 1 x $10^{-7}$ |

Status: Available to users


FOR MORE INFORMATION, CONTACT

Instrument Scientist: John Ankner, anknerjf@ornl.gov, 862.377.4523

Instrument Scientist: Jim Browning, browningjf@ornl.gov, 865.209.5273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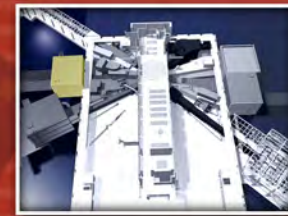
# INSTRUMENT *Fact Sheet*

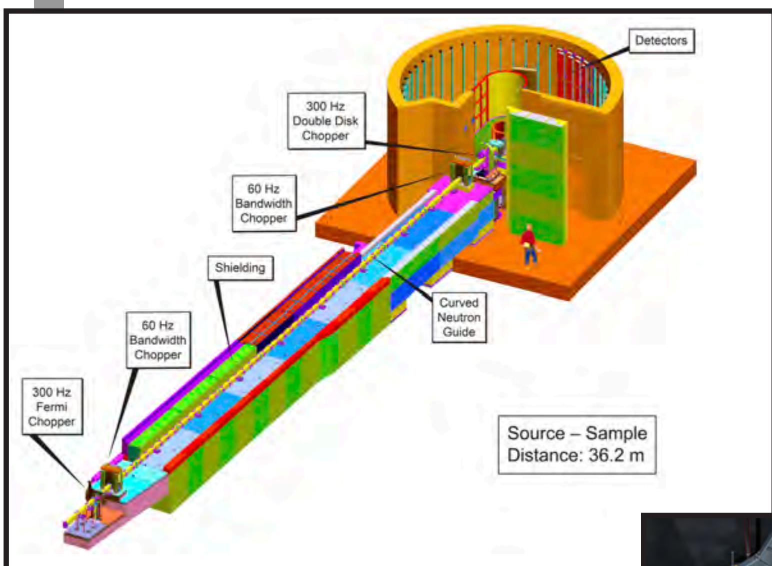
BEAM LINE 5

SPALLATION NEUTRON SOURCE

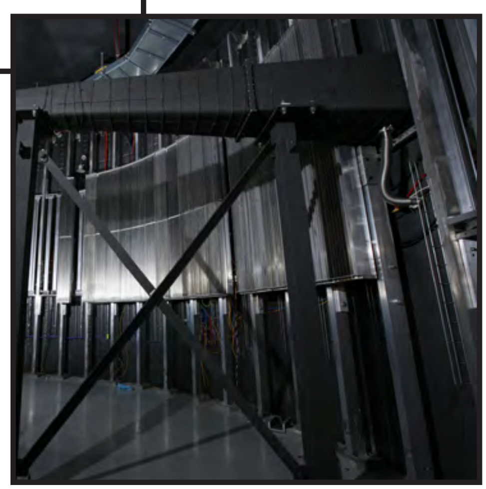


## CNCS – COLD NEUTRON CHOPPER SPECTROMETER

CNCS is a high-resolution, direct-geometry, multichopper inelastic spectrometer designed to provide flexibility in choice of energy resolution and to perform best at low-incident energies (2–50 meV). Although the current detector coverage around the sample is 1.7 sr, a later upgrade to 3 sr is possible. CNCS experiments typically use an energy resolution between 25 and 500 $\mu$eV. A broad variety of scientific problems, ranging from complex and quantum fluids to magnetism and chemical spectroscopy, can be addressed through experiments on the CNCS.




*Engineering design of the CNCS beam line from the target monolith to the instrument satellite building.*



### APPLICATIONS

CNCS is applicable primarily to studies in the following:

- Complex fluids: dilute protein solutions, biological gels, selective absorption of molecules on surfaces
- Dynamics in confined geometries
- Magnetism: low-dimensional systems; non-Fermi liquids; frustrated, disordered, or molecular magnets

### SPECIFICATIONS

| | |
|---|---|
| Source-to-sample distance | 36.2 m |
| Sample-to-detector distance | 3.5 m |
| Angular coverage | -50 to +135° horizontally ±16° vertically |
| Energy resolution | 10–500 $\mu$eV |
| Incident energy range | 0.5–80 meV |
| Momentum transfer range | 0.05–10 Å$^{-1}$ |
| Detector type | $^{3}$He, LPSD |

Status: Available to users

### FOR MORE INFORMATION, CONTACT

Instrument Scientist: Georg Ehlers, ehlersg@ornl.gov, 865.206.0824
Instrument Scientist: Andrey Podlesnyak, podlesnyakaa@ornl.gov, 865.242.7920

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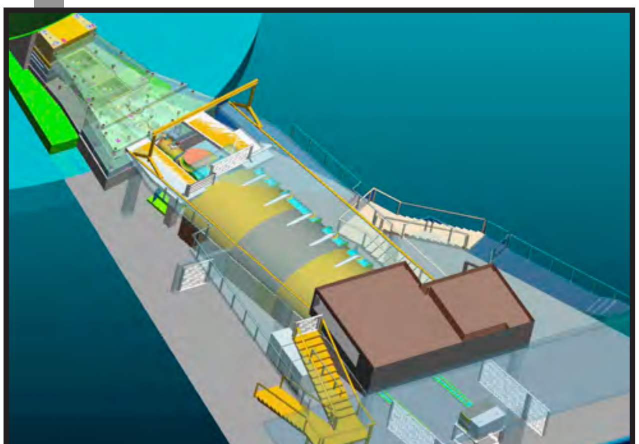
# Instrument Fact Sheet

BEAM LINE 6

SPALLATION NEUTRON SOURCE

## EQ-SANS — Extended Q-Range Small-Angle Neutron Scattering Diffractometer

The EQ-SANS Diffractometer is designed for the study of materials across length scales ranging from 0.1 to 100 nm. The high intensity provided by the EQ-SANS enables both high-throughput experiments and time-resolved experiments facilitated by the pulsed source of SNS. EQ-SANS enables measurements over a wide Q-range at a single instrument configuration, providing improved throughput. The high maximum Q of the instrument allows both large-scale and local structure to be studied by the instrument. The versatility of SANS makes EQ-SANS broadly applicable to a wide range of materials from science and industry.



### Specifications

| | |
|---|---|
| Source-to-sample distance | 14 m |
| Bandwidth | 3–4.3 Å |
| Moderator | Coupled supercritical hydrogen |
| Integrated flux on sample | ~$10^7$–$10^9$ n/cm$^2$/s |
| Q range | 0.004 Å$^{-1}$ < Q < 1.5 Å$^{-1}$ |

| Low-Angle Detector | |
|---|---|
| Sample-to-detector distance | 1.3–10 m |
| Detector size | 1 x 1 m |
| Detector resolution | 5.5 x 4.3 mm |

Status: Available to users

### Applications

Life science

- Solution structures of proteins, DNA, and other biological molecules and molecular complexes
- Protein-protein and protein-ligand interactions, kinase regulation
- Protein-membrane interaction
- Materials for drug delivery

Polymer and colloidal systems

- Block copolymers and dendrimers
- Micelles and emulsions
- Polyelectrolytes and ion distribution at solid-liquid interfaces

Materials science

- Simultaneous study of domain and crystalline structures
- Crystallization and precipitation
- Nanoparticles

Earth and environmental sciences

- Pore structure in soils
- Structure of geologic materials

### For more information, contact

Instrument Scientist: William Heller, hellerwt@ornl.gov, 865.241.0093
Instrument Scientist: Chris Stanley, stanleycb@ornl.gov, 865.574.6669
Instrument Scientist: Changwoo Do, doc1@ornl.gov, 865.576.6981
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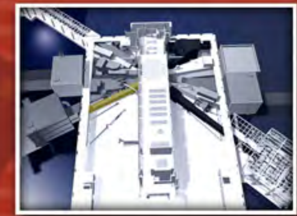
# INSTRUMENT Fact Sheet

BEAM LINE 7

SPALLATION NEUTRON SOURCE



## VULCAN – ENGINEERING MATERIALS DIFFRACTOMETER

VULCAN is designed to tackle a variety of problems in materials science and engineering, including deformation, phase transformation, residual stress, texture, and microstructure studies. VULCAN provides rapid volumetric mapping with a sampling volume of 1 $mm^3$ and a measurement time of minutes for common engineering materials. In extreme cases, VULCAN has the ability to study kinetic behaviors in sub-second times. Through these measurements, VULCAN can help scientists and engineers predict the reliability of structural components and better understand how materials behave under extreme conditions. A small-angle detector will be installed in the near future to provide more wide-angle detector coverage. This will allow users to conduct fast, simultaneous measurements using small-angle scattering, opening new research opportunities for the study of structure evolution at multiple length scales. Available sample environments and equipment include a unique load frame capable of multi-axial loading and fatigue tests with an induction heater at up to 1273 K, a high-temperature vacuum furnace at up to 1,873 K, a controlled atmosphere furnace at up to 1473 K, a battery cycler, a high-voltage ac/dc field, and standard equipment from the sample environment group.

### APPLICATIONS

- VULCAN covers a broad range of applications in materials science and engineering, from residual stress determination in engineering components to understanding the fundamental aspects of material behaviors during synthesis, processing, and service. Research areas that VULCAN can benefit include but are not limited to the following:
- In situ studies of materials behavior during processing: phase formation, temperature distribution, texture changes, stress development, precipitation.
- In situ loading studies of crystalline/amorphous materials at high temperatures: phase transformation, fatigue damage, deformation in nanostructured materials, creep behaviors, piezoelectric and shape-memory alloys.
- Residual stress and microstructure changes in engineering components.
- Phase transformation/transition kinetics during material synthesis.

### SPECIFICATIONS

| | |
|---|---|
| Sample-to-detector distance | ~ 2 m |
| Detector angular coverage | 33.5° < 2θ < 56.5° ± 15° out of horizontal plane |
| Wavelength bandwidth/ d-spacing band (Å) | ~1.44 at 60 Hz d: 0.5-1.5<br>~2.88 at 30 Hz d: 0.5-2.5<br>~4.32 at 20Hz d:0.5~3.6 |
| Resolution | ~0.25% in high-resolution mode<br>~0.45% in high-intensity mode |
| Flux on sample (n/s/$cm^2$) at 60 Hz | 2.2 x 107 in high-resolution mode<br>6.7 x 107 in high-intensity mode |
| Gauge volume (mm) | strain/phase mapping: 8–20<br>insitu loading and/ or heating: 100–250 |
| Collimation | incident slit:17mm in horizontal direction, 12mm in vertical direction |
| Receiving | 2 or 5 mm |

Status: Available to users


FOR MORE INFORMATION, CONTACT

Instrument Scientist: Ke An, kean@ornl.gov, 865.919.5226
Instrument Scientist: Alexandru D. Stoica, stoicaad@ornl.gov, 865.684.3337
Instrument Scientist: Dong Ma, dongma@ornl.gov, 865.806.9872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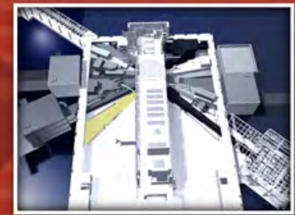
# Instrument Fact Sheet

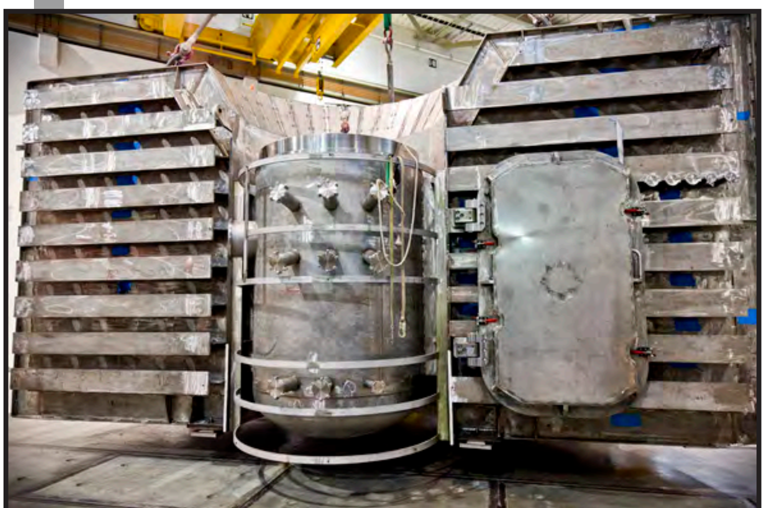
Beam Line 9



Spallation Neutron Source

## CORELLI – Elastic Diffuse Scattering Spectrometer

CORELLI is a statistical chopper spectrometer with energy discrimination. CORELLI is designed and optimized to probe complex disorder in crystalline materials through diffuse scattering of single-crystal samples. The momentum transfer ranges from 0.5 to 12 Å$^{-1}$, and the energy of incident neutrons ranges from 10 to 200 meV. This instrument combines the high efficiency of white-beam Laue diffraction with energy discrimination by modulating the beam with a statistical chopper. A cross-correlation method is used to reconstruct the elastic signal from the modulated data. Accurate modeling of the short-range order associated with the diffuse scattering requires measurements over large volumes of three-dimensional reciprocal space, with sufficient momentum resolution to distinguish the diffuse signal from the strong Bragg peaks.



### Applications

- Diffuse scattering in material science, including colossal magnetoresistance materials, ferroelectric relaxors, and fast ion conductors
- Diffuse scattering in condensed matter physics, including high-temperature superconductors, geometrically frustrated systems, and quantum critical phenomena
- Diffuse scattering in molecular systems including molecular solids and microporous framework systems

### Specifications

| | |
|---|---|
| Moderator | Ambient $H_2O$ decoupled poisoned |
| Source-to-sample distance | 20 m |
| Sample-to-detector distance | 2.5 m |
| Anular coverage | -23 to +152° horizontally ±28.5° vertically |
| Energy resolution | 1 meV at 10 Å$^{-1}$ |
| Momentum resolution | ΔQ/Q~0.005 |
| Incident energy range | 10–200 meV |
| Momentum transfer | 0.5–12 Å$^{-1}$ |
| Beam size at sample position | ~ 1 $cm^2$ |

Status: Under construction


### For more information, contact

Instrument Scientist: Feng Ye, yef1@ornl.gov, 865.576.0931



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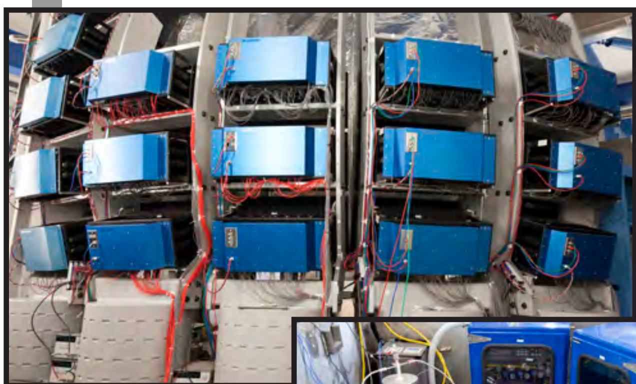
# Instrument Fact Sheet

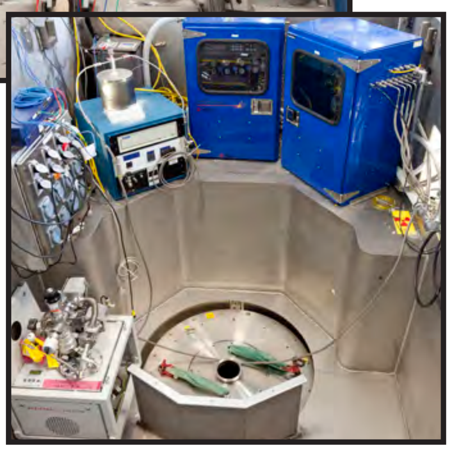
Beam Line 11A

Spallation Neutron Source

## POWGEN – Powder Diffractometer

POWGEN is a general-purpose powder diffractometer useful for a wide range of structural studies. It can cover d-spacings from ~0.3 Å, or less, to 3 Å in a single measurement. Rietveld measurements for traditional neutron-size samples can be completed in a few hours, with a <0.2% resolution at short d-spacings and <1% resolution for nearly all d-spacings of interest. Alternatively, much of this resolution can be traded for intensity, making it possible to take shorter measurements while still maintaining good resolution. It is also possible to collect data from much smaller samples with longer collection time. The adjustable bandwidth-limiting choppers allow for large variations in the incident wavelengths and pulse repetition rate. Insertable guide sections and the ability to trade resolution for intensity at the analysis stage allow users great latitude to optimize the data range, resolution, and statistical precision for each experiment.





## Applications

Scientific studies at this instrument encompass a wide range of novel materials. These include, but are not limited to, structural studies of magnetic materials such as high-Tc superconductors, metal-insulator phase transitions, charge and orbital ordering transitions, and molecular magnets. Additional possibilities include nonmagnetic materials such as zeolite and aluminophosphate frameworks; metals and semiconductors; dielectrics, ferroelectrics, and thermoelectrics; and ab initio structure solutions of complex polycrystalline materials such as pharmaceutical compounds. In addition, POWGEN is capable of acquiring refineable data sets in rapid data collection mode, making it an ideal instrument for parametric studies and time-resolved in situ studies of the electrochemistry of catalysts, ceramic membranes, hydrogen storage materials, and charging and discharging of battery materials.

## Specifications

| | |
|---|---|
| Moderator | Decoupled poisoned super critical $H_2$ |
| Source-to-sample distance | 60 m |
| Sample-to-detector distance | 2.5–4.5 m |
| Detector angular coverage | 30° < 2θ < 150° |
| Total detector coverage | 6.9 $m^2$ |
| Bandwidth | ~1 Å |
| Frame 1 | 0.1–2.0 Å at 60 Hz<br>0.2–4 Å at 30 Hz |
| Frame 5 | 2.2–10.2 Å at 60 Hz |
| Resolution | 0.001 < Δd/d < 0.016 |
| Sample Environment | 24 Sample changer: 12–300 K<br>Orange cryostat: 2–300 K<br>ILL furnace: 1200°C<br>Gas atmosphere furnace (with RGA and $pO_2$ sensor): 850°C |

Status: Available to users

## For more information, contact

Instrument Scientist: Ashfia Huq, huqa@ornl.gov, 630.986.7321
Instrument Scientist: Andrew Payzant, payzanta@ornl.gov, 865.235.4981

neutrons.ornl.gov/powgen

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05-03082F/gim

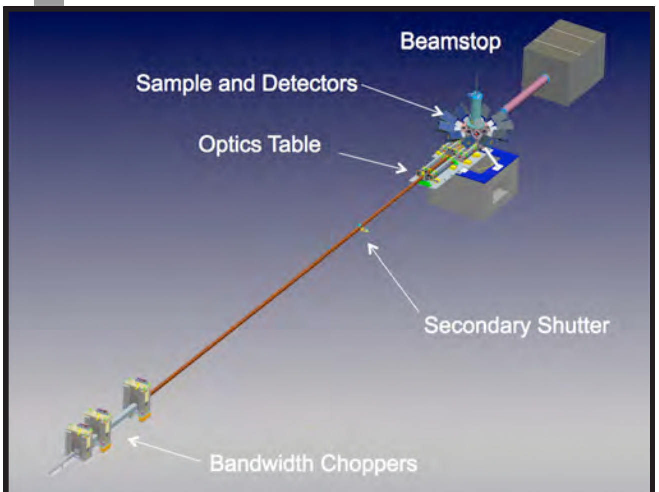
# INSTRUMENT Fact Sheet

BEAM LINE **11B**

SPALLATION NEUTRON SOURCE

## MaNDi – Macromolecular Neutron Diffractometer

MaNDi allows the study of single crystals and is optimized for rapid data collection from large macromolecular structures. MaNDi can achieve 1.5 - 2.0 Å resolution from crystal volumes between 0.1 and 1.0 $mm^3$, with lattice repeats on the order of 150 Å. With larger crystals (>1 $mm^3$), it is possible to obtain useful data in the resolution range of 2.0 to 2.5 Å for unit-cell repeats of up to 300 Å, a revolution in neutron macromolecular crystallography (NMC). Experimental duration times are between one and seven days, revolutionizing NMC for applications in the fields of structural biology, enzymology, and computational chemistry.




The MaNDi detectors are designed to cover a large solid angle to record most of the neutrons scattered from a single-crystal sample, regardless of the reflection angle. This capability is accomplished through the instrument design, which places the detectors approximately spherically around the sample. The detector design follows a modular approach. A spherical detector mount is constructed to accommodate the appropriate number of individual modules of two-dimensional, time-sensitive detectors with front face dimensions of 150 × 150 mm, leaving openings for the sample orienter/environment (top) and the incident and exiting direct neutron beam (horizontal plane). The spatial resolution of the detector is 1 mm, with a minimal sensitivity to gamma rays, hence preserving the signal-to-noise ratio of the Bragg peaks. The efficiency of this type of detector using a 1.5-mm-thick scintillator is 78% for neutrons with a wavelength of 1 Å. An increase in neutron wavelength is coupled with an increase in detection efficiency.

Precision mounting places the 0.1-$mm^3$ crystals within the neutron beam, and the sample-positioning system allows translation and rotation in x, y, and z to precisely align the sample. These operations are remotely controlled and motor driven by a user-friendly graphical user interface.

### Applications

- Molecular magnets, computational chemistry, and fibers
- Protein studies to provide better drug molecules for the treatment of cancer and HIV
- Studies of enzyme mechanisms to accelerate important industrial reactions
- Mechanisms used by plants to convert light into energy

### Specifications

| | |
|---|---|
| Moderator | Decoupled hydrogen |
| Source-to-sample distance | 30 m |
| Sample-to-detector distance | 0.45 m |
| Initial angular detector coverage | 2 sr |
| Optional angular detector coverage | 7 sr |
| Detector pixel size | 1.2 mm |
| Detector angles | 0–180° |
| Wavelength bandwidth | 2.16 Å |
| Resolution | $\Delta d/d = 0.0015$ |
| Sample size | >0.1 $mm^3$ |
| Divergence | 6–16 mrad |

Status: Under construction

### For more information, contact

Instrument Scientist: Leighton Coates, coatesl@ornl.gov, 865.241.3427
neutrons.ornl.gov/mandi

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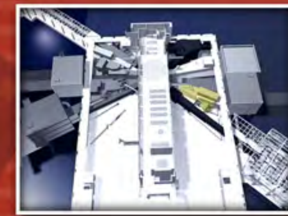
07-G00833E/gim

INSTRUMENT Fact Sheet

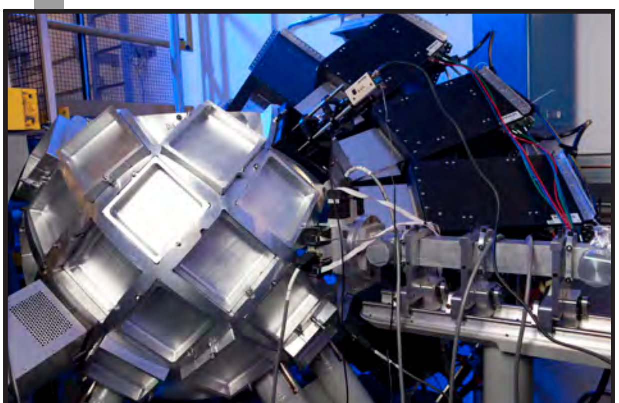
BEAM LINE 12

SPALLATION NEUTRON SOURCE



# TOPAZ – Single-Crystal Diffractometer

TOPAZ can address problems in chemistry, earth sciences, materials science and engineering, solid-state physics, and biology. A wavelength resolved (= time-of-flight) Laue neutron single-crystal diffractometer with extensive area detector coverage, it is well suited for three-dimensional reciprocal or Q-space mapping of Bragg peaks and magnetic and diffuse scattering patterns from a stationary crystal at multiple setting angles. Experiments can be conducted in ambient conditions or in controlled sample environments. A nitrogen cold stream provides temperature control in the range of 100 to 450 K to collect data as a function of temperature. Two tunable neutron wavelength bands are available for data collection: magnetic and nuclear scattering are collected simultaneously. Moreover, the sample can be oriented with high precision to collect magnetic peaks in specific directions. Currently, 11 of 48 detector locations are populated with Anger camera modules covering a scattering angle of about 16–158° 2θ, matching 1.4 sr in an almost spherical arrangement around the sample. A full dataset for structure analysis can be collected in 15–30 settings, depending on crystal symmetry, with a minimum exposure time of about 15 minutes each, depending on scattering strength and sample size



## Applications

TOPAZ is well suited for determining atomic positions and displacement parameters of light elements (such as hydrogen) next to heavy metals and for the study of magnetic structures, phase transitions, disorder, and local structure phenomena. Examples span a wide range of materials:

- Functional inorganic materials for the study of the interplay of nuclear and magnetic structure and spin arrangements such as magnetic superstructures in perovskites and spinels and single-molecule magnet materials.
- Hydrogen storage and other porous framework materials for the study of the guest-host interaction and guest mobility such as in metal organic framework materials and zeolites.
- Catalytic and dihydrogen activation or exchange materials for the study of metal-hydrogen bonding such as for catalytic precursors, metal-hydrides, and organometallics.
- Expansive organic molecules for the study of the hydrogen network, interaction at the active site or cavity, such as for enzymes and supramolecules.

## Specifications

| | |
|---|---|
| Moderator | Decoupled poisoned hydrogen |
| Source-to-sample distance | 18 m |
| Sample-to-detector distance | 39–45 cm |
| Angular detector coverage | 1.7 sr (14 detectors) |
| Detector pixel size | 1 mm |
| Detector angles | 20–160° |
| Wavelength bandwidth | 3.0 Å |
| Accessible wave length | 0.5–3.5 Å |
| Frame 1 | 0.5–3.5 Å |
| Resolution | ~0.4 |
| Sample size | 1 $mm^3$ < S < 10 $mm^3$ |
| Neutron beam divergence on sample | 15 mrad < d < 25 mrad |

Status: In commissioning


## For more information, contact

Instrument Scientist: Christina Hoffmann, hoffmanncm@ornl.gov, 865.576.5127
Instrument Scientist: Xiaoping Wang, wangx@ornl.gov, 865.200.2500


neutrons.ornl.gov/topaz

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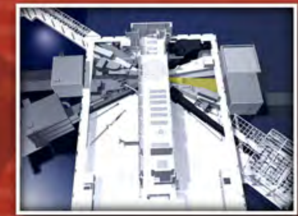
# INSTRUMENT Fact Sheet

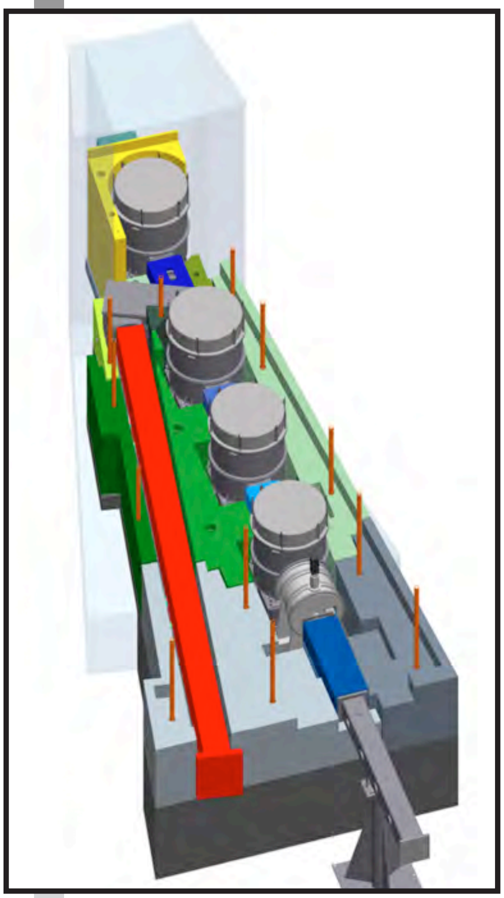
BEAM LINE 13

SPALLATION NEUTRON SOURCE



## FNPB – FUNDAMENTAL NEUTRON PHYSICS BEAM LINE

The FNPB provides neutron beams for a variety of experiments in nuclear and particle physics. This facility is designed to accommodate two classes of experiments: (1) cold neutron experiments that require intense, broad-spectrum beams and (2) ultracold neutron experiments in which neutrons of ~1 meV are "down-converted" to near zero energy in superfluid liquid helium. Experiments at the FNPB include precise measurements of the parameters that describe neutron beta decay, studies of the weak interaction between quarks, and a search for a non-zero neutron electric dipole moment. Each of the experiments at the FNPB requires the development, construction, and installation of major pieces of experimental equipment, and each experiment can take beams for periods of from several months to a few years.



*Design model of the FNPB guide system showing the curved cold beam with four frame overlap choppers, as well as the monochromator housing and the ballistic ultracold neutron guide. The cold guide and choppers share a common vacuum to reduce window losses.*

FNPB is funded and operated by the Oak Ridge National Laboratory Physics Division.

### APPLICATIONS

The FNPB is designed to address questions of interest in cosmology, nuclear and particle physics, and astrophysics. Among the questions that will be addressed are the origin of the light elements (big bang nuclear synthesis), the source of the cosmic matter-antimatter asymmetry, and the origin of parity violation.

### SPECIFICATIONS

| Cold Neutron Beam Line | |
|---|---|
| Supermirror guide | Curved, m = 3.6 |
| Beam area | 100 x 120 mm |
| Choppers | 4 frame over-lap |
| Peak wavelength | 3.5 Å |

| |
|---|
| Independent secondary shutter |
| Floor pit for superconducting magnet |

| Ultracold Neutron Beam Line | |
|---|---|
| Guide | 33 m ballistic |
| Wavelength | 8.9 Å |
| Monochro-mator | Double-crystal alkali intercalated graphite |

| |
|---|
| External building experimental area |

Status: Available to users

FOR MORE INFORMATION, CONTACT

Project Manager: Geoff Greene, greenegl@ornl.gov, 865.574.8435

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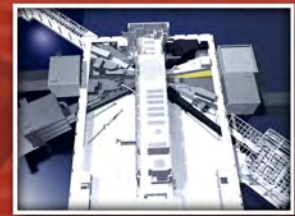
# Instrument Fact Sheet

Beam Line 14B

Spallation Neutron Source



## HYSPEC – Hybrid Spectrometer

HYSPEC is a high-intensity, direct-geometry instrument optimized for measurement of excitations in small single-crystal specimens. The incident neutron beam is monochromated using a Fermi chopper with short, straight blades and is then focused onto the sample using Bragg scattering optics. Neutrons are detected in a bank of position-sensitive detector tubes that can be positioned over a wide range of scattering angles about the sample axis. This combination of Fermi chopper and Bragg focusing optics, plus a position-sensitive detector bank, leads to a highly flexible instrument in which the energy and wave vector resolution can be independently varied by nearly an order of magnitude. Either full or partial neutron polarization analysis can be deployed on HYSPEC. This is accomplished by using a Heusler crystal array to polarize the incident beam and either a $^{3}He$ spin filter or supermirror wide-angle polarization analyzers for the scattered beam.

## Applications

- Superconductors
- Strongly correlated electron materials
- Ferroelectrics
- Lattice and magnetic dynamics
- Phase transitions
- Quantum critical points
- Complex phases in intermetallic compounds
- Frustrated magnets
- Low-dimensional magnetic excitations
- Transition metal oxides
- Spin and lattice dynamics in nanostructures

## Specifications

| | |
|---|---|
| Moderator | Coupled cryogenic hydrogen |
| Moderator-to-Fermi chopper distance | 37.2 m |
| Chopper-to-sample distance | 3.2 m |
| Focusing crystals-to-sample distance | 1.4–1.8 m |
| Sample-to-detector distance | 4.5 m |
| Incident energy range | 3.6–90 meV |
| Energy resolution (elastic scattering) | $0.02 < (\Delta E/E_I) < 0.2$ |
| Scattering-angle range | $2° < 2\theta_S < 135°$ |

Status: In commissioning


## For more information, contact

Instrument Scientist: Barry Winn, winnbl@ornl.gov, 865.805.6819

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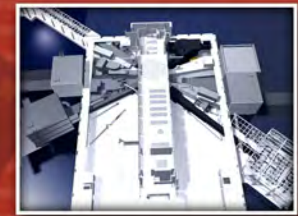
06-G01632D/gim

# Instrument Fact Sheet

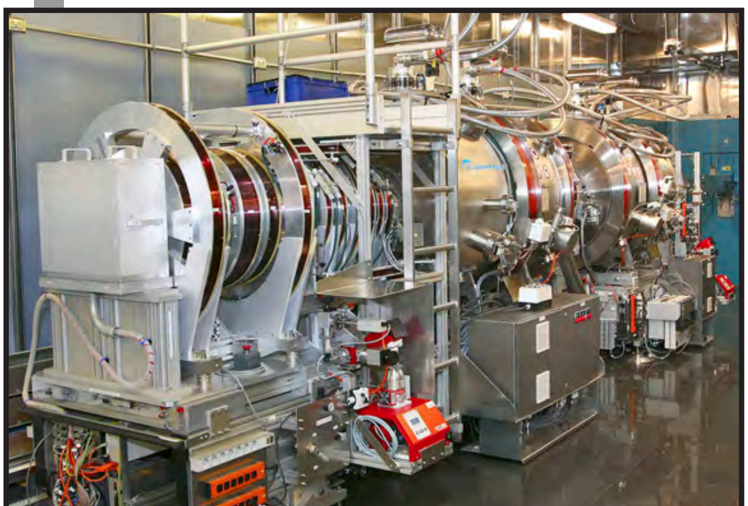
BEAM LINE 15

SPALLATION NEUTRON SOURCE



## NSE – Neutron Spin Echo Spectrometer

Neutron spin echo spectrometers provide both the highest resolution and best dynamical range in neutron scattering. Exploiting superconducting technology and developing novel field correction elements, the NSE instrument aims at a maximum achievable Fourier time τ of at least 1 µs (ΔE ≅ 0.7 neV). Using wavelengths of 2 Å < λ < 20 Å, this would yield an unprecedented dynamical range of six decades from 1 ps < τ < 1 µs. The design of the spectrometer takes advantage of recent progress in neutron optics and polarizing supermirror microbenders, resulting in considerable gains in polarized neutron flux over a wide wavelength range. Performance is also extended by a position-sensitive, two-dimensional detector with a broad detection region. As a result, the effective data rate will gain an additional factor of 5 in addition to the estimated time-averaged sample flux of $10^7$ n/cm$^2$ s around λ = 10 Å. This yields the highest available data accumulation rate (especially at wavelengths up to 0.7 Å). In addition, the wavelength distribution width at any time is well below 0.5%, causing the resolution in momentum transfer to increase significantly compared with reactor instruments with 10% or more wavelength distribution width.



NSE is operated by a satellite office of the Jülich Center for Neutron Science.

### Applications

Although the NSE spectrometer is designed primarily for soft-matter research, its capabilities also make it useful for all fields of modern condensed matter physics, materials science, and biophysics. This instrument is especially suited for analyzing slow dynamical processes and thereby unraveling molecular motions and mobilities at nanoscopic and mesoscopic levels. This feature is highly relevant to soft-matter problems in research on the molecular rheology of polymer melts, related phenomena in networks and rubbers, interface fluctuations in complex fluids and polyelectrolytes, and transport in polymeric electrolytes and gel systems. NSE could also aid studies in magnetism.

### Specifications

| | |
|---|---|
| Moderator | Cold-coupled hydrogen |
| Neutron guide h × b | Ni coated, 4 × 8 cm$^2$, m = 1.4 |
| Wavelength selection | Chopper system consisting of four choppers and selecting wave length bands of up to 3.66 Å |
| Accessible wavelength frame | 2 Å < λ < 20 Å |
| Declination angle | 3.5° |
| Maximum scattering angle | ≅79.5° |
| Q range | 0.05–3.5 Å |
| Maximum field integral | J = 1 Tm |
| Dynamic range | 5 ps < τ < 400 ns |
| Typical sample size | 30 × 30 mm$^2$ |
| Analyzer | m=3 rotatable supermirror |
| Detector | 2D $^3$He counter (300 × 300 mm$^2$, 32 x 32 px) |
| Typical scanning time with 10% scatterer | 5 hours/ spectrum |

Status: Available to users


For more information, contact

Instrument Scientist: Michael Ohl, ohlme@ornl.gov, 865.574.8426
Instrument Scientist: Nikolas Arend, arendn@ornl.gov, 865.576.1965
Instrument Scientist: Laura Stingaciu, l.stingsciu@fz-juelich.de, 865.576.9125
Instrument Scientist: Melissa Sharp, sharpma@ornl.gov, 865.241.7319
Instrument Scientist: Piotr Zolnierczuk, zolnierczukp@ornl.gov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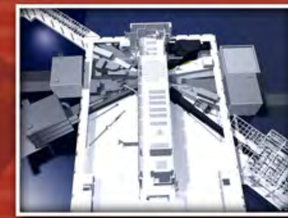
# INSTRUMENT Fact Sheet

BEAM LINE **16B**

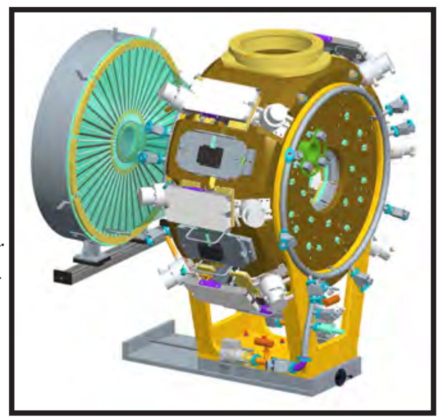
SPALLATION NEUTRON SOURCE



## VISION – VIBRATIONAL SPECTROMETER

VISION is best thought of as the neutron analogue of an infrared-Raman spectrometer. It is optimized to characterize molecular vibrations in a wide range of crystalline and disordered materials over a broad energy range (<5 to >500 meV), while simultaneously recording structural changes using diffraction detectors in the backscattering position and at 90°. This inverted-geometry instrument offers enhanced performance by coupling a white beam of incident neutrons with two banks of eight analyzer modules, equipped with double-focusing crystal arrays, that focus the desired neutrons on a small detector. This arrangement leads to improved signal noise, and the overall count rate in the inelastic signal is at least two orders of magnitude beyond that of similar spectrometers that are currently available.

*Engineering model of VISION, including $T_0$ chopper, bandwidth chopper, secondary spectrometer, and utility rooms.*



*Secondary spectrometer with detector and analyzer modules.*

## APPLICATIONS

Leading-edge studies involving scientific disciplines such as nanotechnology, catalysis, biochemistry, geochemistry, and condensed/soft-matter science.

## SPECIFICATIONS

| | |
|---|---|
| Moderator | Decoupled ambient water |
| Source-to-$T_0$ chopper distance | 7.6 m |
| $T_0$ chopper-to-sample distance (primary flight path) | 6.4 m |
| Sample-to-detector distance (secondary flight path) | 0.732 m |
| Incident energy range | 3.5–500 meV |
| Analyzer Bragg angle | 45º |
| Total analyzer area (in 14 identical units) | 0.7 $m^2$ |
| Energy resolution | Exceeds 1.5% (>5 meV) – 5% (<5 meV) |
| Elastic line width | 90 µeV |
| Annular diffraction detector | 1.3–14 $Å^{-1}$ |
| Backscattering diffraction detector | 1.5–30 $Å^{-1}$ |
| Δd/d | 0.001 |

Status: In commissioning


FOR MORE INFORMATION CONTACT

Instrument Scientist: Christoph Wildgruber, wildgrubercu@ornl.gov, 865.574.5378

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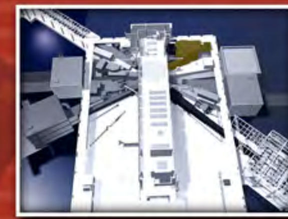
06-G01636E/gim

# Instrument Fact Sheet

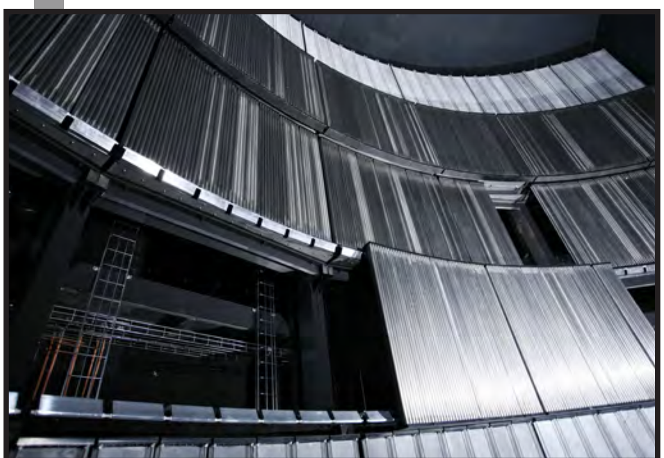
BEAM LINE **17**

SPALLATION NEUTRON SOURCE



## SEQUOIA – Fine-Resolution Fermi Chopper Spectrometer

SEQUOIA is optimized to provide a high neutron flux at the sample and fine energy resolution. The spectrometer can select neutrons with incident energies from several thousandths of an electron volt to a few electron volts and thus can study excitations over this wide energy scale. An elliptically shaped supermirror guide in the incident flight path boosts the performance at the lower end of this range. The sample and detector vacuum chambers provide a window-free final flight path and incorporate a large gate valve to allow rapid sample changeout. A new $T_0$ neutron chopper blocks the prompt radiation from the source and eliminates unwanted neutrons from the incident beam line.



### Specifications

| | |
|---|---|
| Moderator | Decoupled ambient water |
| Source-to-Fermi chopper distance | 18 m |
| Chopper-to-sample distance | 2.0 m |
| Sample-to-detector distance | 5.5–6.3 m cylindrical geometry |
| Incident energy range | 4–2000 meV |
| Resolution (elastic) | 1–5% $E_i$ |
| Vertical detector coverage | $^-$18–18° |
| Horizontal detector coverage | $^-$30–60° |
| Minimum detector angle | 2.5° |

Status: Available to users

### Applications

With its capability to acquire data quickly and relate them to three-dimensional momentum transfers, SEQUOIA allows new studies of single crystals and novel systems such as the following:

- High-temperature superconductivity: spin dynamics in superconductors and precursor compounds and incommensurate spin fluctuations at varying doping levels
- Model magnetic systems, such as one-dimensional spin chains and spin ladders, and crossover effects from one- to three-dimensional magnetism
- Excitations in quantum fluids, quantum critical phenomena, and non-Fermi liquid systems
- High-resolution crystal field spectroscopy reaching into the 1-eV range
- Coupling of electronic and spin systems in correlated-electron materials
- Water in confined structures and extreme conditions
- Hydrogen and other gasses under confinement, including nano-confinement
- Hydrogen in minerals


### For more information, contact

Instrument Scientist: Garrett Granroth, granrothge@ornl.gov, 865.805.0631

Instrument Scientist: Sasha Kolesnikov, kolesnikovai@ornl.gov, 865.576.9145

neutrons.ornl.gov/sequoia



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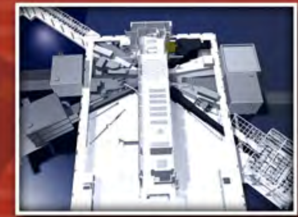
06-G00806G/gim

# INSTRUMENT Fact Sheet

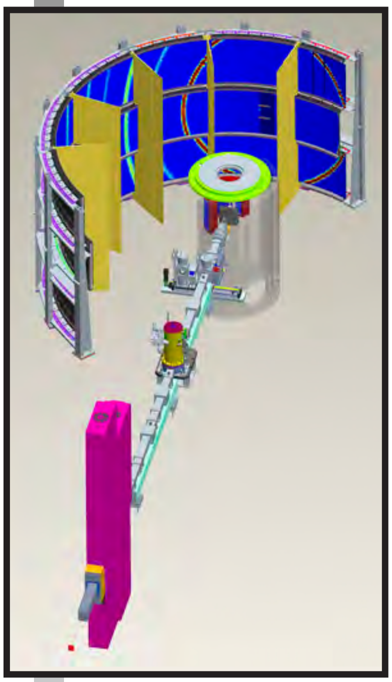
BEAM LINE 18

SPALLATION NEUTRON SOURCE



## ARCS – WIDE ANGULAR-RANGE CHOPPER SPECTROMETER

ARCS is optimized to provide a high neutron flux at the sample and a large solid angle of detector coverage. This spectrometer is capable of selecting incident energies over the full energy spectrum of neutrons, making it useful for studies of excitations from a few to several hundred milli-electron volts. An elliptically shaped supermirror guide in the incident flight path boosts the performance at the lower end of this range. The sample and detector vacuum chambers provide a window-free final flight path and incorporate a large gate valve to allow rapid sample changeout. A new type of neutron $T_0$ chopper blocks prompt radiation from the source and eliminates unwanted neutrons.



*Engineering model of ARCS with neutron powder diffraction data superimposed on the large detector array.*

### APPLICATIONS

The increased sensitivity of ARCS offers new opportunities for scientific studies
in the following:

Lattice Dynamics

- Entropy and the effects of vibrational modes on stability and phase transitions of solids
- Excitations in disordered materials; effects of nanoscale features on vibrational entropy and thermodynamic stability
- Equations-of-state from the measured phonon density-of-states versus temperature and pressure
- Phonons in correlated-electron materials; coupling of lattice and electronic degrees of freedom in high-Tc, heavy-fermion, and mixed-valence materials

Magnetic Dynamics

- High-temperature superconductivity; spin dynamics in superconductors and precursor compounds and crystal field spectroscopy
- Low-dimensional systems; one-dimensional quantum magnets and low-dimensional conductors
- Magnetism in actinide materials; heavy-fermion magnetism and superconductivity

Chemical Physics

- Deep inelastic neutron scattering studies of hydrogen and helium

### SPECIFICATIONS

| | |
|---|---|
| Moderator | Decoupled ambient water |
| Source-to-Fermi chopper distance | 11.6 m |
| Chopper-to-sample distance | 2.0 m |
| Sample-to-detector distance | 3.0 to 3.4 m cylindrical geometry |
| Incident energy range | 20–1500 meV |
| Resolution (elastic) | 2–5% $E_i$ |
| Detector coverage horizontal | -28–135° |
| Detector coverage vertical | -27–26° |
| Minimum detector angle | 3° |

Status: Available to users


### FOR MORE INFORMATION, CONTACT

Instrument Scientist: Doug Abernathy, abernathydl@ornl.gov, 865.617.5624
Instrument Scientist: Matthew B. Stone, stonemb@ornl.gov, 865.202.6898


neutrons.ornl.gov/arcs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