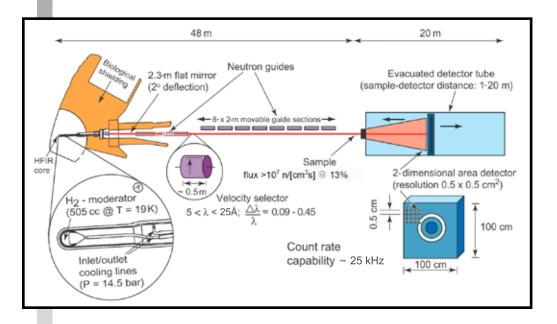
GENERAL-PURPOSE SANS - SMALL-ANGLE NEUTRON SCATTERING DIFFRACTOMETER

The general-purpose SANS diffractometer is optimized for providing information about structure and interactions in materials in the size range of 0.5–200 nm. It will have cold neutron flux on sample and capabilities comparable to those of the best SANS instruments worldwide, including a wide range of neutron wavelengths λ 5–25 Å, resolution $\delta\lambda/\lambda$ 9-45%, and a 1-m² area detector with 5- \times 5-mm² pixel resolution with a maximum counting capability of up to 25 kHz. The sample-to-detector distance can be varied from 1 to 20 m, and the detector can be offset horizontally by up to 45 cm, allowing a total accessible Q range of from <0.001 to 1 Å-1. The 2-m sample environment area will accommodate large, special-purpose sample environments such as cryomagnets, furnaces, mechanical load frames, and shear cells.



APPLICATIONS

- Soft condensed matter: molecular self-assembly and interactions in complex fluids; intermediate order in glassy systems, polymer solutions, gels and blends, colloids, micelles, and microemulsions
- Hard condensed matter: phase separation, grain growth, and orientation in metallurgical alloys, nanocomposites, advanced ceramics, and porous catalytic and adsorbent materials
- Magnetic systems: flux lattices in superconductors, ferrofluids, and the relationship between structural and magnetic domains and ordering

FOR MORE INFORMATION, CONTACT

Instrument Scientist: Ken Littrell, littrellkc@ornl.gov, 865.574.4535

Instrument Scientist: Yuri Melnichenko, melnichenkoy@ornl.gov, 865.576.7746 Scientific Associate: Katherine Bailey, atchleykm@ornl.gov, 865.574.3989

http://neutrons.ornl.gov/hfir instrument systems/CG-2.shtml

SPECIFICATIONS

Beam spectrum	Cold
Monochromator	Helical slot selector
Incident wavelength	4 < λ < 25 Å
Resolution range	Δλ/λ 9–45%
Collimation	Eight removable guide sections, each 4 × 4 cm² and 2 m long; 2-m open area at sample stage to mount automatic changers, furnaces, magnets, cryostats, pressure cells, etc.
Q range (Å ⁻¹) 1.5-m collimation	0.038 < Q < 1.0 Å ⁻¹ (5 Å); 0.019 < Q < 0.50 Å ⁻¹ (10 Å)
20-m collimation	0.004 < Q < 0.074 Å ⁻¹ (5 Å); 0.002 < Q < 0.037 Å ⁻¹ (10 Å)
Sample- detector distances	1 < D < 20 m
Detector	2-D (³ He) position-sensitive detector with 1-m ² active area and 5.1 x 5.1 mm ² pixels
Max counting rate	25 kHz

Status: Operational



BIO-SANS - BIOLOGICAL SMALL-ANGLE NEUTRON SCATTERING INSTRUMENT

Bio-SANS was designed and optimized for analysis of the structure, function, and dynamics of complex biological systems. Bio-SANS is the cornerstone of the Center for Structural Molecular Biology (CSMB) at Oak Ridge National Laboratory. The



Detector tanks for the new SANS instruments at HFIR. The Bio-SANS detector is on the left.

CSMB capabilities that include development of advanced computational tools for neutron analysis and modeling, as well as biophysical characterization and X-ray scattering infrastructure. A dedicated biological sample preparation laboratory is located adjacent to the instrument.

Bio-SANS instrument is

supported by additional

CENTER CAPABILITIES

SPECIFICATIONS

Wavelength

Wavelength

resolution

Sample-

distance

Detector

resolution/ pixel size

to-detector

6< λ <25 Å

 $\Delta \lambda / \lambda =$

12-45%

1-15 m

5.1 x 5.1 mm²

Q range | 0.001-1 Å-1

Detector 2-D 3He

Detector size 1 x 1 m

Max count 25 kHz

Status: Operational



http://www.csmb.ornl.gov





APPLICATIONS

- Bio-macromolecules and their assemblies
 - Protein complexes
 - Protein/DNA complexes
 - Lipids
 - Viruses
 - Carbohydrates
- Hierarchical biological structures
 - Gels
 - · Fibers and fibrils
 - Vesicles
 - Microemulsions
- Membrane diffraction
- Biomimetic and bio-inspired systems

USER ACCESS

Bio-SANS is operated as a user facility and is sponsored by DOE's Office of Biological and Environmental Research. The instrument is managed under the CSMB User Program.

FOR MORE INFORMATION, CONTACT

Instrument Scientist: Volker Urban, urbanvs@ornl.gov, 865.576.2578 Instrument Scientist: William Heller, hellerwt@ornl.gov, 865.241.5694

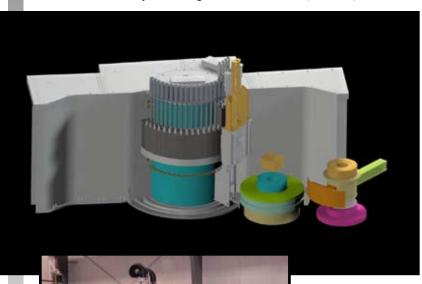
Center Director: Dean Myles, mylesda@ornl.gov, 865.574.5662

http://neutrons.ornl.gov/hfir_instrument_systems/factsheet_pdf/Instrument_cg3.pdf



US/JAPAN COLD NEUTRON TRIPLE-AXIS SPECTROMETER

The US/Japan Cold Neutron Triple-Axis Spectrometer is a conventional triple-axis spectrometer with variable incident energy and variable monochromator-sample and sample-analyzer distances. The cold guide 4 bender and guide hall shielding reduce background levels at CG-4C, and the 15-cm-tall guide profile is well exploited by CG-4C's vertically focusing monochromator (PG 002). To enhance accommodation



of strong magnetic fields at the sample position and to simplify future polarization analysis, the amount of ferromagnetic material has been minimized in the construction of this instrument.

CG-4C is a collaboration of the Neutron Scattering Science Division

at Oak Ridge National Laboratory, the Neutron Scattering Group at Brookhaven National Laboratory, and the Neutron Science Laboratory, Institute for Solid State Physics, at the University of Tokyo.

SPECIFICATIONS

Incident energy range (PG 002)	2–20 meV
Final energy range (PG 002)	>2.8 meV
Sample scatter angular range	Geometry dependent (<160°)
Collimation before mono- chromator	Guide dependent (40' at 2 meV, 20' at 20 meV)
Collimation after mono- chromator	10', 20', 40', 80'

Status:

To be commissioned in 2010

APPLICATIONS

- High-resolution measurement of low-energy excitations with high signal-to-noise ratios due to the low background
- Studies of magnetic phenomena, exploiting the energy range that matches achievable applied field at sample

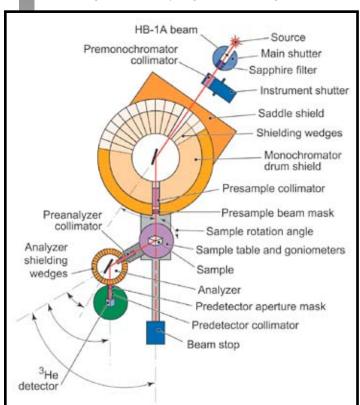
FOR MORE INFORMATION, CONTACT

Principal Investigator: Steve Shapiro, shapiro@bnl.gov, 631.344.3822 Principal Investigator: Hideki Yoshizawa, yoshi@issp.u-tokyo.ac.jp Instrument Scientist: Barry Winn, bwinn@bnl.gov, 865.241.0092 http://neutrons.ornl.gov/hfir instrument systems/CG-4C.shtml



POLARIZED TRIPLE-AXIS SPECTROMETER

The HB-1 Polarized Triple-Axis Spectrometer is designed primarily for the study of excitations in crystalline solids at intermediate energies. Thanks to the vertical beam focusing and the very high time-averaged flux at HFIR, its geometry is optimal for



investigating small samples and weak scattering in specific areas of energy-momentum space. The sample goniometers and a full software implementation of the three-dimensional sample orientation matrix allow measurements outside the traditional single-scattering plane. The unique capability of HB-1 is the polarized configuration for studies of excitations, phase transitions, structures, and density distributions in magnetic materials. Use of a beryllium lowpass filter makes the instrument suitable for hypothermal neutron measurements with incident or final energy below 5 meV.

APPLICATIONS

The following are some of the scientific applications for which the Triple-Axis Spectrometer is particularly well suited.

- Spin waves in ordered magnetic materials
- Exotic excitations in low-dimensional, molecular, itinerate, and other "quantum" magnets
- Spin and lattice excitations in high-T_c superconductivity, colossal magnetoresistance materials, and multiferroic systems
- Spin density distributions in magnetic compounds
- Phonon dispersion curves in alloys and phonon-driven phase transitions

SPECIFICATIONS

Beam spectrum	Thermal
Monochro- mators	Unpolarized PG(002)
	Polarized Heusler (1 1 1)
Analyzers	Unpolarized PG(002), Be(101), Be(002)
	Polarized Heusler (1 1 1)
Monochro- mator takeoff angle	$2\Theta_{\rm M} = 18 \text{ to}$ 75°
Sample angles	360°
Scattering angle	–90 to 140°
Analyzer angles	–40 to 140°
Collimations (FWHM)	Premono- chromator: 15', 30', 48'
	Monochro- mator-sam- ple: 20', 40', 60', 80'
	Sample- analyzer: 20', 40', 60', 80'
	Analyzer- detector: 70', 120', 240'

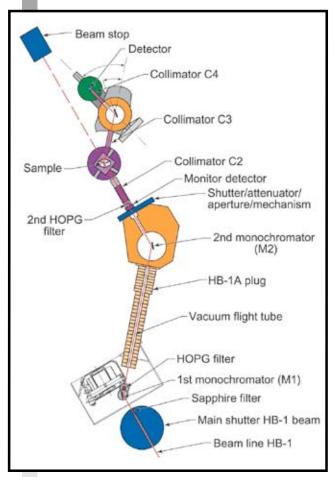
Status: Operational



FOR MORE INFORMATION, CONTACT

FIXED-INCIDENT-ENERGY TRIPLE-AXIS SPECTROMETER

The Fixed-Incident-Energy (14.6 meV) Triple-Axis Spectrometer uses a double pyrolitic graphite monochromator system. The first monochromator is vertically focused, and the second can be either a vertically or doubly focused unit. Two highly oriented pyrolytic graphic filters (HOPG), one after each monochromator, are used to reduce $\lambda/2$ contamination. These filters, together with the double monochromator system, provide HB-1A with an exceptionally clean beam in terms of higher-order contamination neutrons: $I_{\lambda/2} \approx 10^{-4}$ x I_{λ} . This spectometer also has one of the most intense beams at this



energy at the HFIR, as well as a very low γ and fast neutron background. Typical energy resolution is \sim 1 meV, but, using the beryllium analyzer, the energy resolution width can be reduced to \sim 0.5 meV.

HB-1A development and operation is a collaborative effort of the Oak Ridge National Laboratory and Ames Laboratory neutron scattering groups.

APPLICATIONS

- Excitation spectra to ~35 meV using neutron energy gain and low-lying excitations, 1–9 meV, using neutron energy loss
- Elastic studies on crystallographic and magnetic structures and transitions in a Q range of 0.2 to 4.9 Å⁻¹
- Elastic studies and excitations in thin films and other small-volume samples where high flux and very low higher-order contamination of the beam are critical

Recent experiments on this instrument include measurement of phonon dispersion curves in martensitic, shape-memory, and magnetostrictive alloys; crystallographic and magnetic structure determinations in giant magnetocaloric, magnetoresistive, and intermetallic alloys; magnetic structures and spin-density waves in thin films; magnetism in low-dimensional systems; and spin waves and magnetic structures in magnetoelectric materials.

SPECIFICATIONS

Beam spectrum	Thermal
Monochro- mator	PG(002) double crystal
Monochro- mator takeoff angle	2Θ _M = 41.3° E, = 14.7 meV
Analyzers	PG(002), Be(101), Be(002), Si(111), Ge(111)
Sample angle	0° to 360°
Scattering angle	-5° to 135°
Analyzer angles	-60° to 120°
Collimations (FWHM)	Premonochro- mator: 48'
	Monochromator-sample: 10', 20', 30', 40'
	Sample-ana- lyzer: 10', 20', 30', 40'
	Analyzer-detector: 70', 140'
Beam size	40 × 150 mm max
Filters	Sapphire pre- monochro- mator 2 HOPG; after M1 and M2
Flux at sample	~ 2 × 10 ⁷ n/ cm ² /s (est.)
Momentum range	0.2 to 4.9 Å ⁻¹ (elastic configuration)
Energy transfer	~-35 meV to ~+11 meV at q = 3 Å ⁻¹

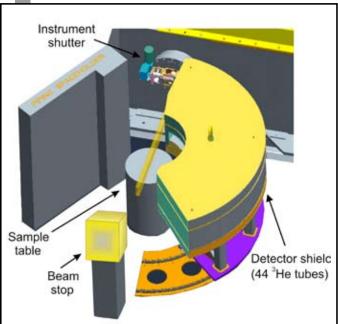
Status: Operational



FOR MORE INFORMATION, CONTACT

NEUTRON POWDER DIFFRACTOMETER

The Neutron Powder Diffractometer has a Debye-Scherrer geometry. The detector bank has 44 ³He tubes, each with 6' Soller collimators. A germanium wafer-stack monochromator is vertically focusing and provides one of three principal wavelengths, depending on which reflection is in the diffracting condition: (113) 2.41 Å, (115)



1.54 Å, and (117) 1.12 Å. The takeoff angle from the monochromator is fixed at 90°, and the minimum peak full width at half maximum (FWHM) is 0.2°. There are two choices of premonochromator collimation (α_1 = 12' or open) and three choices of presample collimation (α_2 = 16', 21', or 31') that allow the operation of the instrument in high-resolution or high-intensity modes.

APPLICATIONS

The HB-2A Neutron Powder Diffractometer is a workhorse instrument used to conduct crystal structural and magnetic structural studies of powdered and ceramic samples, particularly as a function of intensive conditions (T, P, H, etc.). Technologically important materials amenable to study by neutron powder diffraction include (but are not limited to) catalysts, ionic conductors, superconductors, alloys, intermetallic compounds, ceramics, cements, colossal magnetoresistance perovskites, magnets, minerals, waste forms, H-storage, thermoelectrics, zeolites, and pharmaceuticals. Powder diffraction data collected on this instrument are ideally suited for the Rietveld method. In addition to traditional crystal structural refinements, studies of phase transitions, thermal expansion, quantitative analysis, residual stress, and ab initio structure solution can be undertaken from the powder data. A full range of ancillary sample environments can be used, including cryofurnaces (4–800 K), furnaces (to 1800 K), cryostats (to 0.3 K), and cryomagnets (to 7 T).

SPECIFICATIONS

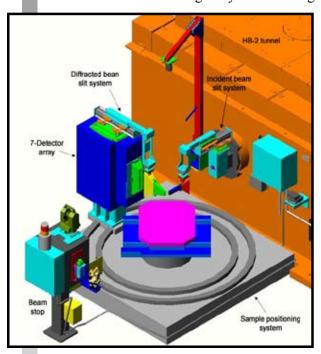
Beam spectrum	Thermal
Monochro- mator	Vertically focusing Ge (115) 20
Monochro- mator angle	$2\Theta_{\rm m} = 90^{\circ}$
Wavelengths	λ=1.54 Å(115) 2.41 Å(113) 1.12 Å(117)
Sample angles	0° < ω < 360°
Scattering angle	0° < 2Θ < 150°
Collimations (FWHM)	$\alpha_{_{1}}$ =12' or open $\alpha_{_{2}}$ =16', 21', or 31'
Detector bank	44 ³ He detectors
Beam size	25 x 25 mm ² at sample position
Resolution	2 x 10 ⁻³ \(\Delta d/d \)

Status: In commissioning



NRSF2 - NEUTRON RESIDUAL STRESS MAPPING FACILITY

NRSF2 at the HFIR HB-2B beam port is optimized for strain measurement and determination of residual stress in engineering materials. The large-specimen "XYZ" instrument is designed for spatial scanning of strains at depths from submillimeters to centimeters. The sample orienter can be used to determine the stress tensor and texture as a function of location. The sample orienter can also be used for mapping strain in large-grained materials and within single crystals. The high flux and large detector coverage allow



real-time, in situ studies or high-resolution mapping. Ancillary equipment available for use at NRSF2 includes a 2,267-kg uniaxial (tension or compression) load frame, a Huber Eulerian cradle, high-temperature furnaces (vacuum or air), and a 5-T superconducting magnet with an induction furnace insert. Custom-built sample environment systems can be installed on the XYZ sample positioning system. A metrology system consists of a Laser ScanArm, Laser Tracker, and SScanSS virtual instrument software. These tools are used to plan experiments, establish measurement locations in the sample coordinate system, calculate beam attenuation, check for potential collisions, and generate the script file for running NRSF2. Together they reduce neutron beam time used for alignment and increase accuracy of location of measurement.

APPLICATIONS

The penetrating power of neutrons is useful in mapping residual stresses in engineering materials. Examples of applications include residual stress maps of welds, heat-treated samples, forgings, extrusions, bearings and races, fasteners, and composites. Neutron diffraction studies of materials under applied stress reveal phase- and grain-level knowledge of deformation processes, which is fundamental for developing finite-element method and self-consistent field models of materials behavior. Also characterized are strains in functional materials, such as piezoelectrics under the influence of electrical fields, shape memory alloys, and hydrogen storage materials.

USER ACCESS

NRSF2 at HB-2B is sponsored by the Assistant Secretary for Energy Efficiency and Renewable Energy, Vehicle Technologies Program, as part of the High Temperature Materials Laboratory User Program (HTML), Oak Ridge National Laboratory. Information about the HTML rapid access proposal process can be obtained from html.ornl.gov.

FOR MORE INFORMATION, CONTACT

Instrument Scientist: Camden Hubbard, hubbardcr@ornl.gov, 865.574.4472 http://neutrons.ornl.gov/hfir_instrument_systems/HB-2B.shtml

SPECIFICATIONS

Beam spectrum	Thermal
Monochromator	Stacked Si wafers with vertical and horizontal focusing
Monochromator takeoff angle	88° (fixed), λ = 1.452 Å (Si 511); 1.540 Å (Si 422); 1.731 Å (Si 331); 1.886 Å (Si 400); 2.275 Å (Si 311); 2.667 Å (Si 220)
Flux on sample	3 x 10 ⁷ n/cm ² /s (Si 331 and Si 400)
Detector angle range	70-110° optimal
Detection system	7 linear position- sensitive detectors
Position- sensitive detector coverage	5° 2⊖ ±17° out of plane
Sample positioner	Ω ± 180° X ± 200 mm Y ± 100 mm
Z elevator Z translation	Z ± 100 mm, 500 Kg Z ± 200 mm, 50 Kg
Nominal gage volume	Width: 0.3–5 mm; Height: 0.3–20 mm
Peak location precision	0.003° 2⊖
Sample environments	Load frame for tension and compression (2,267-kg) Huber Eulerian cradle for tensor

Status: Operational



and texture

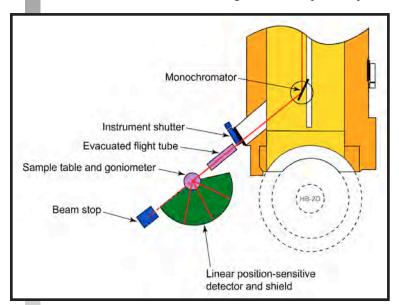
 Vacuum and environmental furnaces

5-T superconduct-

ing magnet with induction heater

WAND - US/JAPAN WIDE-ANGLE NEUTRON DIFFRACTOMETER

The US/Japan WAND at the HFIR HB-2C beam tube was designed to provide two specialized data-collection capabilities: (1) fast measurements of medium-resolution powder-diffraction patterns and (2) measurements of diffuse scattering in single crystals using flat-cone geometry. For these purposes, this instrument is equipped with a curved, one-dimensional ³He position-sensitive detector covering 125° of the scattering angle with the focal distance of 71 cm. The sample and detector can be tilted in the flat-cone geometry mode. These features enable measurement of single-crystal diffraction patterns in a short time over a wide range of the reciprocal space, as well as performance of time-



resolved experiments for structural transformations having short time constants. The WAND detector (ORDELA 1410N) is a multianode type (624 anodes and a 0.2° pitch) ³He gas counter specially designed for this instrument. This detector has an intrinsic angular resolution of 0.25° and a maximum counting rate per anode of 10⁵ counts/s.

SPECIFICATIONS

Beam spectrum	Thermal
Monochro- mator	Vertically focused Ge(113). Ge(115) is also available to provide λ =0.95 Å
Monochro- mator angle	$2\Theta_{\rm M} = 52.0^{\circ}$
Wavelength	$\lambda = 1.5 \text{Å}$
Scattering angles	10° < 2Θ < 135°
Sample angles	0° < Ω < 135°
Detector	Multiwire (624 anodes, 0.2° pitch) He³ curved PSD

Status: Operational

APPLICATIONS

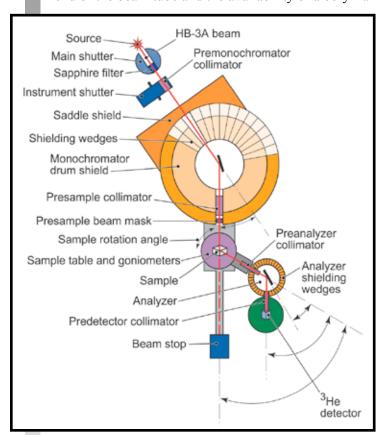
WAND is ideal for the study of time-resolved phenomena and for the study of diffuse scattering in single crystals. Research performed at WAND includes studies of the growth of ferroelectric ice-XI, hole and charge ordering in colossal magnetoresistance materials, and studies of magnetic structures and correlations in low-dimensional magnetic systems and other magnetic materials.

WAND is operated in collaboration with the Japan Atomic Energy Research Institute under the US/Japan Cooperative Program on Neutron Scattering Research.



TRIPLE-AXIS SPECTROMETER

HB-3 is a high-flux thermal neutron three-axis spectrometer designed for inelastic measurements on single crystals over a wide range of energy and momentum transfers. Although the energy and momentum range for measurements is quite large at HB-3, the instrument is the ideal location for performing experiments at high-energy transfers (up to about 100 meV). This is due to a combination of its location directly at the end of the beam tube and the availability of a beryllium monochromator. The HB-3



monchromator provides three crystal choices (PG 002, Be 002, and Si 111) with variable vertical focus. This focus is calibrated to maintain the smallest beam size at the sample position, thus optimizing incident neutron flux as the incident energy varies. Of the three monochromators, pyrolitic graphite provides the highest neutron intensity as a result of its very high neutron reflectivity. The high-quality beryllium monochromator allows measurements with good energy resolution at higher energy transfers, whereas the silicon 111 monochromator has the advantage of an absent secondorder reflection, providing a higher order contaminationfree beam

SPECIFICATIONS

Beam spectrum	Thermal
Monochro- mators	PG (002), Be (002), Si (111)
Analyzer	PG (002)
Monochro- mator takeoff angle	$2\Theta_{\rm M} = 18 \text{ to}$ 75°
Sample angle	0–360°
Scattering angle	-90 to 115°
Analyzer angle	⁻ 120–120°
Collimations (FWHM)	Premono- chromator: 15', 30', 48' Monochro- mator- sample: 20', 40', 60', 80' Sample- analyzer: 20', 40', 60', 80' Analyzer- detector: 70',
	90', 120', 180', 240'

Status: Operational

APPLICATIONS

The availability of three different monochromator crystals makes HB-3 an extremely versatile instrument for studies of excitations in materials with energies ranging from 2 to 100 meV. Typical applications include spin and lattice dynamics in high-temperature superconductors and related compounds; low-dimensional magnetic model systems; magnetic excitations and phonons in colossal magnetoresistive materials, multiferroics, and ruthenates; and spin waves in magnetically ordered materials. The high incident neutron flux makes HB-3 well suited to studying samples that have a small volume or weak scattering characteristics.

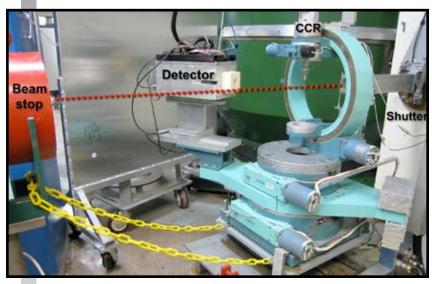
FOR MORE INFORMATION, CONTACT

Instrument Scientist: Mark Lumsden, lumsdenmd@ornl.gov, 865.241.0090 http://neutrons.ornl.gov/hfir_instrument_systems/HB-3.shtml



FOUR-CIRCLE DIFFRACTOMETER

The Four-Circle Diffractometer goniometer has a full χ circle with a 4-K closed-cycle helium refrigerator. The detector is 3 He with a 7-anode array in a honeycomb pattern. The upper 2Θ limit is 100° . A multilayer-[110]-wafer silicon monochromator with the reflection from planes of the <011> zone ensures sharp diffraction peaks in specified ranges of detector angles by control of the horizontal radius of curvature. Any plane from the <011> zone can be set in Bragg position, but only the (331), (220), and (111) reflections are of practical interest. For the fixed monochromator angle of 48°, these reflections provide principal incident wavelengths of 1.01, 1.56, and 2.55 Å, respectively. A PC-based system provides user-friendly diffractometer control and



data acquisition. The beam size is $5 \times 5 \text{ mm}^2$, and the minimum crystal size is 1 mm^3 . The maximum crystal dimension is about 4 mm. The flux on the sample is estimated to be greater than $5 \times 10^6 \text{ n/cm}^2/\text{s}$.

APPLICATIONS

This instrument is suitable for a wide range of small-unit-cell crystallography studies, from structure refinement and solution to charge and nuclear density mapping. Problems from chemistry, physics, materials science, and mineralogy have been addressed. Specific areas of study include hydrogen bonding and weak interactions, organometallics, supramolecular chemistry and crystal engineering, metal hydrides, charge density, pharmaceuticals, and magnetic structures. More general solid-state physics problems in magnetism, diffuse scattering, and ordering phenomena can also be addressed.

SPECIFICATIONS

Beam spectrum	Thermal
Monochro- mators	Vertically focusing silicon
Monochro- mator angle	48°
Incident wavelength	1.01 Å (331), 1.56 Å (220), 2.55 Å (111)
Goniometer	Huber, full chi circle, with 4 K CCR
Scattering angle	100° < 2θ < -90°
Detector	7 anode ³ He (honeycomb pattern)
Crystal size requirement	>1 mm³
Unit-cell size	<15,000 ų
Flux at sample	>5 × 10 ⁶ n cm ⁻¹ s ⁻¹ (est.)

Status: In commissioning

FOR MORE INFORMATION, CONTACT

