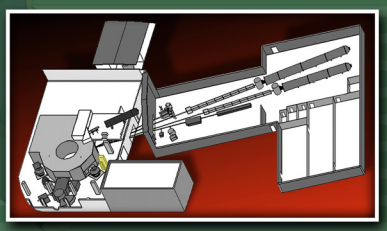
Instrument Fact Sheet

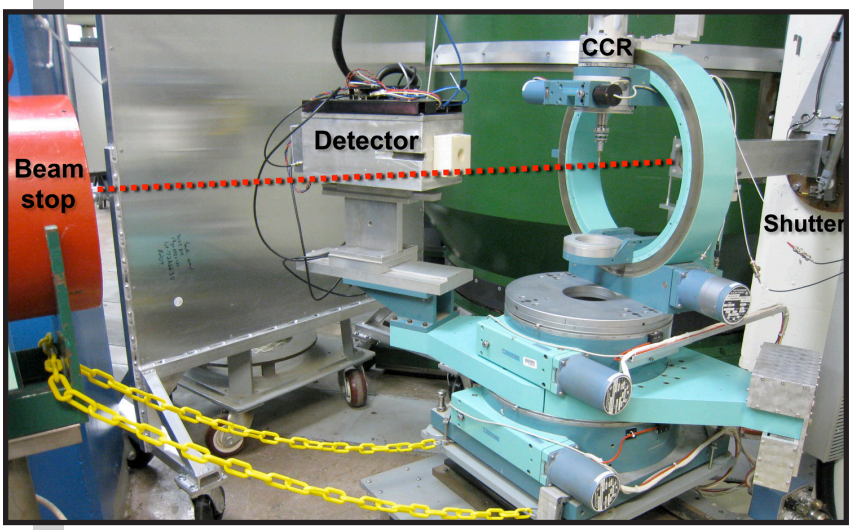
BEAM LINE **HB-3A**

High Flux Isotope Reactor



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 155°. 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) with (044), and (111) with (333) reflections are of practical interest. For the fixed monochromator angle of 48°, these reflections provide principal incident wavelengths of 1.000, 1.536, and 2.540 Å, respectively. A PC-based system provides user-friendly diffractometer control and data acquisition. The beam size is 5 × 5 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 up to 2.2 × 10^7 n/cm^2/s. Both high-resolution or high-intensity modes are possible by tuning the horizontal bending of the monochromator.



Specifications

Beam spectrum	Thermal
Monochro-mator	Silicon (fixed vertical focus with adjustable horizontal bending)
Monochro-mator angle	48°
Incident wavelengths	1.000 Å (331), 1.536 Å (220), 2.5405 Å (111)
Goniometer	Huber, full chi circle, with 4 – 450 K CCR
Scattering angles	2θ < 155°
Detector	7 anode ^{3}He (honeycomb pattern)
Crystal size requirement	>1 mm^3
Unit-cell size	<15,000 Å^3
q-resolution	Δq/q ~ 0.01
Flux at sample	>2.2 × 10^7 n cm^{-1} s^{-1}

Status: Available to users

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 can be 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 are also feasible. Unit cell volumes of less than ~7000 Å^3 are practical.

For more information, contact

Instrument Scientist: Huibo Cao, caoh@ornl.gov, 865.241.9428
Instrument Scientist: Bryan Chakoumakos, chakoumakobc@ornl.gov, 865.574.5235

neutrons.ornl.gov/hb3a

HFIR

May 2012

06-G01639H/gim