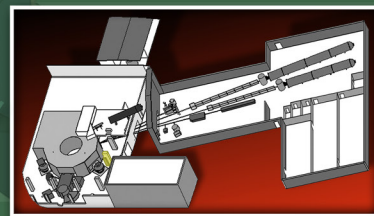


INSTRUMENT

HB-3A

BEAM LINE

HIGH FLUX ISOTOPE REACTOR



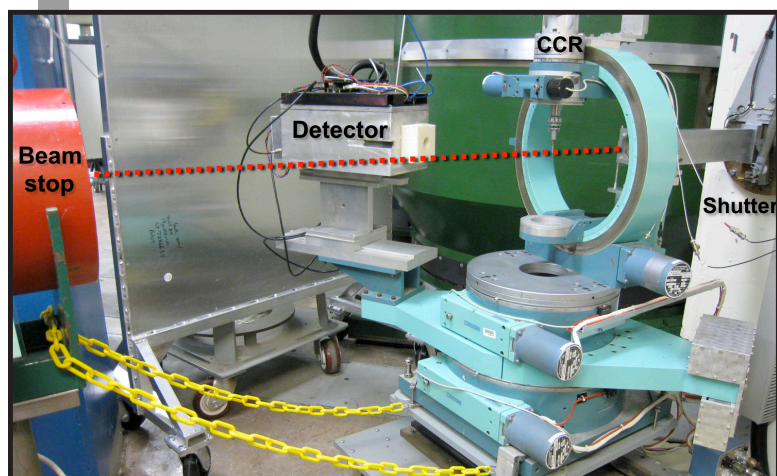
FOUR-CIRCLE DIFFRACTOMETER

SPECIFICATIONS

Beam spectrum	Thermal
Monochromator	Vertically focusing silicon
Monochromator angle	48°
Incident wavelengths	1.003 Å (133), 1.542 Å (022), 2.541 Å (111)
Goniometer	Huber, full χ circle, with 4.5 – 450 K CCR
Scattering angles	5° < 2 θ < 155°
Detector	³ He (single-point)
Crystal size requirement	>1 mm ³ , maximum crystal dimension 5mm
Flux at sample	2.2 × 10 ⁷ n/cm ² /s

Status: Available to users

The Four-Circle Diffractometer goniometer has a full χ circle with a 4.5–450 K closed-cycle helium refrigerator. The detector is ³He with a 7-anode array in a honeycomb pattern. Currently, only the center anode is used with the remaining 6 anodes not active. The upper 2 θ 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 (440), and (111) with (333) reflections are of practical interest. For the fixed monochromator angle of 48°, these reflections provide principal incident

wavelengths of 1.003, 1.542, and 2.541 Å, respectively. A PC-based LabView system provides user-friendly diffractometer control and data acquisition. The beam size is 6 × 8 mm², and the minimum crystal size is 1 mm³. The maximum crystal dimension is about 5 mm. The flux on the sample can be up to 2.2 × 10⁷ n/cm²/s. The horizontal bending of the monochromator can be changed to optimize the resolution or intensity depending upon the needs of the measurement. The longer wavelength of 2.541 Å has ~5% $\lambda/3$ contamination, the 1.542 Å-wavelength has ~2.28% $\lambda/2$ contamination, and the 1.003 wavelength is monochromatic.

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. It can be used to study superlattice structures and atomic anharmonicity. The instrument is particularly suitable for studying magnetic structures, phase transitions and possible accompanied structural changes, as well as measuring order parameters and exploring the phase diagram. Users have researched problems in chemistry, physics, materials science, and mineralogy. Recent specific areas of study include magnetic structure and nuclear superstructure in iron pnictide superconductors, multiferroic oxide phase transitions and diagrams, magnetic/orbital frustration in spinels, temperature dependence of atomic displacement parameters in battery and thermoelectric materials, hydrogen bonding in rock-forming minerals, crystallography of novel scintillators, and diffuse scattering.

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