Pacific Northwest Consortium

University of Washington Simon Fraser University Pacific Northwest National Laboratory

X-Ray Diffraction Capabilities

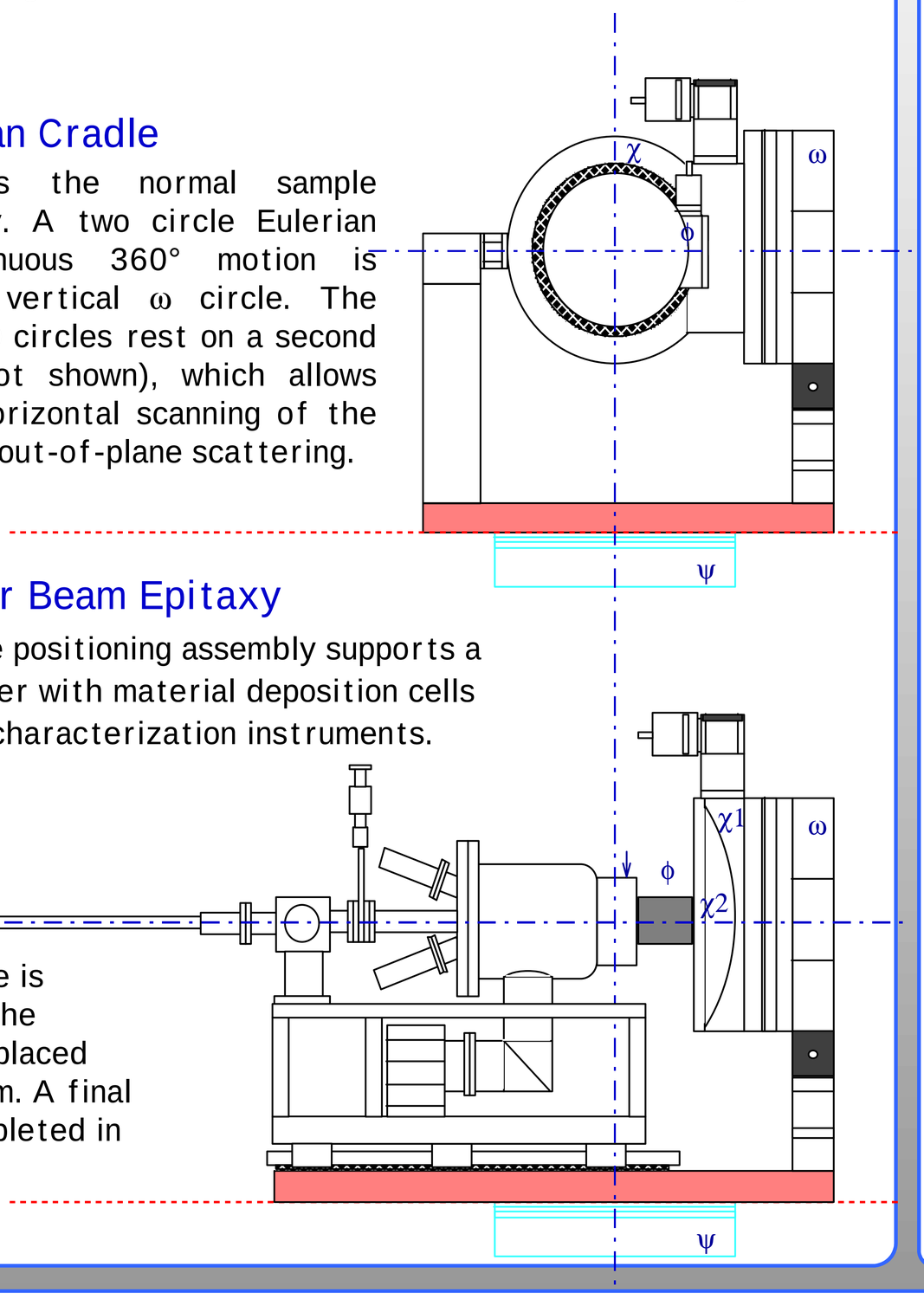
PNC-CAT comprises several research institutions with diverse experimental interests. Because of this, our diffractometers must accomodate a wide range of experiments, with samples and sample environments ranging in size from a few millimeters to a full-sized UHV chamber. In order to meet these requirements, we have installed two general-purpose goniometers on the ID and Bending Magnet lines.

Eight-Circle Psi Goniometer

The basic instrument is a Huber Ψ 8-Circle goniometer with two interchangeable sample positioning assemblies. The two assemblies rest on matching base plates, which use precision tapered steel pins for reproducible mounting. This modular approach provides a true general-purpose instrument.

Standard Eulerian Cradle

This figure shows the normal sample positioning assembly. A two circle Eulerian cradle with continuous 360° motion is supported on the vertical ω circle. The detector arm and 2θ circles rest on a second horizontal stage (not shown), which allows both vertical and horizontal scanning of the detector for in- and out-of-plane scattering.



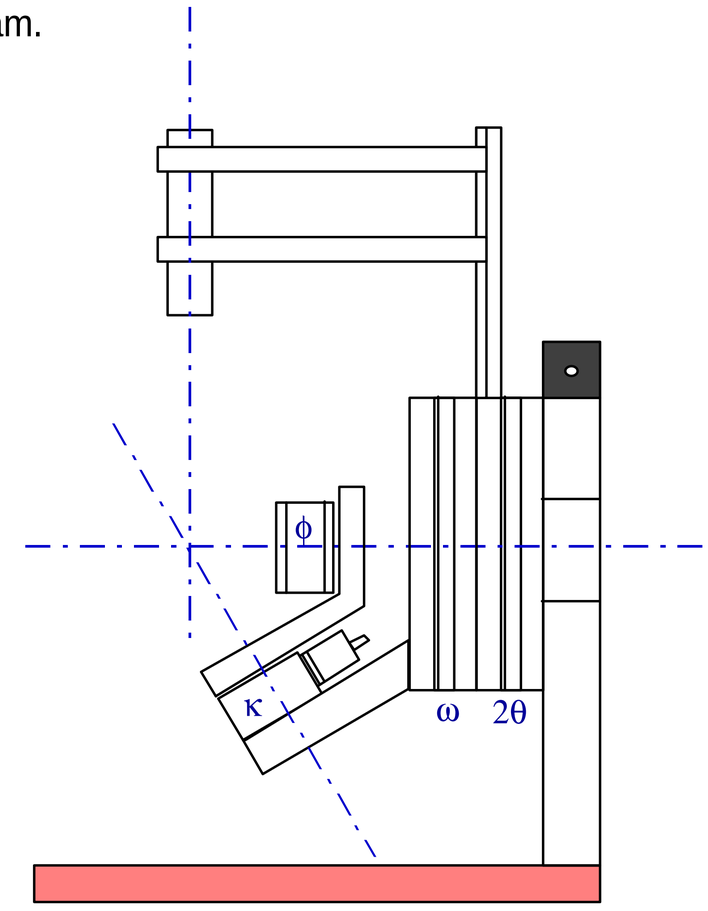
In Situ Molecular Beam Epitaxy

The alternate sample positioning assembly supports a full-size UHV Chamber with material deposition cells and several surface characterization instruments.

A conceptual image is shown here, with the Eulerian Cradle replaced by the UHV system. A final design will be completed in Summer 2000.

Four-Circle Kappa Goniometer

The κ geometry allows unrestricted access to the sample from one side of the goniometer. Although it can only accommodate small samples, due to mechanical limitations of the cantilever arm, the small sphere of confusion (10μm) and minimal sample eclusion makes this the geometry of choice for protein crystallography, in which samples are cryogenically cooled by a continuous nitrogen stream.

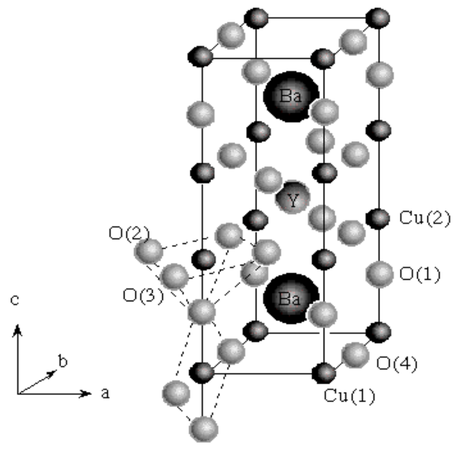


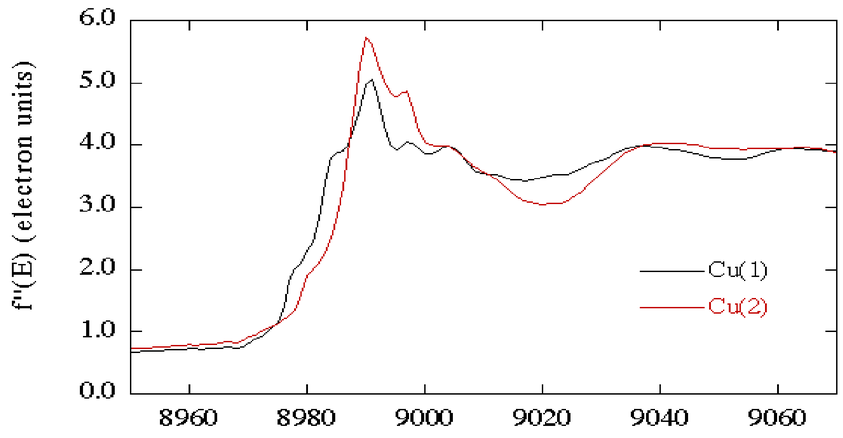
The PNC-CAT κ goniometer is a table top instrument that uses the scanning optical tables in ID-B and BM-B as its base. A precision x-y-z stage with 0.1 μm resolution supports the sample.

Diffraction Anomalous Fine Structure

J.O. Cross, L.B. Sorensen (University of Washington), C.E.Bouldin, J.C. Woicik (NIST), M. Newville (University of Chicago), H.J. Stragier (At Large)

Diffraction anomalous fine structure (DAFS) measures elastic Bragg reflection intensities versus photon energy. This new method combines the long-range order and crystallographic sensitivities of x-ray diffraction with the spectroscopic and short-range order sensitivities of x-ray absorption techniques. DAFS allows spectroscopic information to be isolated from subsets of resonant atoms in complex crystals based on their long-range order





In-plane (a-b) polarized XANES isolated from the inequivalent Cu sites in $YBa_2Cu_3O_{6.8}$ using DAFS

Planned Experiments

Surface Holography

Direct 3-dimensional density maps are generated from two-beam interference patterns measured along crystal truncation rods.

Diffraction Anomalous Fine Structure

Resonant x-ray diffraction in the vicinity of the absorption gives XAFS-like information about subsets of absorbing atoms selected by the diffraction condition.

Powder Diffraction from Aerosols

Evolution of salt crystal formation in sea spray is studied by x-ray diffraction from atomized droplets flowed through a capillary.

Diffraction Tensor Mapping

Out-of-plane resonant diffraction from cations in low symmetry local environments to test ab initio calculations of f' and f" based on the XAFS path formalism