X-ray Powder Diffraction (XPD)

Scientific scope

XPD is a tunable facility with the ability to collect diffraction data at high x-ray energies (40keV-80keV), offering rapid acquisition (milli-second) and high angular resolution capabilities on the same instrument.

XPD addresses future scientific challenges in, for example, hydrogen storage, CO_2 sequestration, advanced structural ceramics, catalysis, and materials processing. Such materials of high technological value often are complex, nanostructured and heterogeneous. The scientific grand challenge is to obtain robust and quantitative (micro)structural information, not only in the ground state at ambient conditions, but also *in situ* or *in operando* with varying temperature, pressure, magnetic/electric/stress field, chemical environment, etc. The beam size is adjustable to match the graininess and heterogeneity scales above the micron scale.

The beamline is of novel optical design, making use of techniques and instrumentation being pioneered at the NSLS (Laue optics and Ge strip array detectors), as well as being matched to the high flux of a full 7m NSLS-II damping wiggler.

In the longer term, the combination with a complementary parallel-operation station dedicated to high-Q, pair distribution function studies will permit determination of both long- and short-range structures.

Beamline description

XPD is designed to operate two independent branch lines simultaneously. In the main branch, the upstream endstation hosts a three-circle diffractometer fitted with a 1D strip detector and a high-resolution detector bank to cover most powder diffraction measurements. The second endstation accommodates more elaborate/complex setups: large pressure cells, non-routine reaction chambers, combined spectrometry, gas handling, user-defined specific devices. The side station will operate at a fixed high energy (60 or 80keV), optimized for total scattering measurements over a large Q range.

Techniques

- Diffraction of polycrystalline materials
- Pair distribution function analysis
- Diffraction tomography

Schematic layout of the beamline

3D CAD view

Conceptual Design Report

Current status:	preliminary design
Construction:	starts January 2012
Commissioning:	begins June 2014
User operation:	begins June 2015

Beamline Performance

Source	Damping Wiggler
Energy range (keV)	40-100
Wavelength range (nm)	0.03-0.012
Energy resolution @50keV	$\Delta E/E = 1.1 \times 10^{-3}$
	$\Delta E/E = 2.0 \times 10^{-4}$ (1)
Beam size at sample (mm^2 FWHM)	2-0.7(h) x 1-0.05(v) (2)
Flux at sample @50keV ph/s	6.3×10^{12}
ph/s/mm^2	2.2×10^{14}

(1) The high resolution mode will be progressively implemented.
(2) Depending on focusing configuration.

Signing of agreement between NSLS-II Project Director Steve Dierker and the XPD Beamline Advisory Team, November 24, 2008. From left to right: (seated) Steve Dierker, Simon Billinge, (standing) Qun Shen, Jonathan Hanson, Lars Ehm, Jim Kaduk, Andy Broadbent, and Peter Chupas. Not present: John Parise. BAT chair.

Equipment in Endstation 1

Sample environments

Furnace	capillary/flat 300 – 1700 K
Hot air blower	ambient - 1300 K
He cryostat	10 – 300 K
Cryostream	80 – 500 K
Flow cells	
Pressure cells	< 100 GPa

Detectors

Scintillation counters	
Si strip detector	120□2θ range - 0.014□2(pixel
2D CCD	
CMOS flat panel	

Contacts

E. Dooryhee	edooryhee at bnl.gov
S. Ghose	sghose at bnl.gov