X-RAY POWDER DIFFRACTION (XPD-1)

BROOKHAVEN NATIONAL LABORATORY

NATIONAL SYNCHROTRON LIGHT SOURCE II

SCIENTIFIC SCOPE

The X-ray Powder Diffraction (XPD-1) beamline at NSLS-II operates at high energies (30 keV-70 keV), and offers exceptional capabilities such as fast (sub-second) readout rates and high angular resolution on the same instrument. The scientific goals are to structurally characterize materials at the frontier of complexity, whether the frontier is nanostructure, heterogeneity or *in situ/in operando* environments. XPD enables powder diffraction and PDF/total scattering measurements on a wide range of functional materials.

BEAMLINE CHARACTERISTICS

TECHNIQUES:

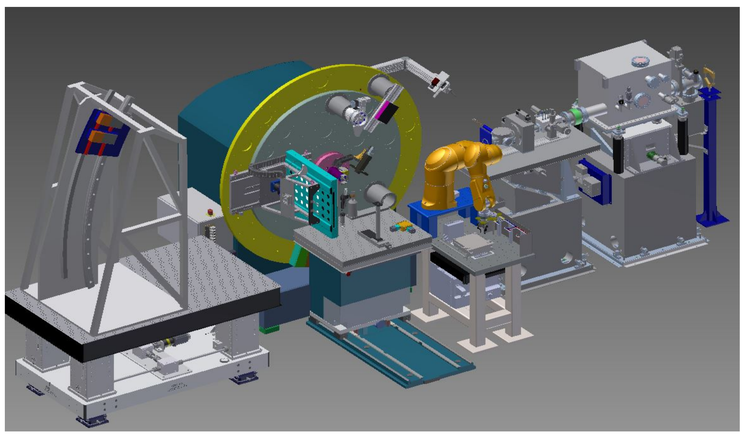
- X-ray Powder Diffraction.
- 2 configurations: high resolution/high flux.
- Stress-Strain scanning.
- Medium Angle X-ray Scattering (MAXS).

ENDSTATION DETAILS:

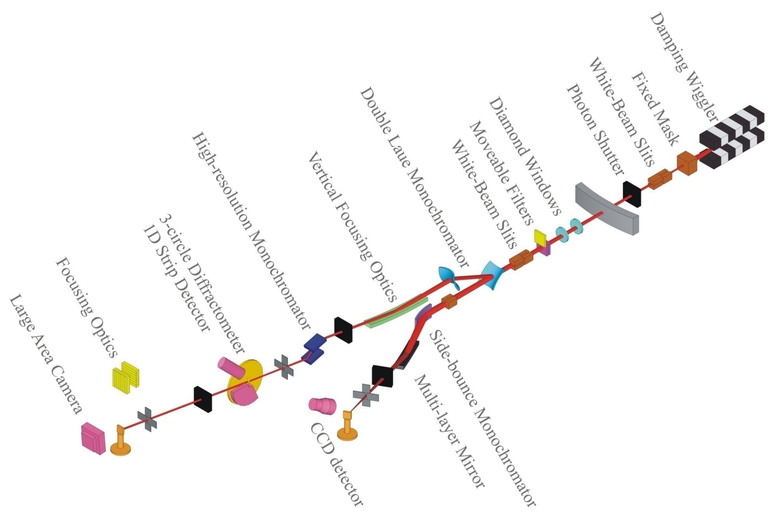
- 3-circle diffractometer.
- A range of detectors (0D to 2D).
- Cryosystems (4K- 500K), furnaces (≤1500°C), high-pressure DAC, high pressure liquid/gas flow cells.
- Robot for high-throughput, combinatorial and screening investigations.

XPD at NSLS-II:

- High-flux configuration enabling time-resolved studies of phase transitions and catalytic reactions vs. T, p or chemical gradients.
- High-resolution measurements for identification and structure solving of new phases.
- New trends in x-rays Materials Science: higher x-ray energy, faster acquisition rates, *in situ*, extreme environments, combined methods.
- Future scientific challenges in hydrogen storage, CO_2 sequestration, advanced structural ceramics, catalysis, and materials processing.



The XPD1 endstation equipment includes: i) a large-area detector for *in situ* time-resolved studies; ii) a multi-crystal array analyzer system; and iii) a Pixel Array Detector for high-resolution, high-energy diffraction.



Schematic layout of XPD showing the two branchlines XPD-1 and XPD-2.

Overview

PORT: 28-ID

SOURCE: Damping Wiggler (DW100)

ENERGY RANGE: 30 – 70 keV

ENERGY Bandpass: $\Delta E/E = 10^{-3}$ to 2×10^{-4}

SPATIAL RESOLUTION: 50 µm

CONSTRUCTION PROJECT: PROJECT

BEAMLINE STATUS: Commissioning

AVAILABLE TO USERS: Spring 2015

Beamline Team

STAFF

Eric Dooryhee: lead beamline scientist

Sanjit Ghose: beamline scientist

Milinda Abeykoon: beamline scientist

Hengzi Wang: mechanical engineer

Wayne Lewis: controls engineer

John Trunk: technician

ADVISORS

Simon Billinge (BNL/Columbia University)

Peter Stephens (Stony Brook University)

John Parise (BNL/Stony Brook University)

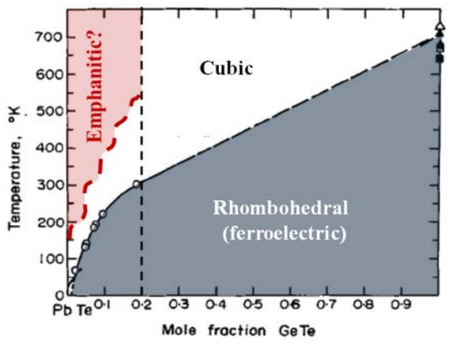
Peter Chupas (Argonne National Lab)

Jonathan Hanson (BNL)

James Kaduk (PolyCrystallography)

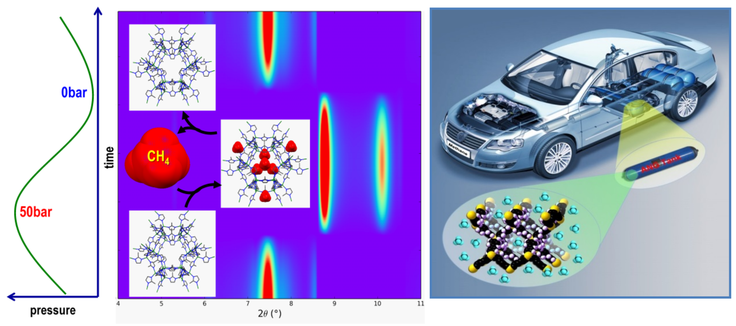
Angus Wilkinson (Georgia Institute of Technology)

SCIENTIFIC APPLICATIONS



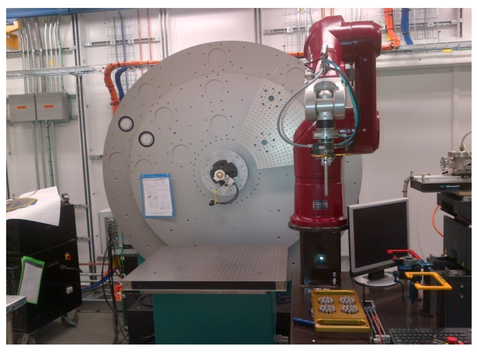
Local structural effects in High Performance Electronic Materials:

- Nanoscale symmetry breaking electronic fluctuations are implicated in novel electronic properties from high temperature superconductivity to high performance thermoelectricity but are difficult to study.
- XPD enables to generate "local phase diagrams" for a range of materials and to relate them to their properties.
- Figure shows for the first time the full short-range and long-range structural phase diagram of $Pb_{1-x}Ge_xTe$.



Modulation Enhanced Diffraction (MED):

- Observe dynamic changes and response of materials, *i.e.* non-equilibrium states and intermediates, all difficult to detect in steady state conditions.
- Application of MED to structural investigations of CH_4-loaded porous materials under pulsed reactant conditions. The on-board methane storage target set by DOE is 500mg/g at 295K, 35bar.
- Direct the development of next-generation materials with improved fuel storage properties.



Nuclear Applications:

- High throughput, combinatorial approach, unmanned operation with hazardous samples.
- Quantitative analysis of the effects of Mn-Ni-Si Late Blooming Phases (LBP) in Irradiated Reactor Pressure Vessel Steels, ferritic-martensitic steels and austenitic stainless steels.
- Effort directly impacts Nuclear Energy (NE) mission on Light Water Reactor sustainability and leverages previous and current NE research programs.