X-RAY POWDER DIFFRACTION 2 (XPD-2)

BROOKHAVEN NATIONAL LABORATORY

NATIONAL SYNCHROTRON LIGHT SOURCE II

SCIENTIFIC SCOPE

Nanoscale fluctuations play an important role in a wide range of technologically important complex materials, such as, strongly correlated systems, multiferroics, thermoelectrics, catalysts, nanomaterials, etc. The X-ray Powder Diffraction 2 (XPD-2) beamline is the dedicated Atomic Pair Distribution Function (PDF) beamline at NSLS-II. XPD-2 enables studies of nanoscale fluctuations in complex materials giving key insights into their structure-property relationship. The high energy and flux available at the XPD-2 will ensure excellent PDF data up to a high momentum transfer resulting in high real-space resolution Atomic Pair Distribution Functions necessary for characterization of these materials.

BEAMLINE CHARACTERISTICS

TECHNIQUES:

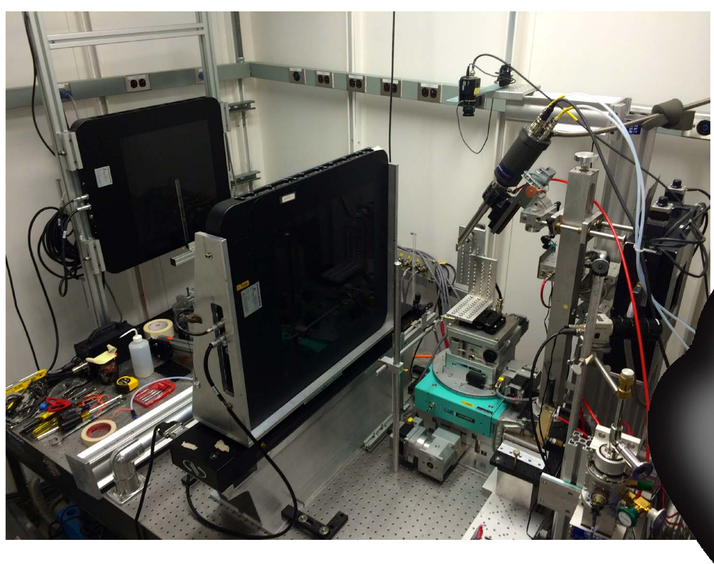
- Atomic Pair Distribution Function
- Small-Angle X-ray Scattering (SAXS) (Q_{min}= 0.01 Å)
- Wide Angle X-ray Scattering (WAXS)

ENDSTATION DETAILS:

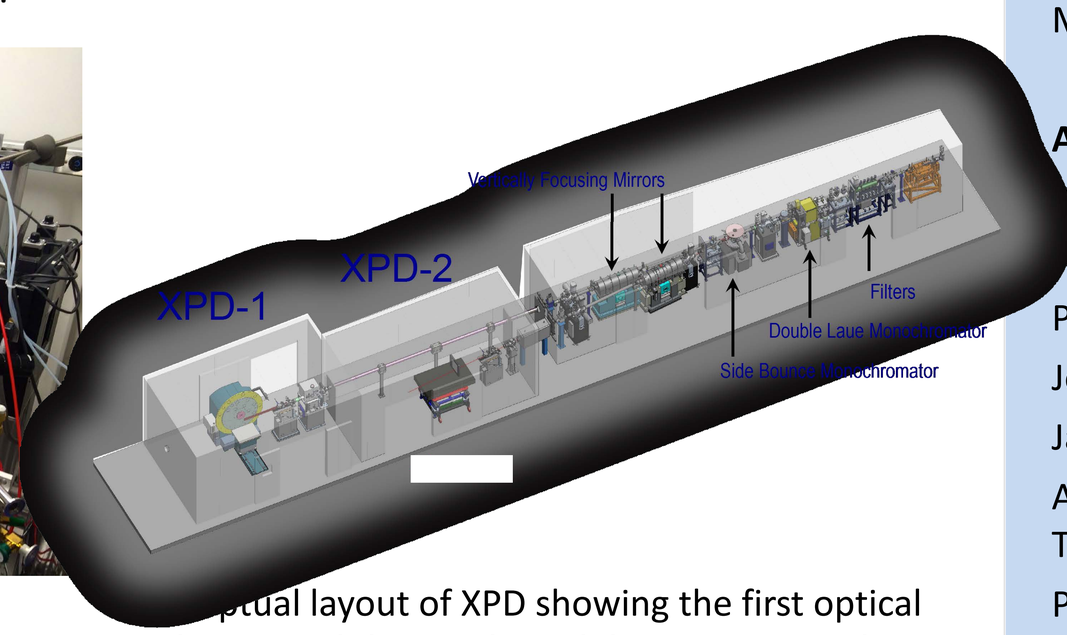
- Two large area detectors.
- (5-500) K temperature range.
- A wide variety of sample environments including electric and magnetic fields, gas-flow and chemical reaction cells.

XPD-2 at NSLS-II:

- Fast frame rates required for in-situ or operando PDF, SAXS and WAXS studies of complex functional materials under real working conditions.
- User friendly real time data processing and visualization software.
- Complementary SAXS, WAXS, along with PDF data
- Combined sample environments. (Ex. Low-T and magnetic fields)



Prototype endstation for XPD-2, X17A/NSLS



ptual layout of XPD showing the first optical enclosure and the two branch lines, XPD-1 and XPD-2

Overview

PORT: 28-ID

SOURCE: Damping Wiggler (DW100)

ENERGIES: 39, 64, 75 and 117 keV

ENERGY RESOLUTION: $\Delta E/E = 10^{-2} - 2 \times 10^{-3}$

SPATIAL RESOLUTION: ~ 200 µm

CONSTRUCTION PROJECT: XPD

BEAMLINE STATUS: Procurement

AVAILABLE TO USERS: April 2017

Beamline Team

STAFF

Eric Dooryhee: lead beamline scientist

Milinda Abeykoon: beamline scientist

ADVISORS

imon Billinge (Columbia University/BNL)

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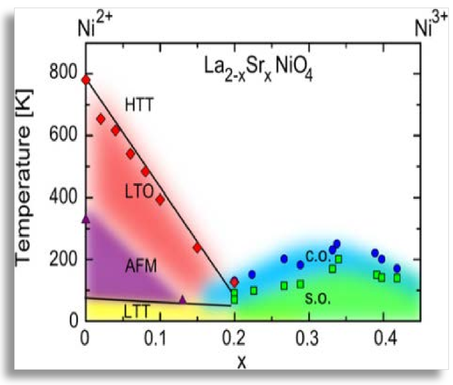
Jonathan Hanson (BNL)

James Kaduk (PolyCrystallography)

Angus Wilkinson (Georgia Institute of Technology)

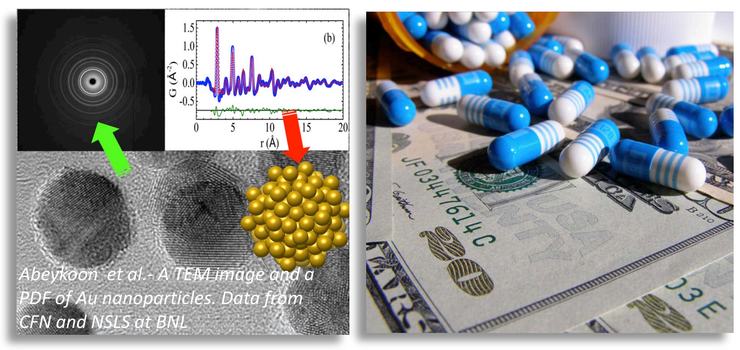
Peter Chupas (Argonne National Lab)

SCIENTIFIC APPLICATIONS



Studies of the electronic state of strongly correlated materials over full phase diagrams

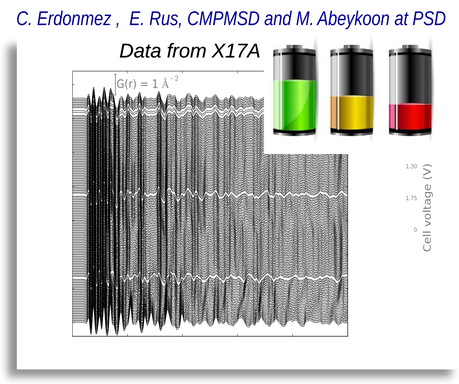
High-throughput, high r-space resolution PDF measurements at XPD-2 will enable local structural studies of the full phase diagrams of strongly correlated systems giving key insights into their structure-property relationship.



Local structural studies of partially disordered low-scattering materials

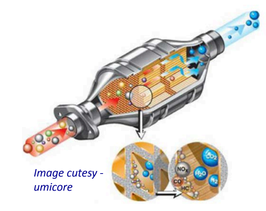
PDF is an excellent tool to study the structure of technologically important low-scattering materials which exhibit Bragg peaks accompanied by diffuse scattering due to nanoscale disorder. High flux and energy available at the XPD-2 will ensure excellent PDF data from energy related nanomaterials and pharmaceuticals up to a high momentum transfer leading to a better understanding of their structure-property relationship.

C. Erdonmez , E. Rus, CMPMSD and M. Abeykoon at PSD

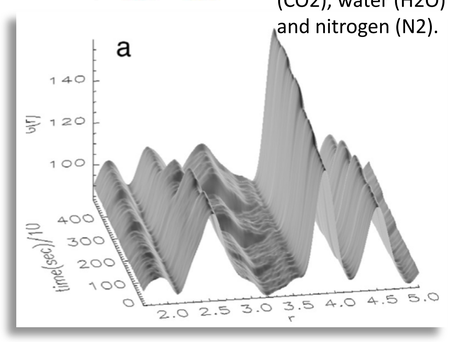


Local structural studies of batteries during charging and discharging cycles

Combining time series PDFs with voltage-current measurements can shed light on local structural changes in batteries during charging/discharging cycles leading to high-efficiency battery technology.



An automotive catalytic converter activates oxidation and/or reduction reactions to transform harmful pollutants into carbon dioxide (CO2), water (H2O) and nitrogen (N2).



In-situ characterization of catalysts

XPD-2 provides high flux and rapid acquisition (<1s) necessary for the in-situ characterization of catalysts under real working environments leading to more efficient materials.

Figure (a) shows time resolved series of PDF's taken during pulse sequence of CO/He/O_2 /He over fully reduced CeO_2/Cu at 200°C. Hanson et al., Catal. Today 229 (2014) 64