IN SITU X-RAY DIFFRACTION (IXD)

BROOKHAVEN NATIONAL LABORATORY

NATIONAL SYNCHROTRON LIGHT SOURCE II

SCIENTIFIC SCOPE

In Situ X-ray diffraction (IXD) is a diffraction beamline optimized in the medium x-ray energy range (6 – 25 keV). The beamline is complementary to the high energy x-ray powder diffraction beamline (XPD) with emphasis on in situ powder diffraction measurements, in the sub-minute time scale , to study structural, morphological and chemical transformations under various conditions. IXD will continue and enhance research programs in materials science (battery, catalysts, functional materials , and industrial applications) that were developed on the NSLS powder diffraction beamlines: X7B, X14A, X16C.

BEAMLINE CHARACTERISTICS

TECHNIQUES:

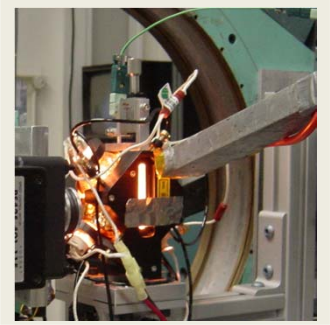
- X-ray Powder Diffraction
- Residual stress measurement
- X-ray reflectivity

ENDSTATION DETAILS:

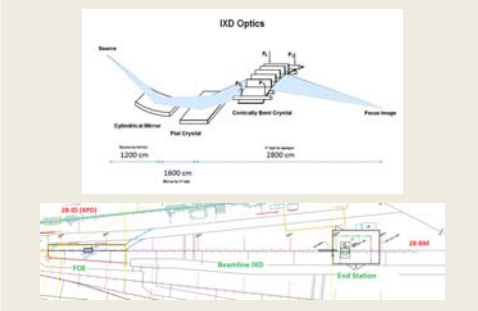
- Si strip detector
- Perkin Elmer 2D detector
- Six-circle Huber Diffractometer
- High temperature furnaces

IXD at NSLS-II:

- Will enable high resolution x-ray powder diffraction for structural characterization of materials
- Time-resolved in situ XRD measurements in the sub-minute time scale to study phase transitions.
- Element selective and surface sensitive XRD measurements.



Quadrupole lamp furnace, capable of heating capillary or small plate samples to 2000 K



(Top) IXD optical components: Focusing mirror and the double crystal sagittal focusing monochromator (Bottom) IXD beamline layout

Overview

PORT: 28 BM
SOURCE: Three-Pole-Wiggler (TPW)
ENERGY RANGE: 6 – 25 keV
ENERGY RESOLUTION: $\Delta E/E = 10^{-4}$
BEAM SPOT SIZE: 1.0 mm x 0.5 mm
BEAM FLUX: ~5×10^{11} photon/s at 20 keV
CONSTRUCTION PROJECT: NxtGen
BEAMLINE STATUS: Construction
AVAILABLE TO USERS: December 2017

Beamline Team

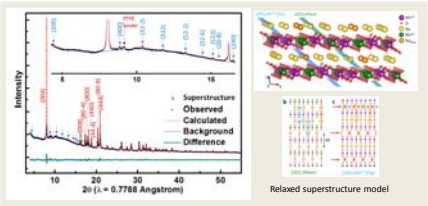
STAFF

Jianming Bai: lead beamline scientist
Lukas Lienhard: mechanical engineer
Michael Johanson: designer

BEAMLINE DEV. PROPOSAL LEAD

John B. Parise (Stony Brook University)

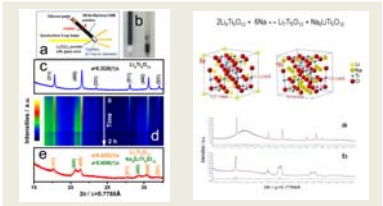
SCIENTIFIC APPLICATIONS



Materials Science: Cooperative Jahn-Teller effect in $Na_{5/8}MnO_2$

High Resolution X-ray Powder Diffraction for Structural Characterization

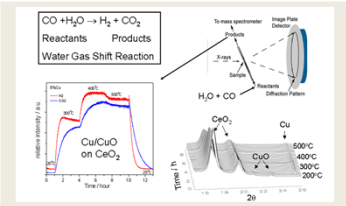
IXD provides highly collimated and focused x-ray beam and quick detecting systems for high resolution powder diffraction measurement, as an indispensable structural characterization tool in materials science studies. The capability of resolving weak superstructure peaks (as shown in above example) and indexing Bragg peaks in adequate Q-range are essential for solving complex structures.



Battery: Sodium storage mechanism in $Li_4Ti_5O_{12}$

In Situ X-ray Powder Diffraction Studies on Chemical Reaction and Crystallization Processes in Solution

Time-resolved in situ x-ray powder diffraction is an important tool in the investigation of the mechanism, pathways and kinetics of chemical reactions in solution. This technique has been applied in studies of hydrothermal and solvothermal synthesis, ion-exchange process, chemical lithiation and sodiation procedures etc. and will make unique contributions in developing new electrode materials for the next generation of energy storage devices.



Catalysis: Water gas shift reaction

Real-Time Catalysis: *In-Situ* Structural Studies for Producing and Storing Hydrogen Fuel

Catalysis is the most critical field for sustainable energy production. Since real catalysts and catalytic processes are extremely complex, the availability of techniques for the real time characterization of catalytic systems as they evolve in time with a changing chemical environment is a high priority. The *in-situ* XRD capability of the IXD beamline provides the effective solution to such research needs, and will ensure the continuity of service to existing user groups.