Brookhaven National Laboratory

Overview of capabilities supporting advanced nuclear technology development. Point of Contact: William Horak, <u>horak@bnl.gov</u>

Contents:

- 1. National Nuclear Data Center (NNDC)
- 2. X-ray Powder Diffraction (XPD) Beamline
- 3. X-ray Diffraction-Computed Tomography (XRD-CT) System
- 4. Submicron Resolution X-ray Spectroscopy (SRX)
- 5. Hard X-ray Nanoprobe Beamline

Introduction

Brookhaven National Laboratory's Department of Nuclear Science and Technology conducts research and development related to nuclear technologies (reactors and accelerator-driven systems), reliability and risk assessment, and advanced modeling techniques for reactor simulation and energy systems

The Department serves as a resource in these and related areas to support the missions of the Department of Energy (DOE), the Nuclear Regulatory Commission (NRC), and other national and international organizations. With a world-class staff of professionals with expertise in a broad range of areas related to the design and analyses of commercial, research and advanced nuclear systems, Brookhaven's capabilities and facilities are also available to support and execute experiments in support of these missions. Additional strengths are in the areas of Probabilistic Risk Analysis, Modeling of Complex Energy Systems, Risk Informed Regulation, and technical support to DOE and NRC to improve the safety of nuclear power plants, both domestic, and in the Former Soviet Union.

The Department provides technical expertise in reactor physics, thermal-hydraulics, nuclear fuel design, and structural mechanic, and supports a broad range of DOE research projects on future nuclear energy systems and accelerator-driven systems. It conducts risk analyses of complex technological systems to provide quantitative information to decision-maker and has established expertise in integrated risk and reliability management.

While principally focused on domestic and foreign nuclear power plants, the staff also examines risks in such diverse areas as aircraft performance, chemical spills and electrical reliability. Specific current applications include risk-informing the regulations governing the operation of commercial nuclear power reactors; using risk insights to develop high-level, technology- neutral regulations for advanced reactor concepts; and establishing consensus standards for risk analyses to assure better quality, uniformity and consistency among practitioners.

The Department also conducts programs and projects in nuclear energy and infrastructure systems through the following types of analysis: seismic and structural, plant aging, risk management, human factors, and neutronics/thermal-The Laboratory's work in reactor safety continues a decades-old tradition of providing in-depth support to the Nuclear Regulatory Commission to ensure that operating U.S. nuclear power plants provide electricity safely and reliably. Work in nuclear power reactor safety is focused on structural and seismic analysis, nuclear power plant license renewal and new license review

support, and operational safety inspections. The work includes both engineering and analytical support, and the results of this work contribute to the development of NRC regulatory guidelines, licensing activities, and operating plant safety. Human factors work helps to ensure that the human-system interface in nuclear plants and other industrial facilities contributes to the overall safety of operations conducted there. These projects include development of a risk-informed methodology and human factors review and acceptance criteria in nuclear power plants for the NRC, and human factors guidance documents for digital systems and control rooms for DOE, in collaboration with industry.

The Department is involved in a number of projects related to the safety of research reactors. These include conducting reactor safety analyses for the research reactor operated by the NIST Center for Neutron Research, reviewing the updated Safety Analysis Report for the High Flux Isotope Reactor at Oak Ridge National Laboratory, and supporting license renewal review of several university research reactors. The Department collaborates with industry, both domestic and foreign, on several large projects requiring specialized engineering and analysis capabilities.

1. National Nuclear Data Center (NNDC)

The National Nuclear Data Center (NNDC) collects, evaluates, archives and disseminates nuclear physics data for basic nuclear research and for applied nuclear technologies. The center collects information on nuclear structure and nuclear cross-sections, maintains nuclear databases and makes use of modern information technology to disseminate the results. The data is kept in dedicated numerical libraries, which are periodically reevaluated and updated. The information is the product of the NNDC, cooperating data centers and other interested groups worldwide. In 2006, the Center reached an important milestone of more than one million Web database retrievals.

The NNDC has provided more than a half century of data and expertise to the world community, tracing its roots back to 1952, when the Brookhaven Neutron Cross Section Compilation Group was formed in the Physics Department. This group published the first edition of the well-known reference book BNL-325 (Neutron Cross Sections) in 1955. The group's name was changed to the Sigma Center in 1961, to the National Neutron Cross Section Center in 1967 and finally to the NNDC in 1977, when it was given the additional responsibility for nuclear structure and decay data.

The National Synchrotron Light Source-II (NSLS-II) is a new state-of-the-art, medium-energy electron storage ring (3 billion electron-volts) designed to deliver world-leading intensity and brightness. The NSLS-II enables the study of material properties and function with nanoscale resolution and exquisite sensitivity by providing world-leading capabilities for X-ray imaging and high-resolution energy analysis.

2. X-ray Powder Diffraction (XPD) Beamline

The X-ray Powder Diffraction (XPD) beamline at the NSLS-II is the only high-resolution instrument in the U.S. that is capable of collecting data at high energies, which will make it ideal for structural characterization of heterogeneous, dense high-Z materials, intrinsic to nuclear reactor systems. XPD is a unique facility with the ability to collect diffraction data at high X-ray energies (30keV-70keV), offering rapid acquisition (milli-second, to second time scales) and high angular resolution capabilities on the

same instrument. The XPD endstation hosts a three-circle diffractometer fitted with a multiple flat scintillator panel detectors (Perkin Elmer), a photon-counting detector and a bank of high-resolution counters to cover most powder diffraction measurements. A robotic sample changer is available for the manipulation of radioactive samples and for the rapid collection of x-ray diffraction, Pair distribution function analysis and small angle x-ray scattering patterns for large sample sets. Sample holders and the associated infrastructure for radioactive materials are available for the robot due to a previous investment by DOE-NE. This previous DOE- NE investment has also led to the availability and installation of several XRD and SAXS software packages at XPD and the Nuclear Science and Technology Department (BNL) for the quantitative phase analysis, structural refinement and the analysis of large XRD and SAXS data sets.

3. X-ray Diffraction-Computed Tomography (XRD-CT) System

XPD is currently installing an X-ray Diffraction-Computed Tomography (XRD-CT) system. It will be fully commissioned by March 2019 and available for use with the samples proposed for this research. XRD-CT creates a 3D reconstruction of sample morphology directly from diffraction patterns. Unlike traditional X-ray computed tomography that is based on X-ray absorption, it simultaneously supplies crystallographic structural information with spatial resolution set by the beam size ($10 \times 10 \mu m$). The structural information available includes; phase identification, phase fraction, grain size and lattice strain. Elemental mapping will be provided with a fluorescence detector. It is an ideal mesoscale probe; bridging the gap between bulk characterization techniques such as diffraction and local methods (electron microscopy).

XRD-CT is a non-invasive, quantitative structural and morphological characterization technique that can be applied to heterogeneous "real world" materials. XRD-CT is typically performed at a synchrotron facility with a high-flux, monochromatic "pencil" X-ray beam. The collection of the scattering/diffraction signal is performed in the conventional tomographic set up: measuring two-dimensional diffraction patterns across a series of positions and rotation angles. The image reconstruction and spatial information are extracted using common sinogram reduction methods while quantitative phase analysis (lattice parameter, grain size, strain, etc.) can be performed for any selected area of the tomographic image. Complementary X-ray fluorescence tomography can simultaneously be used for mapping chemical element distribution in the sample. The table below is a comparison between XRD-CT and othe X-Ray imaging techniques. A schematic of the equipment required to perform XRD-CT is shown in Figure 1.

Technique	Description	Crystal Structure	Morphology	Chemical Mapping
Absorption Tomography	Conventional tomography based on differences in X-ray absorption between elements.	No	Yes	No
3D-XRD	Crystal orientation mapping in 3D with X-rays (limited to large grain samples).	Yes	Yes	No
Tomographic Energy Dispersive Diffraction Imaging	Polychromatic X-ray beam for measuring lattice strains and crystal phase (Poor Resolution and sensitivity).	Yes	Yes	No
X-ray Fluorescence Mapping	Elemental distribution from X-ray fluorescence signal does not distinguish between crystalline and amorphous or porous materials.	No	Yes	Yes
XRD-CT	Creates a 3D reconstruction of sample morphology directly from diffraction patterns.	Yes	Yes	Yes

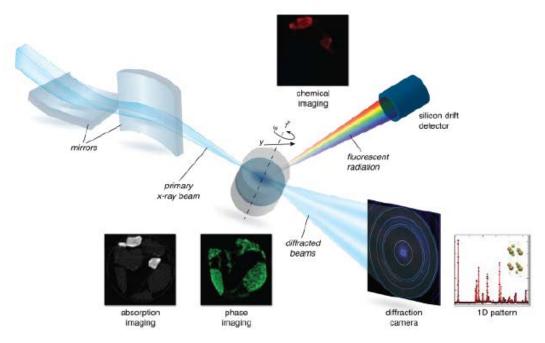


Figure 1. Schematic of the experimental XRD-CT set up.

4. Submicron Resolution X-ray Spectroscopy (SRX)

Submicron Resolution X-ray Spectroscopy (SRX) is an undulator beamline providing world-leading, highthroughput spectroscopic imaging capability (2D and 3D) with sub-100 nm spatial resolution and millisecond dwell times/pixel with fly-scan capability. SRX will enable simultaneous x-ray fluorescence and transmission measurements with sub-µm to sub-100 nm spatial resolution with an incident x-ray beam energy of 4.65-25 keV. Sample stages will enable fast 2D scanning and tomography capabilities. Xray fluorescence imaging and tomography will provide elemental mapping in 2D and 3D, respectively. Spatially resolved X-ray Absorption Near Edge Structure (XANES) spectroscopy can be performed in fluorescence or transmission mode. Several different operation modes including high resolution scanning (sub-100 nm focused beam), high flux (sub-µm focused beam) scanning and full-field imaging are available.

5. Hard X-ray Nanoprobe Beamline

The Hard X-ray Nanoprobe Beamline at the NSLS-II provides scanning microscopy capability for studying materials with resolutions down to ~12 x 13 nm2. An important feature of this beamline is the multimodali imaging capability, where two or more different types of measurements are performed simultaneously, thereby collecting comprehensive data sets. Commonly used imaging modalities include fluorescence, diffraction, differential phase-contrast (DPC) and ptychography. Multimodali imaging can also be performed through 3D tomography measurements.