NATIONAL SYNCHROTRON LIGHT SOURCE II (NSLS-II)

National Institute of Standards and Technology Beamline Development Proposals

(Submitted June 21, 2010)

NIST NSLS-II Spectroscopy Beamline Suite: Materials Measurement to Promote Innovation and Industrial Competiveness

1) Soft and Tender X-ray Spectroscopy and Microscopy (100 eV to 7.5 keV canted undulator sources)

2) Hard X-ray Absorption Spectroscopy and Diffraction (4.5 keV to 40 keV 3-pole wiggler source)

NIST
National Institute of Standards and Technology
U.S. Department of Commerce

NSLS-II Beamline Development Proposal

Type I ☐ Type II ☒

NIST Spectroscopy Beamline Suite: Hard X-ray Absorption Spectroscopy and Diffraction (4.5 keV to 40 keV 3-Pole wiggler source) Three-Letter Acronym (BMM - Beamline for Materials Measurement)
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NIST NSLS-II Spectroscopy Beamline Suite:

Materials Measurement to Promote Innovation and Industrial Competiveness

Executive Summary: The National Institute of Standards and Technology (NIST) and the Department of Energy (DOE) have a 30 year ongoing partnership at the National Synchrotron Light Source (building to NSLS-II) developing advanced synchrotron measurement methods and delivering excellence in material science impacting important societal challenges in energy, health, environment, and national security improving our quality of life. This partnership promotes innovation and enhances US industrial competiveness for inorganic and organic semiconductors, photovoltaics, SAMs, biological and environmental materials, batteries, catalysts, fuel cells, polymers, superconductors, ferroelectrics, and ferromagnets. Located at the NSLS, the NIST Synchrotron Methods Group of nine operates a suite of three state-of-the-art spectroscopy beamlines (U7A, X24A, and X23A2) that span the entire absorption-edge energy range of the periodic table to establish structure function relationships in advanced materials. More than 200 industry and academic researchers each year use the NIST Beamline Suite to accelerate the development of new materials into devices and systems with advanced functionality for a broad spectrum of industries. Building upon this success, NIST proposes to establish an NSLS-II spectroscopy suite of three state-of-the-art high throughput beamlines (with X-ray Diffraction capability) described in two beamline development proposals; Soft and Tender X-ray Spectroscopy and Microscopy (100 eV to 7.5 keV canted sources) and Hard X-ray Absorption Spectroscopy and Diffraction (4.5 keV to 40 keV three-pole wiggler source). Taken together, the NIST NSLS-II Spectroscopy Beamline Suite will be capable of measuring the electronic, chemical, and structural properties of almost any material, often at the nanoscale. NIST is committed to fully funding the construction of its proposed Spectroscopy Beamline Suite and to continuous world leading improvements in synchrotron measurement science and technology. Furthermore, NIST will build upon its NSLS based Synchrotron Methods Group to fully staff its stakeholder relationship in NSLS-II.

A. Science Case: Hard X-ray Absorption Spectroscopy and Diffraction (4.5 keV to 40 keV)

In this proposal, we outline NIST's plans to develop an X-ray absorption fine structure beamline at NSLS-II using a three-pole wiggler source. The beamline will take advantage of the superior beam characteristics of the NSLS-II source for high resolution X-ray absorption spectroscopy (XAS) measurements. The beamline will also add new X-ray diffraction (XRD) capabilities to complement NIST's existing and planned XAS program. X-ray optics will be designed to provide either focused or collimated X-rays at the sample, for both high resolution XAS and diffraction experiments. The X-ray diffraction end station will be equipped to take advantage of the scanning capabilities of the beamline, adding glancing incidence XAS and XAS at constant *q* (reflectivity XAS and diffraction anomalous fine structure (DAFS)) to NIST's many other spectroscopic tools for materials science study. Polarization dependent XAFS measurements will also benefit from the high-precision eight-circle goniometer and its ability to accurately and quickly position samples relative to the X-ray beam.

This beamline will provide high-quality, high-throughput XAS for advanced sample characterization. XAS users will also have access to XRD for sample characterization. XAS and XRD are complimentary materials science probes. XAS measures local (short range) atomic structure while diffraction is more sensitive to a sample's long range order. By offering these combined and complementary measurement capabilities along with a variety of *in situ* sample environments, NIST's beamline will serve a broad range of structural characterization problems in materials science, ranging from the study of bulk mixed phases to epitaxy and strain state of thin films.

The XAS and XRD capabilities of the BMM beamline coupled with NIST's continuous development of automated high-throughput spectroscopy methods and world class high efficiency detectors will combine to have a large scale impact on the materials science of important societal challenges in energy, health, environment, and national security. Some strategic science case examples follow. They illustrate how this beamline will establish structure function relationships in advanced materials often at the nanoscale to accelerate the development of new materials into devices and systems with advanced functionality for promoting innovation and enhancing US industrial competitiveness.

Science cases:

1. Local Structure and Phase Transitions in Electronic Ceramics, *I. Levin (NIST)*
2. Local Structure Function Properties of Strain Engineered Electronic Thin Films, *J.C. Woicik (NIST)*
3. Understanding Radiation Damage in Nuclear Materials with GA-XAS, *N. Hyatt, D. Reid, M. Stennet (U. Sheffield), B. Ravel, J.C. Woicik (NIST)*
4. *In situ* Characterization of Commercial Catalysts: From Understanding to Development, *S.R. Bare (UOP)*

Additional science Case Examples appear in the appendix starting on page 13

5. Proximity and Dimensionality Effects in Ferroelectric Nanostructures Studied by Diffraction Anomalous Fine Structure (DAFS), *J.C. Woicik (NIST)*
6. Local Structure Function Relationships in Thin Dielectric Films for Advanced Microelectronics, *P. Lysaght (SEMATECH)*
7. EXAFS of Phase Change Materials: Characterizing the role of the Local Bonding Environment on the Crystallization Properties of Chalcogenide Materials for Phase Change Memory Applications, *E. Joseph and J. Jordon-Sweet (IBM)*
8. High throughput XAS and an example of its application to chemical science, *B. Ravel, J.C. Woicik, D. Fischer (NIST), S.R. Bare, S.D. Kelly (UOP)*