**6-BM Management Plan**

**(Updated)**

**COMPRES**

**Advanced Photon Source**

**Date: November 17, 2017**

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6-BM Beamline Management Plan

**Executive Summary**

This document replaces the 6-BM Management Plan dated October 14, 2014 and reflects the withdrawal of BNL Photon Sciences from the operation of the beamline. A separate document describes the Safety Plan for 6-BM

1 Introduction and Scientific Scope

**COMPRES Program**

COMPRES-supported beam lines X17B2, X17B3, and X17C at the National Synchrotron

Light Source have a large, active, and very productive user communities. These

hard X-ray beam lines support high-pressure experimentation using large-volume multianvil

presses (LVP’s) and diamond-anvil cells (DAC’s), providing crucial tools for Earth science research, as well as related research in materials sciences, condensed matter physics, chemistry, and planetary science. The dark period between the closing of the NSLS and the opening of NSLS-II will leave the NSLS high-pressure user groups stranded, without the necessary specialized facilities to carry out experiments. The impact on individual funded research programs, and a large number of students who depend on these facilities for carrying out their graduate research, will be severe. Synchrotron facilities with similar experimental capabilities, such as GSECARS at the APS, are already heavily oversubscribed and will not be able to accommodate the current users from COMPRES-supported beam lines at NSLS (which themselves are already heavily oversubscribed). This proposal outlines a plan to manage the NSLS dark period by utilizing a white-beam bending magnet beamline at the APS for a large-volume press, aimed at deformation, rheology, elasticity, and thermal diffusivity studies of solids at high pressures and temperatures. The effort will be led by Donald J Weidner of Stony Brook University. Through a partnership between COMPRES, Stony Brook University, and APS we see this as not only an opportunity to accommodate the current user base from X17B2, but a chance to define the state of the art in a field with growing user demand and vast potential for new and exciting science.

**COMPRES Science Program**

Our understanding of the makeup and evolution of the Earth is strongly tied to our understanding of the materials that comprise the Earth. Pressure and temperature set the environment where these minerals and melts are found, and it is the goal of high-pressure experimental studies to probe and characterize Earth material systems. A 2008 workshop on seismological research frontiers (Seismological Grand Challenges in Understanding Earth’s Dynamic Systems, 2009), funded by the National Science Foundation (NSF), considered promising research directions for the next decades and identified 10 Seismological Grand Challenge research questions including: *How do faults slip?; How does the near-surface environment affect natural hazards and resources?; What is the relationship between stress and strain in the lithosphere?; Where are water and hydrocarbons hidden beneath the surface?; How do magmas ascend and erupt?; What is the lithosphere-asthenosphere boundary?; How do plate boundary systems evolve?; How do temperature and composition variations control mantle and core convection?; and How are Earth’s internal boundaries affected by dynamics?* While these questions drive the agenda of the next decade seismology research, they are also central to the research program of the multi-anvil high-pressure beamline at NSLS.

*Elasticity*

The most robust fingerprint of the chemical and thermal state of the Earth’s interior are the elastic properties of Earth materials. Radial variations in seismic velocity point to phase transitions, melting, and general pressure increase. These transitions require a comprehensive understanding of the elastic properties of materials as a function of all of the relevant variables. The last few years has seen tremendous growth in our data base as well as our experimental tools for defining this information.

The interpretation of seismological profiles of Earth’s interior has long been the principal motivation for measuring the acoustic velocities and the elastic tensors of minerals, both at ambient and high P or T conditions. As the resolution of seismological studies continues to improve, the need for more and better elasticity data, under simultaneous high pressures and high temperatures, increases.

Two specific scientific challenges that can be highlighted include: the interpretation of seismic anisotropy throughout the planet, from uppermost mantle to inner core conditions; and understanding lateral variations of compressional and shear wave velocities (∂Vp and ∂Vs) in terms of composition and/or temperature variations. These goals require the mineral physics community to provide complete characterization of elastic anisotropy, as well as aggregate acoustic velocities, in minerals, and also the variation of these properties with pressure, temperature, and composition.

Simultaneous ultrasonics + XRD investigations in the multi-anvil press permit the EoS and acoustic properties of minerals to be evaluated under high-P,T conditions. The multi-anvil beamline at the NSLS has been the pioneer of such measurements and continues to develop a wider array of possible samples for such high P-T experiments.. In principle this technique can be extended to 25 GPa and 2000K and we plan to reach this capability in the next 5 years. This program will continue at the APS bending magnet.

*Rheology*

The quantitative relationship between stress, strain, and time in minerals forms the basis for our view of the evolving Earth. Plate tectonics, earthquakes, volcanic eruptions all respond to these intrinsic properties of Earth materials. Thermal convection in Earth’s deep interior cools the planet and in the process generates earthquakes and volcanoes, moves tectonic plates, and disturbs the uniform chemical layering of a differentiated Earth. Laboratory measurements of the relationship between deviatoric stress and deviatoric strain rate of rocks and minerals at high pressure are driven by the need to understand this circulation at depth. Current research on global geodynamics strongly suggests that the dynamics and evolution of this planet are controlled largely by materials properties under deep Earth conditions, including rheological properties, phase relationships, elastic properties and chemical properties such as the diffusivity and solubility of certain elements. For instance, the lateral and radial variation of viscosity have an important influence on the convection pattern and generation of deep earthquakes, whereas the solubility and diffusivity of elements in various phases control the chemical evolution associated with mantle convection. Also, the way in which materials are distributed or the flow pattern in Earth can, in principle, be inferred from seismological observations, but the interpretation of seismological data relies entirely on our understanding of elastic and anelastic properties of minerals under deep Earth conditions. Laboratory studies have recently made a significant breakthrough in capability for defining these properties at mantle pressures and temperatures using x-rays generated by synchrotrons at national laboratories. This progress has set the stage for new and exciting research efforts.

The rheology experiments associated with the NSLS beamline have set an entirely new range of conditions for these measurements. We can now conduct experiments uniaxial stress deformation experiments at 10 GPa and 2000K with near the precision of experiments at 0.3 GPa a decade ago. Through these developments, not only can we infer pressure dependence of mineral properties, but we can examine the properties of high-pressure mineral phases that were impossible before. The technical developments have enabled studies on the relevant properties of minerals.

The new pressure cells and measurement tools also allow a wide array of new characterizations that are still being explored including measurements of phase transition kinetics through stress oscillations with frequencies in the seismic zones, Q measurements at high P and T, thermal diffusivity at high P and T.. New science will emerge as these tools are used to study polycrystalline samples, partially molten samples, and single crystal samples. This next five years promises to be a time of great discoveries, taking the tools we have on hand and pushing our understanding of relevant materials.

## Energy Dispersive Diffraction Science Program

Quantifying phase evolution and the measurement of stress-strain relationships using x-ray diffraction are critical in testing engineered systems, such as electrical storage devices.

1) Phase and/or chemical changes: The simplest application of EDXRD diffraction is in the rapid identification of component crystalline phases, such as phase mapping;

2) Science of the deformation of materials;

3) Rapid, high-resolution x-ray physical imaging methods.

Measurements on real devices as they operate (*operando* studies) are critical to understanding function and failure mechanisms, and to validate models that will ultimately be used to translate from short term (hours) to long-term (years) wear/failure tests. Rather than relying only on snap-shots of materials recovered from experimental runs, continuous monitoring of the processes occurring at varying conditions of stress and chemical gradients, in real time, is becoming standard operating procedure.

Fig. 1.1 Cell configuration in beam environment showing gauge volume of the measurement. of a typical coin cell.

**2 Organizational Structure for 6-BM Operations**

Figure 2.1 shows the proposed organizational structure for the operations of the 6-BM- beamline. Below are the roles and responsibilities of the staff associated with 6-BM.

**Roles and Responsibilities**

*XSD Associate Division Director – Stefan Vogt (XSD/APS)*

The XSD Associate Division Director will be the APS point of contact for this beamline, coordinate activities of the APS and COMPRES/BNL-PS programs, and provide oversight for the XSD Beamline Scientist (who is directly supervised by the XSD Materials Physics and Engineering Group Leader). The XSD Associate Division Director will work closely with the 6-BM Directors to ensure safe and efficient operations of the beamline.

*6-BM-B COMPRES EDD Director – Donald J. Weidner (SUNY Stony Brook)*

The COMPRES EDD Director serves as the point of contact for the COMPRES LVP activities at the beamline, will coordinate activities of the COMPRES LVP programs, provide scientific leadership for scientific and technical activities at 6-BM-B and will directly supervise the COMPRES Lead Scientist.

*XSD-MPE Group Leader - Jonathan Almer (XSD/APS)*

The XSD Materials Physics and Engineering (MPE) group leader will supervise the XSD-MPE beamline scientist and help coordinate the EDD experiments in the 6-BM-A station. He will work with both the XSD and BL-PS staff for installation and upgrades of energy dispersive diffraction instrumentation in the 6-BM-A station.

*COMPRES Beamline Scientist –* Haiyan Chen *(Stony Brook, COMPRES)*

The COMPRES 6-BM-B Lead Scientist, reporting to the COMPRES EDD Director, will provide onsite day-to-day operational guidance for all scientific and technical activities on 6-BM-B. This person will be a COMPRES employee.

*XSD Beamline Scientist – John Okasinski (XSD/APS)*

The XSD Beamline Scientist will provide scientific and technical support for the energy dispersive activities at 6-BM-A for APS General Users. This staff will work closely with the BNL-PS Beamline Scientist to provide seamless support for the energy dispersive program. This person will be an APS employee.



Figure 2.1 - Org Chart for 6-BM

**3 Beamline Requirements**

**COMPRES Program**

The intensity (intensity through a pin hole for an unfocused beam) and brightness

(for a focused beam) of the APS bending magnet delivers approximately half of the total X-rays to the sample of the current wiggler at X-17 of the NSLS over the entire energy band of interest (20 kev – 100 kev). We feel that this is adequate for these experiments.

A new high-pressure deformation apparatus, called the Deformation DIA (D-DIA), made its first appearance on a synchrotron beamline at X17 of the NSLS in 2002. Over the years, its use has matured and it has achieved success beyond the initial hope. The system proposed for the APS will have a footprint of about 1.5x2 (along the beam) meters with access space for scientist set up.

Towards this beamline, the APS has committed to provide the following hardware:

White beam compatible stations with operating PSS

White beam mask

White beam slits (from 5 mm to 1 mm wide)

White beam shutter

White beam stop

Various Be windows and spool pieces

Network connections

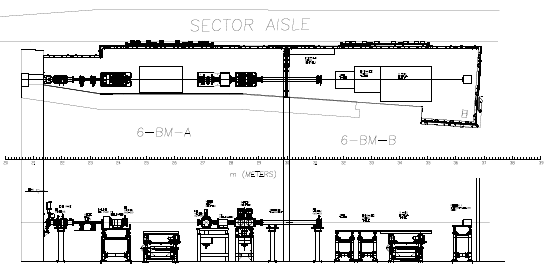


Fig. 3.1 6-BM layout showing APS-provided hardware

*Space*

APS will provide office space for the COMPRES beamline scientist and laboratory space for sample preparation of high-pressure sample assemblies for the LVP experiments.

Stony Brook University will provide the following instrumentation for high pressure studies in 6-BM-B:

DDIA high pressure system complete with hydraulic jacks and pumps (DDIA module on loan from UC Riverside).

Multi-element solid state energy dispersive detector, complete with electronics

Conical slit assembly

Prosilica camera, lenses, fluorescence screen, mounting system for sample imaging

Stages and motors for positioning all systems (about 10 stages, 30 motors)

VME crate and electronics for driving motors

Keithley box for data reading

4 Windows based computers with EPICS based software and 1 Unix computer.

# 4 Funding

**6-BM-A Instruments**

Instruments for this station will be provided by APS. APS will also cover the effort and M&S costs for the XSD Beamline Scientist.

**6- BM-B Instruments**

Instruments for this station (see Section 3 - Instrumentation for high pressure studies) will be provided by Stony Brook University with the oversight of COMPRES. COMPRES will cover the effort and M&S costs for the COMPRES Beamline Scientist.

# 5 Safety

COMPRES and APS are committed to ensuring that all beamline activities are conducted in a safe and environmentally sound manner. All activities at Argonne National Laboratory will conform to the requirements in the ANL Laboratory Management System (LMS) and the APS User Safety Policies and Procedures. (Information contained in ANL LMS and the APS document can be obtained by contacting Paul Rossi, interim XSD ES&H Coordinator.) A detailed Safety Plan for 6-BM can be found in a separate document titled 6-BM Safety Plan.

# 6 Operations and User Access Plan

**Operations and User Program**

At present we are envisioning two FTE staff to support the beamline, one FTE funded through COMPRES to support high-pressure studied and approximately 1 FTE funded though the APS X-ray Science Division to support energy dispersive diffraction. Based on an agreement between COMPRES and APS, the allocation of beamtime will be shared as described in the table below.

Table 6.1 – Beamtime Allocation

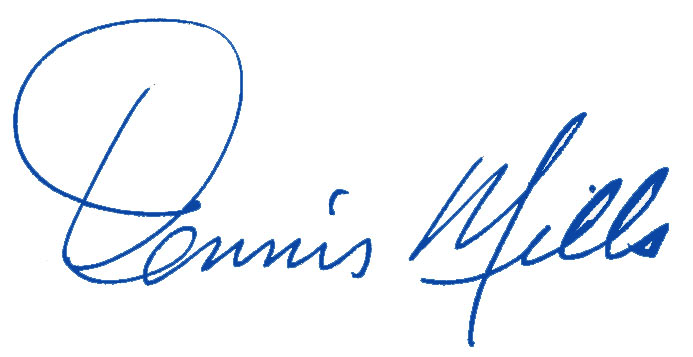
|  |  |  |
| --- | --- | --- |
| **Usage** | **Beamtime (percentage)** | **BL Scientist Responsible (percentage)** |
| High Pressure General Users | 12 | COMPRES |
| High-Pressure Earth Science Users, including Transitioned NSLS COMPRES users | 38 | COMPRES |
| EDD General Users | 40 | XSD |
| XSD BL Scientist | 10 | XSD |

All users (General Users and COMPRES High-Pressure Earth Science Users) will submit general user (GU) proposals and be scored by the APS Proposal Review Panel (PRP).

This will be effective starting the 2018-1 run cycle at the APS and continue through the 2019-2 run cycle.

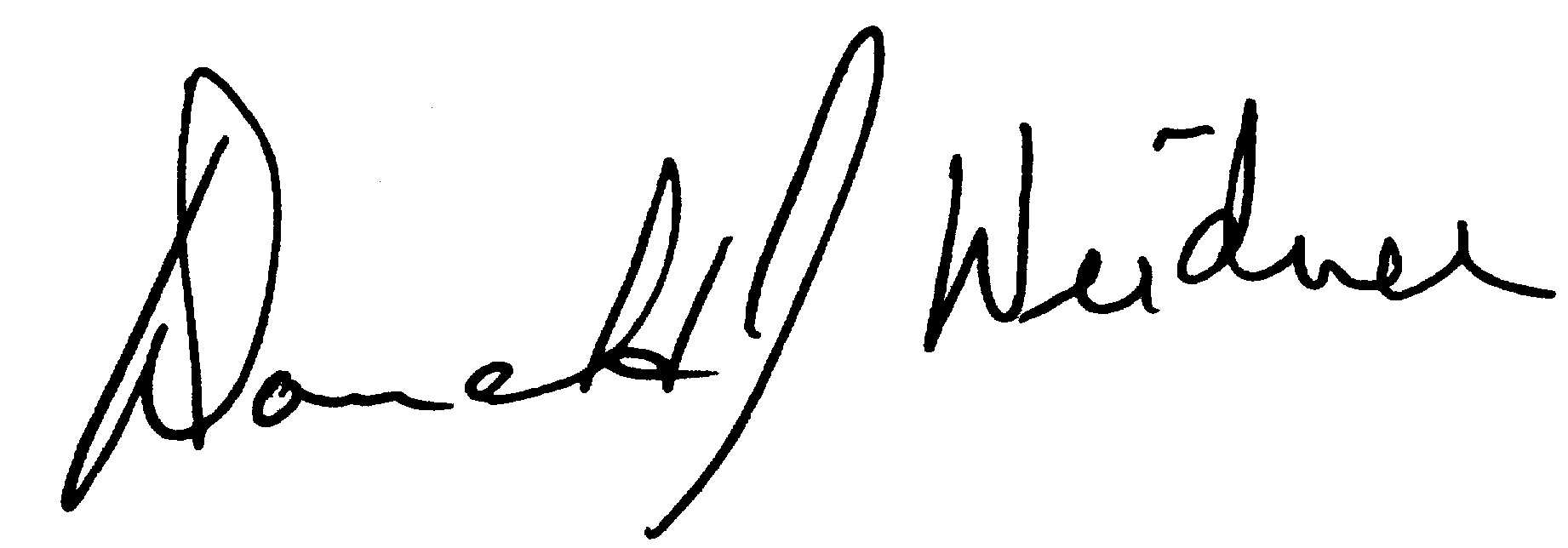
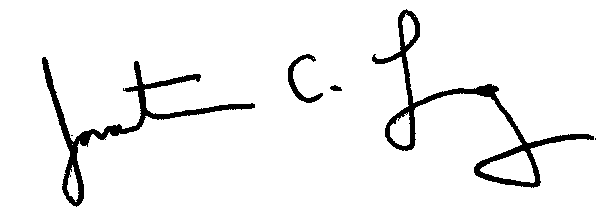
**7 Term of the Agreement**

The term of this agreement shall automatically renew on a year-to-year basis. COMPRES can withdraw from this agreement with 6 months notification to APS.

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XXXXXX Dennis Mills

President, COMPRES APS-PSC Deputy ALD

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Donald Weidner Jonathan Lang

COMPRES EDD Director XSD Div. Dir.