

PHYSICS REQUIREMENT DOCUMENT (PRD)	Doc. No. SP-391-000-33 R0	LUSI SUB-SYSTEM XPP		
Physics Requirements for the XPP Instrument				
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1. Applicable Documents

PRD# SP-391-000-03	LUSI Controls and Data System
PRD# SP-391-000-04	LUSI Pop-in Profile Monitor
PRD# SP-391-000-06	LUSI Data Management
PRD# SP-391-000-08	LUSI Intensity-Position Monitor
PRD# SP-391-000-09	LUSI Pop-in Intensity Monitor
PRD# SP-391-000-10	LUSI Attenuator System
PRD# SP-391-000-11	LUSI X-ray Focusing Lens System
PRD# SP-391-000-13	XPP Diffractometer System
PRD# SP-391-000-14	LUSI Slit System
PRD# SP-391-000-18	XPP Laser System
PRD# SP-391-000-23	LUSI Pulse Picker
PRD# SP-391-000-34	LUSI Harmonic Rejection Mirror System
PRD# SP-391-000-97	XPP 2D Detector

2. Overview

The X-ray Pump-Probe instrument (XPP) will enable the study of stimulated changes in the structures of molecules and condensed matter systems. The XPP instrument will predominantly use a short pulse optical laser to generate transient states of matter, and the hard X-ray pulses from the LCLS to probe the structural dynamics initiated by the laser excitation. The laser pump will have the ability to conduct precise optical manipulations in order to create the desired excited states. The instrument design will emphasize versatility. To maximize the range of phenomena that can be excited, it will be necessary to be able to manipulate the laser pulse energy, frequency, polarization and temporal profile. Additionally, the instrument shall have the capability of accommodating a wide variety of sample environments (cryostat, cryostream, liquid jet, pressure cell, etc...). X-ray scattering will be the dominant tool for probing the laser-induced structural changes, while X-ray emission spectroscopy will probe changes in electronic structure. These experiments require the union of four experimental capacities: the generation and delivery of X-ray and laser pulses to the sample, sample preparation and orientation, and the detection of the X-ray scattering pattern or X-ray emission.

This document contains a general description of the XPP instrument. Specific details of the instrument components are provided in separate PRDs.

The coordinate system is defined in Design Standards Supplement DS31100036.

3. Instrument Performance Goals

3.1. Experimental Versatility

The pump-probe technique can be applied for all X-ray scattering techniques. As such, the XPP instrument shall have sufficient flexibility to accommodate as many classes of experiments as reasonable achievable.

3.2. Temporal Instrument Response

One of the main performance parameters of the XPP instrument is the temporal instrument response function. This function is a convolution of the X-ray pulse duration and the precision that the ultrafast laser is synchronize to the X-ray pulse. The initial design goal of the XPP temporal instrument response is 80 fs (rms).

4. Components

4.1. LUSI Attenuator System (SP-391-000-10)

Attenuators will be used to reduce the X-ray flux during alignment procedures, as well as during some experiments where the sample must be protected from damage by the beam. Attenuators will consist of highly polished foils of damage resistant material. Multiple foils will be used to vary the attenuation.

4.2. LUSI Slit System (*SP-391-000-14*)

Slits will be used to define the sample region that is being probed by the X-ray beam. The slit blades will be engineered to tolerate the full LCLS peak flux and to minimize parasitic scatter. Slit systems will be positioned on the beamline as shown on the layout displayed in Figure 1.

4.3. LUSI X-ray Focusing Lens System (*SP-391-000-11*)

Compound refractive lenses will be used to decrease the X-ray spot size at the sample when required. Three lens assemblies will be accommodated. The lens-to-sample distance shall have ± 20 cm adjustability.

4.4. LUSI Harmonic Rejection Mirror System (*SP-391-000-34*)

A double mirror system will be used to reject high energy X-ray photons from the fundamental X-ray wavelength. This device will be used when experiments are operating with the fundamental radiation and removed when experiments require the 3rd harmonic.

4.5. LUSI Pulse Picker (*SP*-391-000-23)

The LUSI pulse picker is used to select a single LCLS pulse or pulses at a desired frequency below 1 Hz. This device will be used when there are concerns regarding sample damage or relaxation times.

4.6. XPP Diffractometer System (*SP-391-000-13*)

The XPP diffractometer system will be used to orient and position samples as well as position the XPP detector about a spherical surface centered at the interaction region. Two diffractometer assemblies (kappa and tilt platform) will mount to a base setup to accommodate a wide variety of sample environments and orientational degrees of freedom.

4.7. XPP Laser System (*SP-391-000-18*)

A short pulse laser system will be used to photoexcite samples. The system will have the ability to tailor the spectral, temporal, polarization, spatial and intensity properties of the excitation pulse. Also included in the system are: optical tables, optics and optomechanics, diagnostics, laser containment and safety system.

4.8. LUSI Pop-in Profile Monitor (SP-391-000-04)

The Pop-in Profile monitor will be used to characterize the spatial profile of the X-ray beam. This diagnostic will be used to align X-ray optics, diagnostics and samples. The monitor consists of a scintillation screen placed directly into the beam followed by a visible mirror. A CCD camera will capture the scintillation signal from the screen. The monitor is not a transmissive diagnostic. Therefore, the screen will be retracted out of the beam when not in use.

4.9. LUSI Pop-in Intensity Monitor (SP-391-000-08)

The LUSI Pop-In Intensity monitor is an X-ray photodiode placed directly into the beam. The integrated signal is measured in a destructive fashion and is proportional to the incident beam intensity. These monitors will be used for alignment of X-ray optics and samples. It will be retracted out of the beam once alignment is complete.

4.10. LUSI Intensity-Position Monitor (SP-391-000-09)

The LUSI Intensity-Position monitor is a device that will measure the incident X-ray intensity and position in a non-destructive manner. The information obtained from this device will be used to normalize experimental data as well as for alignment of X-ray optics. The device is designed to measure the Compton backscattering from a foil. Upstream of the foil is a tiled photodiode arrangement with a central hole to let the beam pass. The integrated signal is proportional to the incident beam intensity while the relative signal from each tile gives a rough estimate of the beam position. The measurement is not destructive provided the foil is thin, uniform and constructed from a light element.

4.11. XPP 2D Detector (SP-391-000-97)

An X-ray active matrix pixel sensor (XAMPS) is being developed by Brookhaven National Laboratory for the XPP instrument since a detector system with the required characteristics is not commercially available. It will include an array of 1024 x 1024 pixels with a pixel size of 90x90 μ m². To support the breadth of experiments that will be performed at the XPP station, the detector must have the ability to detect a single X-ray photon with high efficiency as well as measure a slight change in an intense Bragg reflection. To accommodate these requirements, the detector will have high quantum efficiency (approaching unity at 8 keV) and a 10⁴ dynamic range per pixel.

4.12. Crane

A crane will be required for introducing or removing heavy equipment to and from the interaction point. In particular, this device is needed to safely reconfigure the sample goniometer system and for moving large sample environments.

5. Global Requirements

5.1. Layout Requirements

- **5.1.1.** Two interaction points will be used for all experimental configurations. One point will be designed for a future monochromatic beam and the second for direct beam operation. These points will be located at a common Z position.
- **5.1.2.** XPP components will be positioned in the order displayed in Figure 2.
- **5.1.3.** The XPP diffractometer will be placed in a location that is as close the northwest corner of the alcove in hutch 3 as possible (see Figure 1), while allowing sufficient clearance for a person to walk between the corner and the diffractometer arm.

5.2. Mechanical Requirements

- **5.2.1.** The faded components in Figure 1 shall be capable of translating into either the direct FEL beam or the future monochromatic beam. This translation does not need to be motorized. However, the aim of the translation system will be to position "aligned" optical components into either beam without the need to re-align. Therefore a 25 micron translational repeatability is needed.
- **5.2.2.** Stringent thermal and vibration requirements apply to the LUSI Slit systems, LUSI X-ray Focusing Lens system, LUSI Harmonic Rejection Mirror system and LUSI Intensity-Position monitors. Once these devices are aligned in the beam, their location shall not deviate with respect to each other by more than 5 microns in position and 10 μ rad in angle over the course of an experiment (~ days).
- **5.2.3.** The thermal and vibration stability of the monochromator and diffractometer are described in PRDs SP-391-000-16 and SP-391-000-13.
- **5.2.4.** All other components require a stability of 25 microns in position and 50 μrad in angle over the course of an experiment (~ days).

5.3. Vacuum Requirements

- **5.3.1.** The vacuum pressure at the location of any optical component along the XPP beamline shall not exceed 1×10^{-7} Torr to avoid contamination.
- **5.3.2.** A level of vacuum should be maintained in the system to permit a 10 year ion pump lifetime.
- **5.3.3.** An X-ray window will be implemented between the laser port and interaction region to provide vacuum isolation between the beamline and either air or a vacuum sample environment. The window shall permit a connection to a vacuum sample environment (i.e. double side flange).

5.4. Access Requirement

- **5.4.1.** The design of the XPP Instrument shall permit entrance into NEH Hutch 3 while beam is being delivered to the FEH or while soft X-rays are being delivered to NEH Hutch 1 or 2.
- **5.4.2.** If a beamsplitting monochromator is added to the instrument, NEH Hutch 3 access shall not interrupt direct beam delivery to the FEH.



Figure 1. Cartoon schematic of NEH Hutch 3. The FEL radiation propagates from left to right in this picture. Besides the optics and diagnostics in NEH Hutch 2, the entire XPP instrument will reside in Hutch 3. The alcove will be used to perform Small Angle X-ray Scattering (SAXS) experiments as a future upgrade to the instrument. The northwest corner of the SAXS alcove is indicated.



