PHYSICS REQUIREMENT DOCUMENT (PRD)	Doc. No. SP-391-000-13 R1	LUSI SUB-SYSTEM XPP

Physics Requirements for the XPP Diffractometer System

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Revision	Date	Description of Changes	Approved
R0	18DEC07	Initial Release	
R1	01APR08	Modified Detector Mover Reach Requirements	

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Table of Contents

1. Overview

The diffractometer system is a critical component for almost all XPP experiments. At its center, the laser beam and the FEL beam intersect with the sample. Henceforth, this point of intersection will be referred to as the interaction point. The diffractometer system serves two purposes simultaneously: control the angular orientation and spatial position of the sample, and to position the XPP detector. The sample position and angular orientation must be manipulated in a precise, reproducible fashion. For some XPP experiments the sample will be confined in a particular environment (vacuum, cryostat system, pressure cell, liquid jet, etc…). In all cases the diffractometer has to guarantee a stable and reproducible position and angular orientation of both the sample and detector. The XPP diffractometer system specification is defined in this document.

The coordinate system is defined in Design Standards Supplement DS31100036.

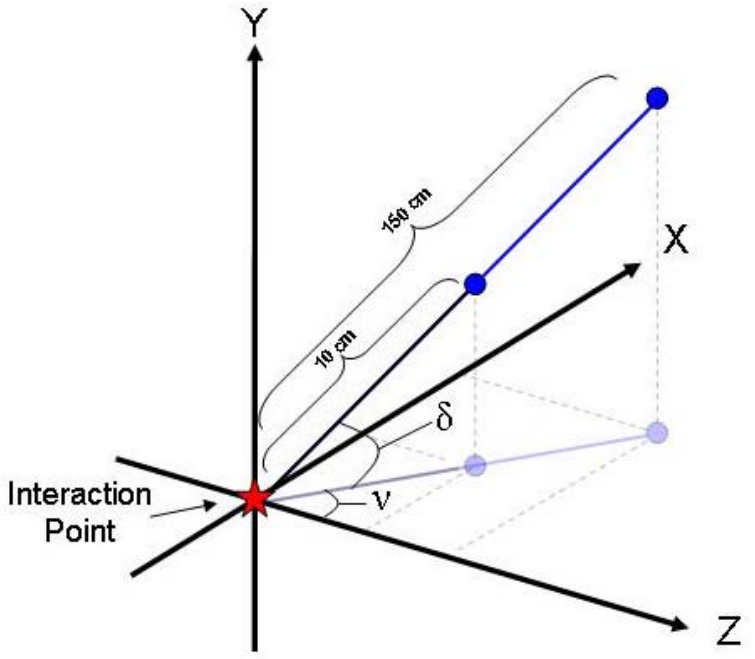

Figure 1. Geometry of the detector motion.

2. XPP Diffractometer System Performance Requirements

2.1. The diffractometer system shall have the flexibility to accommodate a wide variety of sample environments. This includes, but is not limited to, the XPP vacuum chamber (SP 391-000-37), XPP liquid jet (SP 391-000-38) and XPP emission spectrometer (SP 391-000-17).

2.2. The diffractometer system shall have the capability of operating in both the white and monochromatic beamlines.

2.2.1. The repeatability of the positioning of the sample positioner when returning to an operating position (white or monochromatic) shall be better than ±5 μm in X, Y, Z and better than ±5 mDeg in roll, pitch and yaw. These values are intended to provide sufficient precision to reproducible position a 50 μm sample without the need for re-alignment.

2.2.2. The repeatability of the positioning of the detector positioner when returning to an operating position (white or monochromatic) shall be better than ±20 μm in X, Y, Z and better than ±1.5 mDeg in roll, pitch and yaw. This is less than 1 pixel error at a detector distance of 150 cm.

2.3. The diffractometer system (sample and detector movers) shall have the capability of remotely translating the interaction point in the Y direction to accommodate operation with and without the LUSI harmonic rejection mirror system.

2.4. Instrumentation shall be included in the diffractometer system to characterize the sphere of confusion for both the detector and sample movers.

3. Detector Mover and Detector Arm Performance Requirements

3.1. The detector mover shall move XPP detectors about a spherical surface centered at the interaction region.

3.2. The spherical surface shall have a variable radius from 10 cm to 100 cm measured from the interaction point to the XPP detector sensor.

3.3. The integrated sphere of confusion of the detector arm motion about the interaction point shall be less than 120 μm. This number shall include both long term and short term drift due to thermal and vibrational effects.

3.4. A calibration mechanism shall be included on the detector arm to determine the absolute detector-to-interaction region distance for any detector position once the distance is calibrated for a particular location through surveying methods or experimental measurement.

3.5. The detector mover shall have coverage that spans the volume displayed in Figure 2.

3.6. The repeatability of detector motion about the spherical surface shall be better than ±3.0 mDeg for both angular degrees of freedom (ν and δ).

3.7. The clocking angle of the detector sensor shall be known to an accuracy of 0.04 degrees.

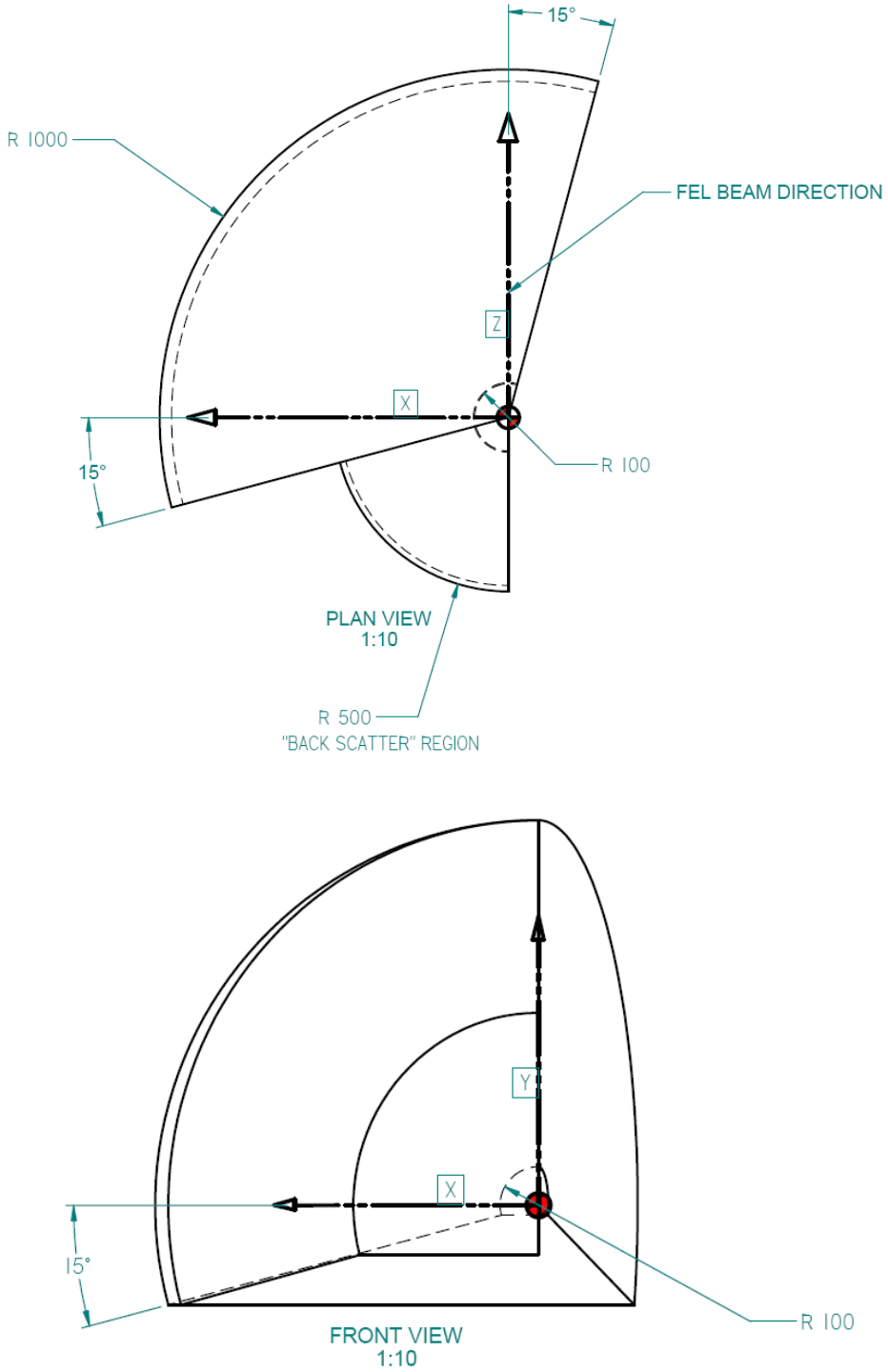

Figure 2. Detector mover reach volume (REF_Detector Face Volume_19FEB08.dft).

4. Sample Mover Performance Requirements

4.1. Open access to the sample shall be accommodated in the sample mover design to the highest extent reasonably achievable. This will permit unobstructed introduction of the X-ray and optical laser beams onto the sample as well as unobstructed detection of X-ray scattering from the sample.

4.2. The integrated sphere of confusion of sample motion shall be less than 30 μm.

4.3. The position of the sample shall not drift by more than 10 μm in X, Y, and Z and 1 arcsec in roll, pitch and yaw over 1 day.

4.4. The interaction point vibration shall be minimized to less than 1 μm. Additional, vibrations shall not cause interaction point angular deviations greater than 0.2 arcsec. However, this requirement is not applicable for the XPP liquid jet environment.

4.5. A remote sample mover configuration is required to accommodate large sample environments (LSE).

4.5.1. The LSE configuration shall accommodate sample environments up to 50 kg.

4.5.2. A distance greater than 200 mm from the sample center to the LSE mounting surface is required.

4.5.3. Pitch, roll, and yaw adjustment shall be provided to the LSE configuration with a range of motion ≥ 5 degrees and a precision and repeatability that is consistent with meeting the Bragg condition for single crystal samples in the monochromatic beam ($\Delta E/E = 1.4 \times 10^{-4}$).

4.5.4. X, Y, and Z adjustment shall be provided to the LSE configuration with a ±30 mm range of motion. The precision and repeatability of these motions shall be consistent with maintaining the Bragg condition of a single crystal sample while being translated.

4.6. A remote precision sample mover configuration is required for small sample manipulation (SSM).

4.6.1. The SSM configuration shall have no limitation on the achievable angular range of the sample (360 degrees for roll, pitch and yaw).

4.6.2. The precision and repeatability of the SSM angular motions shall be consistent with meeting the Bragg condition for single crystal samples in the monochromatic beam ($\Delta E/E = 1.4 \times 10^{-4}$).

4.6.3. Manual adjustment of the sample position shall be provided to center the sample in the diffractometer (Eucentric goniometer head).

4.6.4. A motorized translational adjustment is required to raster the sample in the event of beam damage. The range of motion shall be ≥ 25 mm.

5. Controls Requirements

5.1. Positioning of the XPP detector and sample shall be performed remotely.

5.2. All adjustable electronic limits that will be provided for diffractometer components shall be incorporated into the instrument control system.

5.3. A geometry calculation routine shall be integrated into controls system that will drive the diffractometer and data acquisition system (i.e. ability to control the explored sample in reciprocal space).

Appendix A – Revision 1 Primary Changes Affected Sections

3. Revision 1 Detector Mover and Detector Arm Performance Requirements

3.1. (no change)

3.2. (was) The spherical surface shall have a variable radius from 10 cm to 150 cm measured from the interaction point to the XPP detector sensor.

3.3. (no change)

3.4. (no change)

3.5. (was) The detector mover shall have coverage that spans at least one half of a hemisphere (see Figure 1) when the sample-to-detector distance is greater than 50 cm. This corresponds to a δ value ranging between between 0 and 90 degrees, and a ν value either between 0 and 180 degrees or 180 and 360.

3.6. (was) The repeatability of detector motion about the spherical surface shall be better than $\pm$1.5 mDeg for both angular degrees of freedom (ν and δ).

3.7. (was) The detector arm shall have the capability of accommodating other instrumentation (typically < 10 kg) such as a vacuum flight tube, apertures and attenuators in front of the detector.