

PHYSICS REQUIREMENT DOCUMENT (PRD)	Doc. No. SP-391-001-32 R0	LUSI SUB-SYSTEM XCS
Physics Requirements for the XCS Diffractometer System		
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Table of Contents

1. Overview	2
2. XCS Diffractometer System Performance Requirements	2
3. Local Detector Arm Performance Requirements	3
4. Sample Mover Performance Requirements	5
5. Local Detector requirements	5
6. Controls Requirements	5

1. Overview

The diffractometer system is a component of the XCS Instrument. The detector motion used for performing XPCS experiment (i.e for experimental data acquisition) on the XCS Instrument is not part of the present Physics Requirement Document and is described in SP-391-001-33 (i.e Wide Angle Detector Stage). The diffractometer system has however a detector, referred here as “local detector”.

The diffractometer system serves the two following purposes simultaneously:

- control the angular orientation and spatial position of the sample towards the incident x-ray beam.
- position the local detector.

The sample position and angular orientation must be manipulated in a precise and reproducible fashion. For some XCS-experiments the sample will be confined in a particular environment (vacuum, cryostat system, pressure cell, liquid jet, etc...). The local detector aids to the alignment of the sample/sample environment in the x-ray beam. In all cases the diffractometer has to guarantee a stable and reproducible position and angular orientation of both the sample and local detector.

The XCS diffractometer is a 4-circle horizontal scattering geometry diffractometer and its specification is defined in this document.

The coordinate system is defined in Design Standards Supplement DS39100036.

2. XCS 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 any sample environment built for the XPP instrument with minor modification (i.e. an interface piece is acceptable).
- 2.2.** The diffractometer system shall have the capability of operating in the monochromatic beam, but also to be removed from the beam path, thus leaving a clear floor print. This motion is not required to be motorized. This allows accommodating very large sample environments or equipments which are not compatible with the diffractometer design and thus ensures a very high flexibility of the XCS instrument.

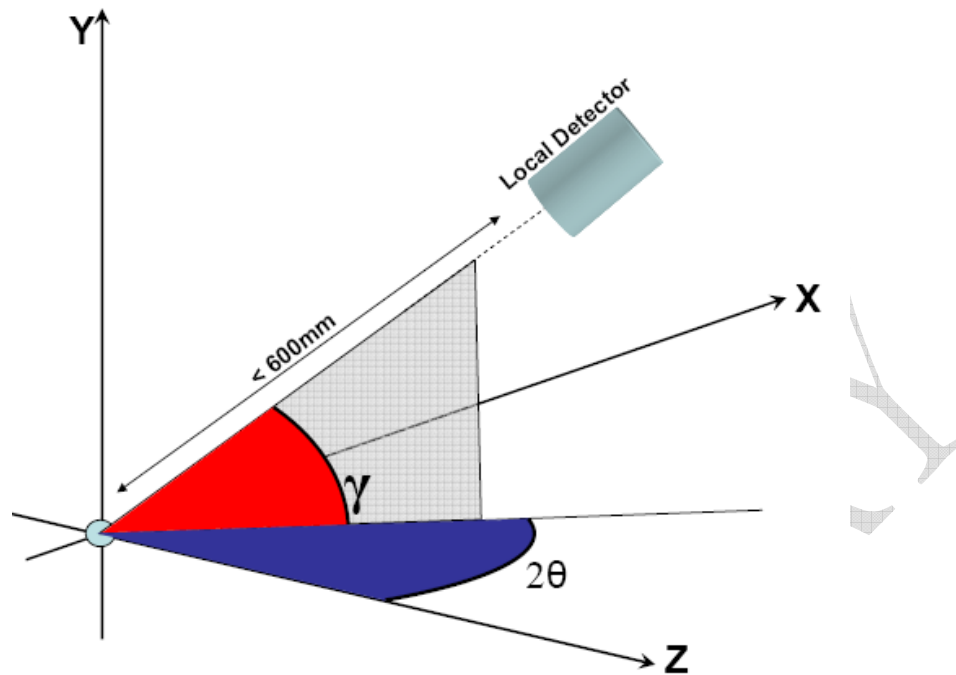


Figure 1. Geometry of the XCS diffractometer local detector.

- 2.3. The repeatability of the positioning of the diffractometer when returning to the operating position (i.e to the monochromatic beam) shall be better than $\pm 5 \mu\text{m}$ in the X direction . This could be realized by a motorized translation of the overall diffractometer components in the X-directions, decoupled from the large motion of the overall assembly. This motion range should be $> \pm 10\text{mm}$.
- 2.4. The diffractometer system shall have the capability of remotely translating its COR in the Y direction to accommodate operation with and without the LUSI harmonic rejection mirror system (i.e vertical offset of the beam, but also use of the mirror to produce a beam impinging at the sample location in grazing incidence).
- 2.5. Instrumentation should include a standard non-motorized goniometer head with a sharp pin for centering the diffractometer in the x-ray beam during alignment procedures.

3. Local Detector Arm Performance Requirements

- 3.1. The detector mover shall move a local detector (such as but not limited to a point detector and associated pairs of slits to control the observed solid angle) about a horizontally truncated spherical surface centered at the COR of the diffractometer. The whole sphere is not required, as the motion will be constrained in the proximity of the horizontal scattering plane.

- 3.2. The detector mover shall have coverage that spans the surface displayed in Figure 2. (i.e. truncated sphere with γ - angle ± 5 degree, 2θ -angle ± 160 degree and distance $< 600\text{mm}$)
- 3.3. The repeatability of the local detector motion about the truncated spherical surface in both the horizontal vertical scattering plane shall be better than ± 1.0 mDeg ($\approx 3.6\text{arcsec}$)
- 3.4. The local detector shall have the capability of moving as close to the COR as reasonably achievable, while minimizing interferences with large sample environments.
- 3.5. Specific care has to be taken regarding the interaction between the motion of the local detector and the possible nearby obstacles (such as the CXI beamline located 600mm south from the XCS monochromatic line but also the Wide Angle Detector Stage). This could be performed by software and electrical limits.
- 3.6. The integrated sphere of confusion of the local detector arm and sample motion shall be less than $100\ \mu\text{m}$. This number shall include both long term and short term drift due to thermal and vibrational effects.
- 3.7. The center of rotation could change in the Y direction. The local detector motion should accommodate a change of the center of rotation in the Y direction (as result of the operation of upstream optical components).

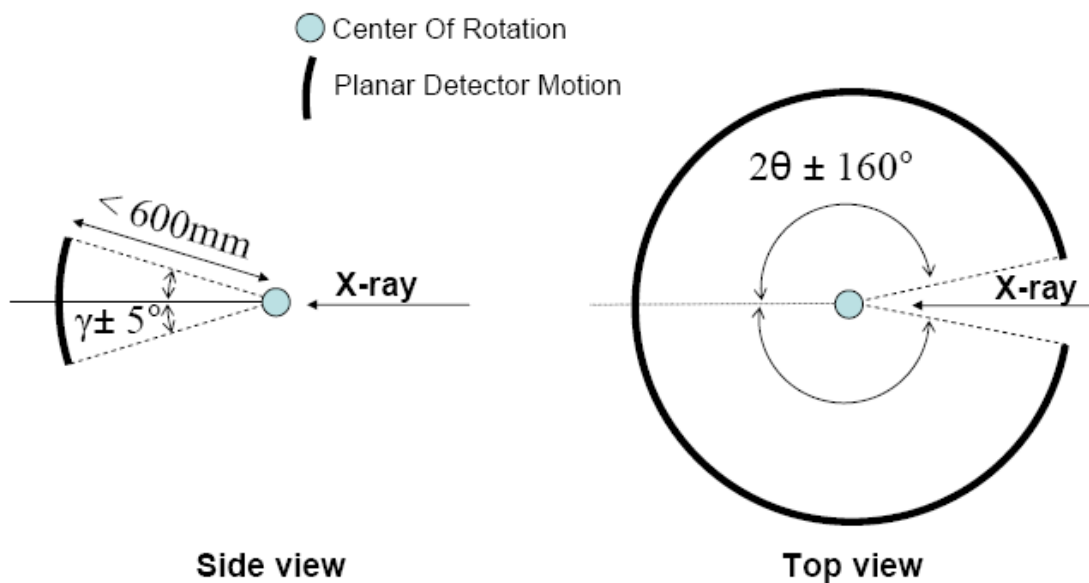


Figure 2. Angular Range of motion $\{2\theta, \gamma\}$ for the local detector. It describes a truncated spherical surface allowing the local detector to move over a limited range in the proximity of the horizontal plane

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 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 70 μm .
- 4.3. The position of the sample shall not drift by more than 10 μm in X, Y, and Z and 0.3mDeg (≈ 1 arcsec) in roll, pitch and yaw over 1 day.
- 4.4. The COR vibration shall be minimized to less than 1 μm . Additional, vibrations shall not COR angular deviations greater than 0.06mDeg (≈ 0.2 arcsec).
- 4.5. The sample mover shall accommodate sample environments up to 50 kg.
- 4.6. A distance greater than 200 mm from the COR to the mounting surface is required This distance should be to the extent of possible similar to the one of the XPP diffractometer system.
- 4.7. Pitch and roll adjustment shall be provided with a range of motion ≥ 5 degrees and a precision and repeatability better than 1mDeg (≈ 3.6 arcsec)
- 4.8. Yaw adjustment shall be provided with a range of motion ± 180 degree and a precision and repeatability better than 1mDeg (≈ 3.6 arcsec).
- 4.9. X, Y, and Z adjustment shall be provided with at least ± 10 mm range of motion with a resolution better than 2 μm .
- 4.10. The capability of adjusting the COR in the Y direction should be incorporated in the design (as result of the operation of upstream optical components) with a resolution better than 5 μm .

5. Local Detector requirements

- 5.1. The local detector will consist of a point detector (such as a diode) and pairs of slits
- 5.2. The assembly (i.e. detector and slits) should be modular and mounted on the local detector motion
- 5.3. The assembly should perform in air.
- 5.4. Sufficient flexibility in the design of the assembly is requested to accommodate another point detector or other slits if necessary.

6. Controls Requirements

- 6.1. Positioning and orientation of the local detector and sample shall be performed remotely.
- 6.2. All adjustable electronic limits that will be provided for diffractometer components shall be incorporated into the instrument control system.
- 6.3. 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).