LUSI — LCLS Ultrafast Science Instruments

ENGINEERING SPECIFICATION DOCUMENT (ESD)	Doc. No. SP-391-001-20 R0	LUSI SUB-SYSTEM XCS

LUSI XCS Diffractometer System Engineering Specification
DRAFT

Approved by: Eric Bong XCS Lead Engineer	Signature	Date
Prepared by: Jim Delor – XCS Design Engineer	Signature	30JUN08 Date
Approved: Aymeric Robert XCS Instrument Scientist	Signature	Date
Approved: Darren Marsh Quality Assurance Manager	Signature	Date
Approved: Nadine Kurita Chief Engineer	Signature	Date
Approved: Jerome Hastings Project Director	Signature	Date

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1. Scope:

This document describes and defines the engineering requirements for a system to precisely translate, rotate, and orient samples and sample environments in the LUSI X-Ray Correlation Spectroscopy (XCS) instrument. The "**Diffractometer System**" is comprised of the two following major elements:

- "**Sample Goniometer**": Precisely positions, rotates, and translates the sample.
- "**Detector Mover**": Precisely positions and orients the "local detector" towards the center of the goniometer.

In all cases the diffractometer system has to guarantee a stable and reproducible position and angular orientation of both the sample and local detector for the life of the instrument. A 'four circle, horizontal scattering diffractometer' has been used as a solution to meet these requirements.

2. Diffractometer System Summary:

2.1. Sample Goniometer Summary:

The LUSI XCS sample goniometer will be used to precisely control the physical location and orientation of a variety of samples and sample environments. The nature of the LUSI XCS instrument requires a level of "flexibility" and accuracy from the diffractometer system. The system must incorporate features to enable the use of sample environments such as: Cryostat, Cyrostream, vacuum/pressure chambers, etc., etc. Features to accommodate alignment fixtures for the sample goniometer and the detector mover must be integral to the overall design to achieve desired levels of accuracy. The sample goniometer design must enable rapid reconfiguration to maximize science output and best utilize limited beam time.

The Sample Goniometer shall be able to position the sample using six degrees of freedom; e.g. translations in X, Y, Z, and rotations about the same three axis. A center of rotation is defined above the sample goniometer top platform at common distance with the XPP diffractometer system to facilitate interchangeability of sample environments.

2.2. Detector Mover Summary:

The local detector aids the alignment of the sample/sample environment in the X-ray beam and the subsequent positioning of the large detector covered in separate ESD/PRDs.

The detector mover is precisely motor-controlled so as to point at the CoR through a range of beam height, and angular changes. The detector mover has three automated degrees of freedom: Translation in the Y direction (lift), tilt in a vertical plane, and a base rotation about the axis of rotation of the diffractometer. An additional manual degree of freedom allows variations of the detector-to-sample radial distance. All these motions are to be independent and uncoupled from the motions of the sample goniometer. Software and control shall be employed to maintain correct pointing of the detector through the variety of heights and radii.

3. Glossary / Definitions:

Accuracy: The measure by which a predetermined value can be achieved with respect to a fixed coordinate system.
CoR: Center of Rotation
Goniometer: Precision positioning device which moves sample to precise angular & spatial position.
Goniometer Foundation: Surface providing attachment for goniometer mount base.
Repeatability: Defines the ability to successively reestablish a position with respect to a fixed coordinate system.
Resolution: Defines the uncertainty of a measurement of a position with respect to a fixed coordinate system. Also defines the minimum measurable difference between two dissimilar values.
SoC: Sphere of Confusion
Stability: Defines accuracy for a specified time.
XPCS: X-ray Photon Correlation Spectroscopy
XRT: X-Ray Tunnel

3.1. Sphere of Confusion:

Rotations of the sample goniometer over all possible axes define a quasi-spherical precession of the CoR due to alignment and manufacturing imperfections when viewed from a fixed coordinate system. This is called the "sphere of confusion" (SoC), the diameter of which defines the accuracy with which the beam can be positioned and maintained over a given spot on the sample.

Determination of the specifications for the sample goniometer hardware are directly related to, and determined by, the desire to minimize the SoC.

4. Applicable Documents, Specifications and Codes:

The coordinate system is defined in Design Standards Supplement DS31100036.

4.1. SLAC Documents and Specifications:

AP-391-000-59: "Engineering Review Guidelines"
DS-391-000-36, "Design Standards Supplement"
GP-391-XXX-XX, "Hutch 4 - XCS Arrangement"
ID-391-XXX-XX, "Sample Goniometer Installation"
GP-391-750-XX, "Hutch 4 - XCS Sub-system Stay Clear Definitive Lay-out"

4.2. General Seismic Considerations:

SLAC is situated in an active seismic zone. All hardware exceeding a weight of 300 Lbs. and / or mounted greater than 4 feet above the floor will be reviewed by a SLAC "citizen safety committee" for seismic loading resistance. Applicable loads and structural behavior will be evaluated for compliance to the 1997 version of the uniform building code and SLAC publication **SLAC-I-720-0A24E-002**: "Specification for Seismic Design of Buildings, Structures, Equipment, and Systems at the Stanford Linear Accelerator".

4.3. Industry Specifications and Codes:

NEC, NFPA 70; "National Electric Code,
NEC, NFPA 70E; "Electrical safety in the Workplace"
UBC 1997: "Uniform Building Code, 1997"

5. Environmental Safety and Health Requirements:

All systems hardware will be subject to SLAC review and approval. Reviews will be conducted in accordance with SLAC document number AP-391-000-59: "Engineering Review Guidelines". SLAC reserves to right to employ an internal (SLAC direct), external independent, or mixed source review panel.

Particular review attention will be devoted to:

- Personnel access restriction methodology
- Emergency stop methodology / mechanisms
- Power failure provision – fault modes
- Electrical subsystem Lock-Out / Tag-Out:
- Training mode functionality
- Maintenance mode functionality
- Machine Protection

As previously stated, all hardware exceeding a weight of 300 Lbs. and / or mounted greater than 4 feet above the floor will be reviewed by a SLAC "citizen safety committee" for seismic loading resistance.

All electrical hardware and connections will be reviewed for compliance to local electrical code(s).

6. General Area / Adjacent Equipment Description:

6.1. Overview:

The Linac Coherent Light Source (LCLS) generates coherent hard x-rays (i.e.: x-ray laser light) in conjunction with the last 1km of the SLAC linear accelerator.

The LCLS Ultra-fast Science Instruments (LUSI) project consists of a suite of three x-ray instruments for exploiting the scientific capability of the LCLS. These instruments will be housed in experiment hutches located in the Near Experimental Hall (NEH) and the Far Experimental Hall (FEH).

6.2. XCS Instrument Overview:

The X-Ray Correlation Spectroscopy (XCS) instrument is one of the instruments built by LUSI. This instrument will investigate dynamical phenomena on condensed matter systems down to nanometric length scales. The XCS instrument is located in hutch 4 in the FEH.

To maximize scientific output, all XCS systems will be designed, constructed and installed to support hardware reconfiguration, realignment and recalibration in 8 hours or less. This includes repositioning the diffractometer from the out-of-beam position, completing the seismic restraint, power and control hook-ups, and performing initial alignment to the X-ray beam.

XCS is comprised of four main subsystems:

- Optical components and diagnostics located in the XRT.
- An X-ray optics-diagnostic section for analysis and optimization of x-ray beam properties within Hutch 4. The optical components can provide vertical steering of the beam.
- A diffractometer system comprised of a sample goniometer and a local detector. This allows very precise placement and orientation of the sample in the FEL beam. This is the subject of this specification.
- A wide angle detector stage holding a pixilated detector to perform XPCS experiments.

6.3. Hutch 4/XCS Equipment Overview:

The hutch 4 floor plan consists of a main experimenter area and a down-beam alcove. Overall hutch 4 dimensions are shown in **figure 1**.

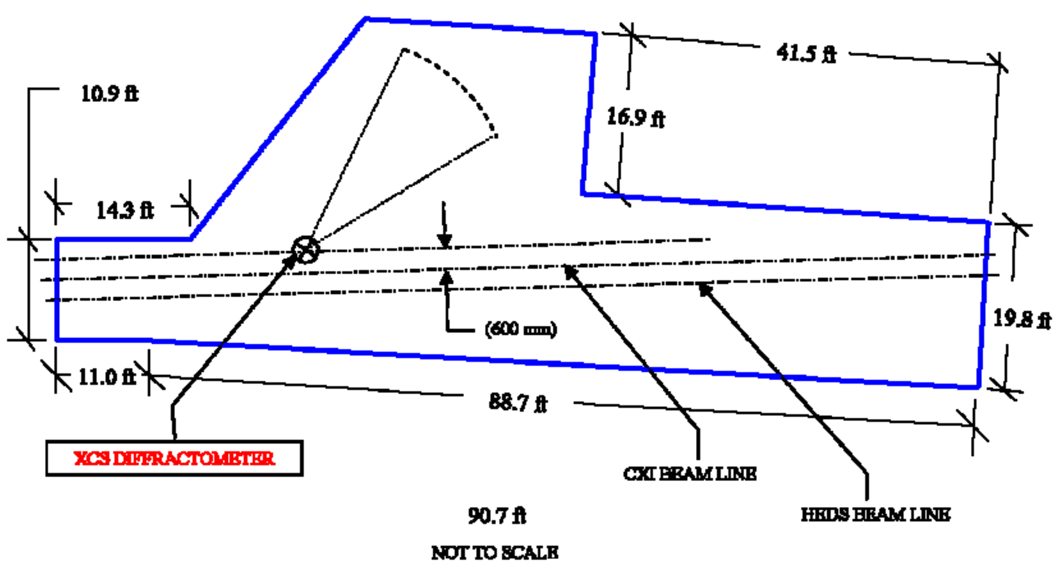

Figure 1

Hutch 4 – XCS Floor Plan

The major XCS subsystem locations are referenced in SLAC drawing GP-391-400-00.

6.4. X-ray beam Positional Uncertainty:

Long transport distances, upstream optics, coupled with variables such as temperature and ground motion of undulator and optical transport elements, can have a significant effect on the position of the x-ray beam entering hutch four.

The low frequency (days-weeks) drift of the X-ray beam in XCS hutch four combined with steering from the upstream optics, can cause a significant shift of the Center of Rotation. For the XCS diffractometer design purposes, the Center of Rotation coordinate is considered variable by up to 4 mm (+/- 2 mm tol.) from nominal. Some classes of XCS experiments will require the X-ray beam to impinge the sample with a grazing incident angle. Elements in the optics-diagnostic section will be employed to steer the x-ray beam to the desired grazing angle. This translates to a vertical offset of the active interaction point. The maximum vertical offset of the active interaction point, from nominal position, will be ____ mm. The total area of the possible active interaction point location is shown in the figure following.

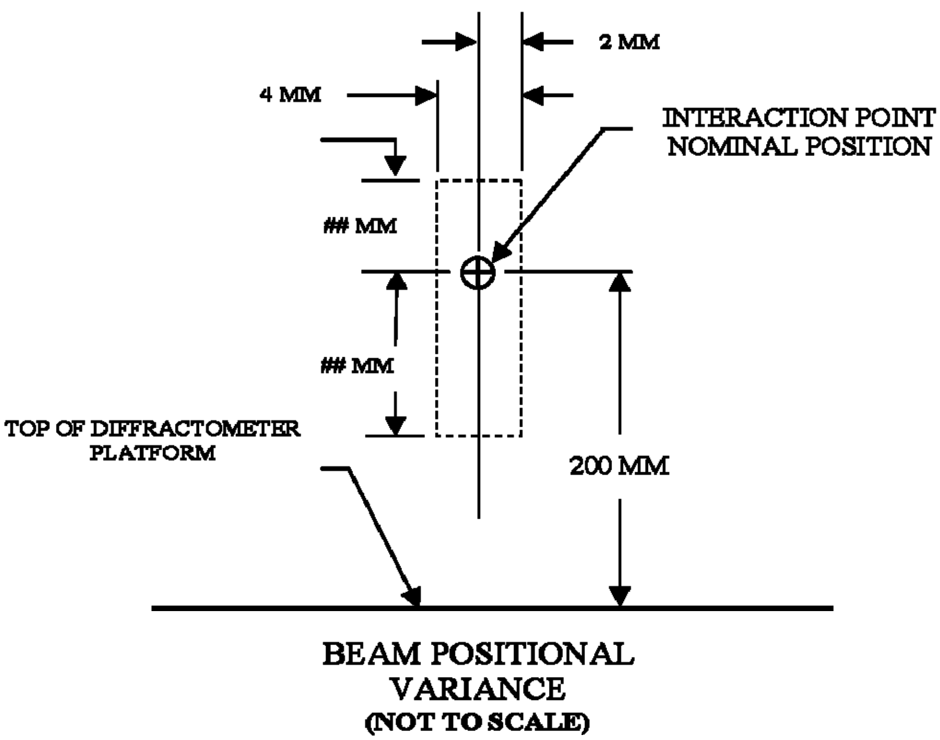

Figure 2

7. Diffractometer Load Capacities:

7.1.1. Sample Goniometer:

The sample goniometer shall accommodate a vertical top mass of up to 50 kg mounted on the top platform. The vertical load may be shifted as much as 50 mm from the goniometer rotation central axis. The sample goniometer must maintain the required sphere of confusion and move accurately with this loading in any position throughout all ranges of motion.

7.1.2. Detector Mover:

The detector mover shall accommodate a vertical top mass of up to 5 kg for the detector unit, and additional components. The vertical load may be shifted as much as 50 mm from the mount center. The detector mover must maintain the required sphere of confusion and move accurately with this loading in any position throughout all ranges of motion.

8. Diffractometer System Motion Description:

Table 8-1: Bottom-to-Top Description of the Goniometer System Motions
*Shaded stages may be removed if permanent alignment of upper stages is within SoC.

Vertical Sequence	I.D.	Function	Direction/Axis	MOTION
Top	**12**	Sample Movement	Y	Translation
	11		X	Translation
	10		Z	Translation
	9	Sample Tilt	PITCH	Rotation Segment
	8	Sample Tilt	ROLL	Rotation Segment
↑	7	Align Tilt Rotation Axes	X	Translation
	6		Z	Translation
	5	CoR Height Adjust	Y	Translation
	4	Sample Rotation	YAW	Rotation
	3	Detector Motion	YAW	Rotation (Decoupled)
	2	Diff. Axis Adjust	X	Translation
Bottom	1	Base Position	X	Air pad Motion

Table 8-2: Bottom-to-Top Description of the Motions for the Local Detector, atop the detector motion described in Table 8.1, I.D. 3 .

Vertical Sequence	I.D.	Function	DIR	MOTION
Detector Mount	**IV**	Vary Detector-Sample distance	Δd	Manual Translation
↑	**III**	Tilt Angle Adjust	Pitch	Rotation
	II	Vertical Adjust	Y	Translation
Base	**I**	Radial Support	ΔR	Manual Translation

9. Diffractometer System Motion Requirements

Table 9-1: Bottom-to-Top Requirements for the Goniometer System Motions
*Shaded stages may be removed if permanent alignment of upper stages is within SoC.

Vertical Sequence	I.D.	Range (mm)	Accuracy (μm)	Repeatability (μm)	Resolution (μm)	Stability (μm/hour)
Top	**12**	+/- 10	+/- 2	1	<1	<1
↑	**11**	+/- 10	+/- 2	1	<1	<1
	10	+/- 10	+/- 2	1	<1	<1
	9	+/- 5º	+/- 5 arc-sec	+/- 1 arc-sec	<2 arc-sec	<2 arc-sec/hr
	8	+/- 5º	+/- 5 arc-sec	+/- 1 arc-sec	<2 arc-sec	<2 arc-sec/hr
	7	+/- 10	+/- 2	1	<1	<1
	6	+/- 10	+/- 2	1	<1	<1
	5	+/- 100	+/- 2	1	<1	<1
	4	360º (w/encoder)	+/- 5 arc-sec	+/- 1 arc-sec	<2 arc-sec	<2 arc-sec/hr
	3	360º (w/encoder)	+/- 5 arc-sec	+/- 1 arc-sec	<2 arc-sec	<2 arc-sec/hr
	2	+/- 40	+/- 2	1	<1	<1
BASE	**1**	3500	+/- 2000	-	-	<1

Table 9-2: Bottom-to-Top Requirements for the Motions for the Local Detector, atop the detector motion described in Table 9.1, I.D. 3 .

Vertical Sequence	I.D.	Range (mm)	Accuracy (μm)	Repeatability (μm)	Resolution (μm)	Stability (μm/hour)
Detector Mount	**IV**	+/- 150	1000	-	-	<5
↑	**III**	+/- 5º	+/- 5 arc-sec	+/- 3 arc-sec	<3 arc-sec	<3 arc-sec/hr
	II	+/- 100	+/- 5	+/- 5	<2	<2
Base	**I**	+/- 50	1000	-	-	<5

9.1. Detector Mover Additional Requirements

9.1.1. Motions Extents:

The Detector Mover is used to move a local detector (such as but not limited to, a point detector and associated pair of slits) about a horizontally truncated spherical surface centered at the CoR of the diffractometer. The detector mover shall be intrinsically aligned to the same vertical axis that positions the sample, and it will moved within an angular range of +/- 5° about the horizontal plane through the CoR. This requires the Detector Mover to have a vertical motion(Y) capability relative to the sample goniometer CoR. This vertical adjustment and the corresponding angular motion (to keep detector pointed at the CoR) shall be a precisely motor controlled motion.

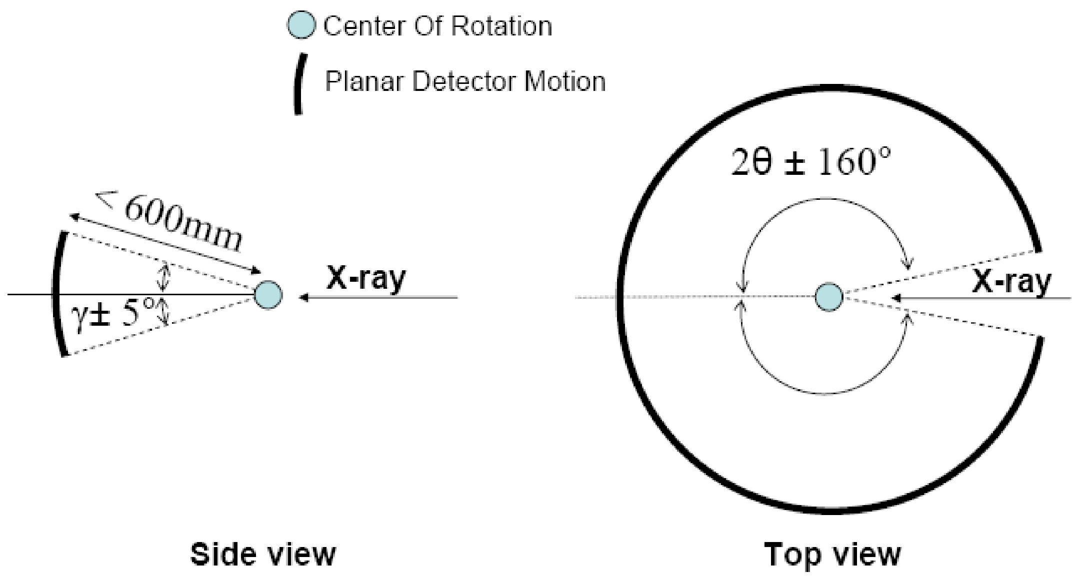

Figure 3

9.1.2. Coverage:

The detector mover shall have coverage that spans the volume displayed in **Figure 4**. (i.e. truncated sphere with γ- angle ± 5 degree, 2θ-angle ±160 degree and distance <600mm)

9.1.3. Radial Distance:

The distance from the local detector to the center of rotation of the diffractometer should be minimized with a small level of tunability in order to accommodate large sample environment if needed. The detector face shall have the ability to be positioned from a nearest distance of _____mm out to a distance of ____mm.

9.1.4. Integrated Sphere of Confusion:

The integrated sphere of confusion of the local detector arm and sample motion shall be less than **100 µm.** This number shall include both long term and short term drift due to thermal and vibrational effects.

9.1.5. Local Obstruction Avoidance:

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). This could be performed by software.

9.2. Sample Goniometer – Additional Requirements

9.2.1. Integrated Sphere of Confusion

The integrated sphere of confusion of the sample motion shall be less than **70 µm.** This number shall include both long term and short term drift due to thermal and vibrational effects.

9.2.2. Long Term Stability Requirement:

The position of the sample shall not drift by more than 10 μm(microns) in X, Y, nor Z, nor more than 0.3 mDeg(~1 arcsec) in roll, pitch, and yaw over a 24 hour period.

9.3. Diffractometer Hutch Position and Alignment:

The diffractometer base shall be initially leveled and aligned to the X-ray beam by the SLAC metrology group. Movement of the diffractometer back from the out-of-beam position (i.e. via air pads) shall re-establish this alignment within the tolerances shown in **Table 9-3** with out the need for metrological realignment activities.

Table 9-3: Diffractometer Leveling & Repositioning Requirement

Direction	Accuracy	Repeatability
Roll, Pitch	< 5 arc-sec	< 5 arc-sec
Yaw	< 360 arc-sec (.1º)	< 360 arc-sec(.1º)

10. Interface Requirements:

All interfaces require mate/de-mate rigidity and durability. Any element mating interface shall have the rigidity required to achieve the sphere of confusion and load capacity requirements defined in this document. Each interface must achieve a minimum five hundred (500) mate/de-mate cycles without requiring overhaul or component replacement. Each mate/de-mate element interface alignment shall achieve a minimum of 50 microns repeatability for at least the 500 mate/de-mate minimum cycle life.

Detailed definition of all mating surface parameters: flatness, bolt pattern, bolt size, alignment interface, bolt torque, etc, are defined in **SC-391-XXX-XX**.

10.1. Sample Goniometer Top Platform (sample interface):

The distance from the top of the sample platform to the goniometer center of rotation shall be 200mm, a distance common with the XPP Diffractometer to facilitate shared experimental set-ups. Use of an interface plate may be required. The dimension of the top platform shall be a minimum of 170 x 170 mm.

11. Power and Data Interface / Cable Management:

Motor power and control interfaces shall be in accordance with accepted and approved standards for environmental safety and health.

All motor connectors shall be located, configured and labeled to provide rapid and intuitive and ‘fool proof’ reconfiguration of the diffractometer system connections. Numerous connect and disconnects on the order of 1000 cycles should be possible without loss of performance or damage to the connections or mounting hardware.

All power and control cabling shall be routed and strain relieved in a manner such that all translation directions and rotation axis can achieve full range capability, plus 10% of full range, without undue load on cable, connector or diffractometer hardware. Rotation axis with a range specification of 360 degree continuous shall be capable of plus/minus ~200 degree of range, from nominal “zero”, without undue load on cable, connector or diffractometer hardware.

12. Materials:

All parts and materials for the device shall be new and compatible with the performance requirements of this specification. No part interfaces should result in galvanic corrosion for the life of the system.

No system, sub-system or part shall be reconditioned or remanufactured.

All applicable material safety data sheets (MSDS) shall be provided and stored in an accessible location.

13. XCS Official Color Definition:

Where it is specified, certain components are to be finished in the XCS official color which is FS 17100 (Purple) in accordance with US Federal Standard 595B.

14. Supplemental System Requirements:

Requirements, including the following topics, will be addressed in detail in subsequent procurement specifications and contracts.

i. Inspection, testing and acceptance
ii. Installation support services
iii. Training support services
iv. Maintenance procedures, schedules and assistance
v. Repair and overhaul services
vi. Storage and machine protection