Engineering specification Document (ESD)	Doc. No. SP-391-000-68 R0	LUSI SUB-SYSTEM CXI instrument

Engineering Specifications for the CXI Ion Time-of-Flight

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R0	14APR09	Initial release	

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1. Overview

Samples illuminated by the LCLS beam in the CXI instrument will get highly ionized and undergo a Coulomb explosion. Detecting the products of this explosion is required in order to provide information about the chemical components of the sample and to provide a diagnostic on whether a particle was hit by the LCLS pulse. This document describes the engineering specifications for an Ion Time-of-Flight (ITOF) mass spectrometer capable of performing these tasks. The document also outlines how the devices will be designed, fabricated and operated. Where applicable, this document specifically addresses how specific requirements from document PRD# SP-391-000-30, *Physics Requirements for the CXI Ion Time-of-Flight* are to be met. In some cases, where a Physics Requirement cannot be met, the reason is given and the expected performance is compared to the requirement

The coordinate system is defined in Mechanical Design Standards Supplement DS-391-000-36.

2. Applicable documents

PRD# SP-391-000-19	Physics Requirements for the CXI Instrument
PRD# SP-391-000-20	Physics Requirements for the CXI 0.1 micron Sample Chamber
PRD# SP-391-000-30	Physics Requirements for the CXI Ion Time-of-Flight
PRD# SP-391-001-41	Physics Requirements for the CXI 1 micron Sample Chamber
ESD# SP-391-000-67	Engineering Specifications for the CXI 0.1 micron Sample Chamber
ESD# SP-391-001-43	Engineering Specifications for the CXI 1 micron Sample Chamber

3. General Requirements

3.1. Location

The CXI Ion TOF shall be located inside the CXI hutch (hutch 5) in the far experimental hall.

3.2. Environment

The humidity and temperature are controlled in the FEH hutches, therefore no component specific temperature stabilizing system shall be provided for the instrument, unless the expected temperature stability is determined to be insufficient to meet the stability requirements.

The temperature and relative humidity in the FEH Hutch 5 will be maintained at 72°F ±1°F (22.2°C ±0.5°C) and 45% ±10%, respectively.

3.3. Maintenance, Accessibility, Operations and Storage

The CXI Ion TOF shall be attached to an 8" flange of the CXI Sample Chambers at a height of roughly 4ft 7in. It will be assembled and disassembled on the order of once every week for the life of the device.

During operations, high voltages will be applied to the device and proper electrical safety shall be followed.

The CXI Ion TOF shall be reasonably easily unmounted from the Sample Chambers for maintenance.

The detector used to measure the arrival time of ions can degrade over time if exposed to atmosphere for too long. It shall therefore be possible to store the ion TOF in a vacuum environment when it is not is use.

3.4. Lifetime

The expected service life of the device is 10 years.

4. Major System Components

The major components of the particle injector are shown on

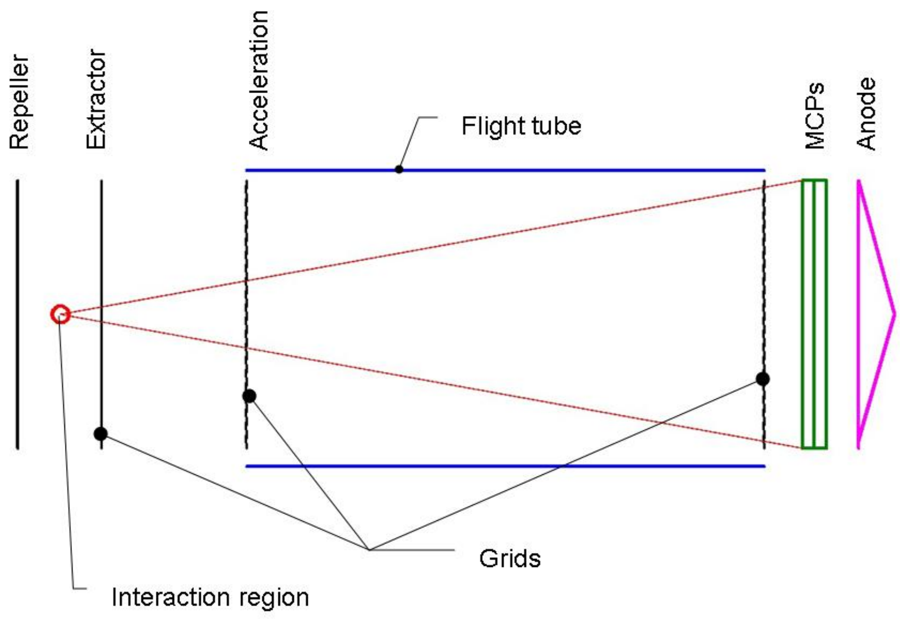

Figure 1: Schematic representation of the Ion TOF showing the typical component of the device.

4.1. Electrodes

Charged particles are created at the interaction region (red dot on Figure 1). These charged particles are extracted from the interaction region with electrodes set to specific voltages in order to accelerate the particles in a given direction.

4.1.1. Repeller Electrode

The repeller electrode is located on the opposite side of the interaction region from the ion detector. Its presence allows better control of the electric field lines and also can increase the strength of the electric field when a positive voltage is applied to it (the ions will always be positively charged). The repeller electrode may be pulsed at the repetition rate of the LCLS beam in order to increase the resolution of the TOF.

4.1.2. Extractor Electrode

The extractor electrode has a negative voltage applied to it to attract positively charged ions toward the detector. It typically has the same voltage as the repeller except for the opposite polarity. This voltage may also be pulsed at 120 Hz. Since the ions pass through the extractor, this electrode must be a grid.

4.1.3. Acceleration Electrode

The acceleration electrode has a negative voltage which is higher than the extractor in order to continue the acceleration of the ions towards the detector. This electrode has a fixed voltage and is also a grid. Only the acceleration electrode is absolutely needed for the Ion TOF.

Both the repeller and the extractor can be omitted, but this comes at the cost of decreased resolution. Possible collisions and interferences with other CXI Sample Chamber components may prevent the use of the repeller and extractor in the device. It shall be a design goal to have a repeller and extractor that are removable.

4.2. Drift or Flight Tube

The drift tube is a simple field-free flight path during which ions of different mass to charge ratios get spatially separated. All ions get accelerated by the electrodes and their final velocity when entering the drift tube depends only on the mass to charge ratio. The ions are subject to no force in the drift tube and get separated in space due to their different velocities. The longer the flight tube is, the more temporal separation one can get between different mass to charge ratios. However, a long narrow tube is not desirable since the ions also possess some transverse momentum and will eventually hit the tube wall if the tube is too long.

4.3. Detector Grid

At the end of the flight tube, there needs to be another grid electrode at the same voltage as the acceleration electrode to ensure that there is no electric field within the flight tube.

4.4. Detector

The detector consists of a multichannel plate (MCP). When ions enter the MCP, a shower of electrons is created and detected by the anode. These detectors are commercially available. Detectors are available either entirely in vacuum or flange mounted. Ideally, the CXI Ion TOF detector should be flange mounted but the limitations on the drift tube size and the distance from the interaction region to the flange may preclude this.

4.5. Flange and Support

The Ion TOF components shall all be mounted to a single flange in a manner similar to that shown on Figure 2, which shows the design of the AMO Ion TOF. The CXI Ion TOF will be similar.

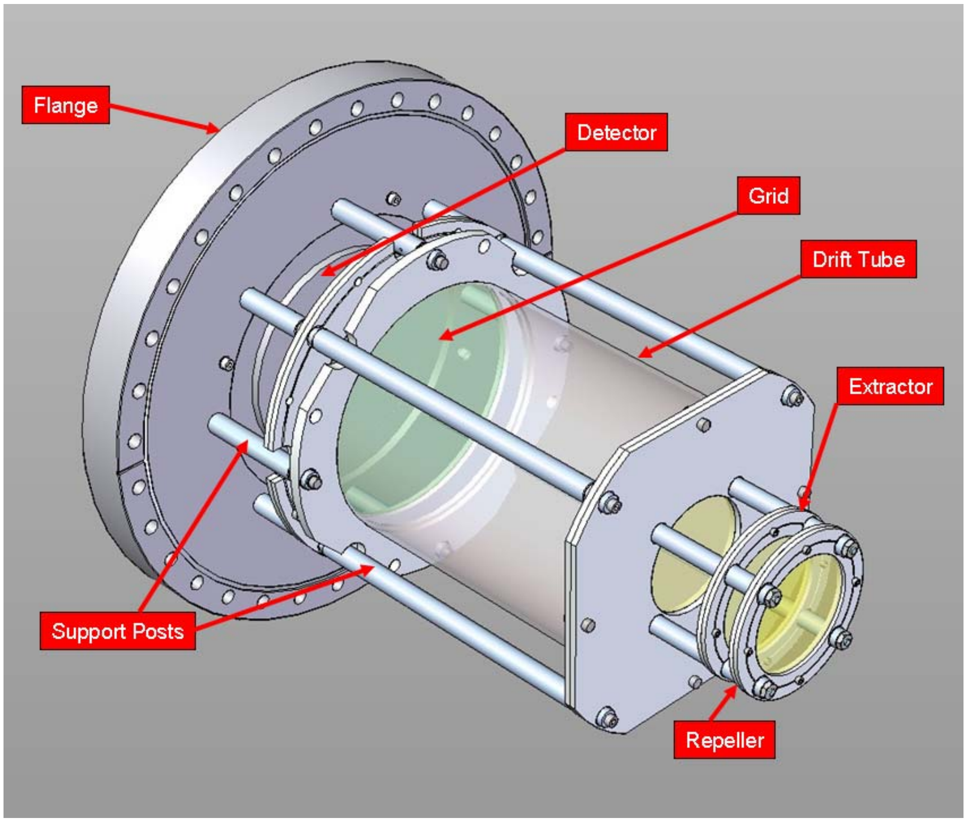

Figure 2: Design of the AMO Ion TOF. The CXI Ion TOF design will resemble with small packaging modifications.

4.6. Electrical Feedthroughs

All the electrical signal and power connectors shall be included in the single Ion TOF flange.

5. Performance Requirements

5.1. The ion TOF shall detect the arrival time of charged particles at the ITOF detector plane.

A multichannel plate (MCP) detector shall be used.

5.2. The ion TOF shall have a mass resolution of 1 atomic mass unit over a range up to 100 atomic mass units, assuming the initial kinetic energy of the created ions is 10 eV or less.

5.3. For more energetic ions, in the range of 1-10 keV that will be produced with the 0.1 micron KB system of the CXI instrument, the resolution of the ion TOF shall be 1 atomic mass unit up to at least a mass of 20 AMU.

The kinetic energy of the ions created by the LCLS pulse will vary greatly depending on the sample. The kinetic energy spread of the ions will be proportional to the average kinetic energy. Achieving 1 AMU resolution for heavy ions with a large kinetic energy spread would likely require a much larger TOF than is realistic for the CXI Sample Chambers or would require extremely high voltages which would be unsafe. Therefore, it is accepted that the performance parameters of the Ion TOF will fade rapidly for samples creating highly energetic ions.

5.4. The ion TOF shall be used to veto diffraction images with the ITOF signal used to determine if a particle was hit by a given LCLS pulse.

Whether the Ion TOF has a good resolution or not, it will always detect created ions and therefore it shall be possible to differentiate between an LCLS pulse where no sample was hit and a shot where an object was in the beam and get ionized by the LCLS beam. This will be used to flag pulses where a sample was hit.

6. Cyclic Requirements

6.1. There are no moving parts in this system so no mechanical cyclic requirements apply. Electrical power will be cycled in this device and these requirements are addressed in Section 13.

7. Mechanical Interfaces

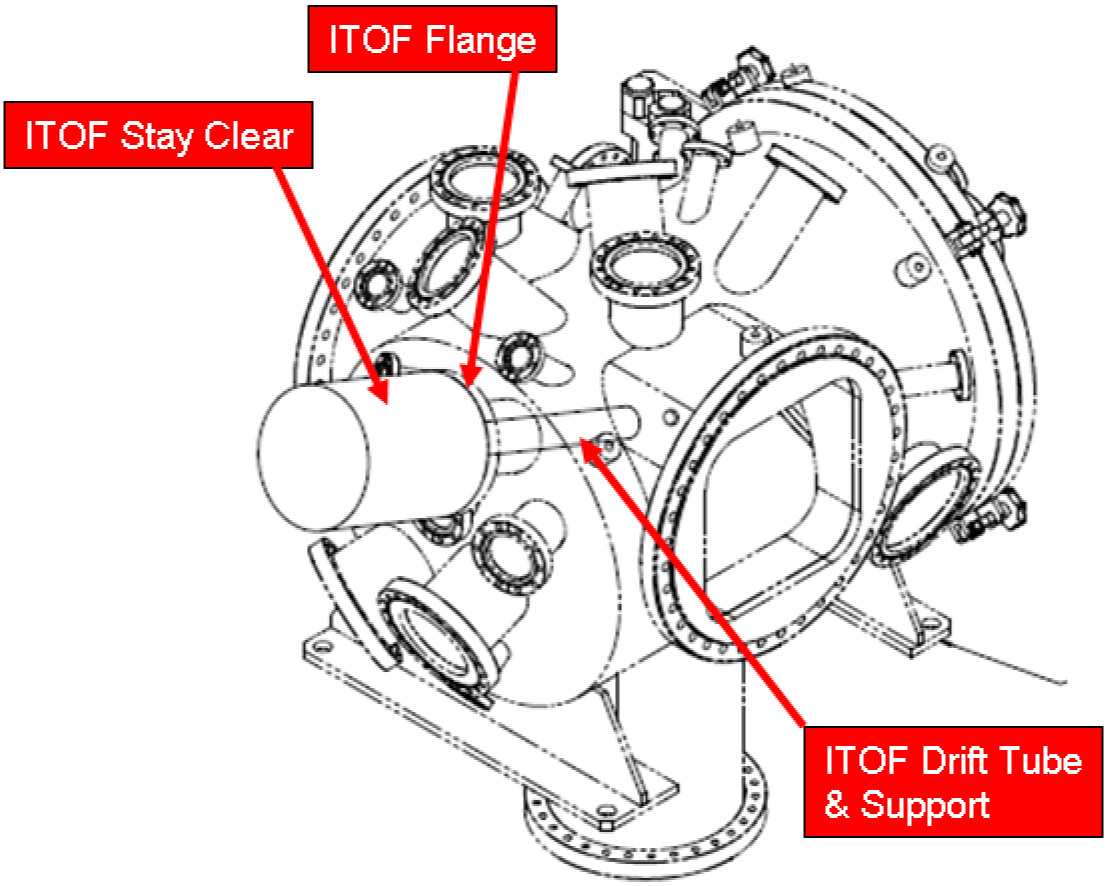

Figure 3: Design of the 1 micron Sample Chamber with a cartoon of the Ion TOF.

7.1. The ion TOF shall be mounted on either of the CXI Sample Chambers (1 micron Sample Chamber PRD# SP-391-000-20 and 0.1 micron Sample Chamber PRD# SP-391-001-41).

An 8" CF flange will be identified and reserved for the Ion TOF in each sample chamber, as shown on Figure 3.

7.2. The drift tube and the repeller electrode, along with their respective supports shall not encroach under any circumstance on the ±45 degree angle from the interaction region to the 2D X-ray Detector (LCLS PRD # 1.6-002) which is mounted inside the CXI Detector Stage (PRD # SP-391-000-28).

7.3. In the case where functionality of the ion TOF is in conflict with the functionality of the imaging system in the CXI Sample Chamber, the functionality of the Sample Chamber shall have precedence and lead to reduced functionality of the Ion TOF.

7.4. The ion TOF shall be designed so it cannot interfere or collide with any of the components inside the Sample Chambers (PRD # SP-391-000-20 and PRD# SP-391-001-41).

The repeller electrode may need to be removed to avoid interferences. In such a case, the repeller electrode will only be used if the sample chamber components are not in use. It is expected that the repeller electrode will interfere with the sample stage and the third aperture stage inside the Sample Chambers. The repeller electrode shall therefore be designed to be removable. (See Figure 4 and Figure 5).

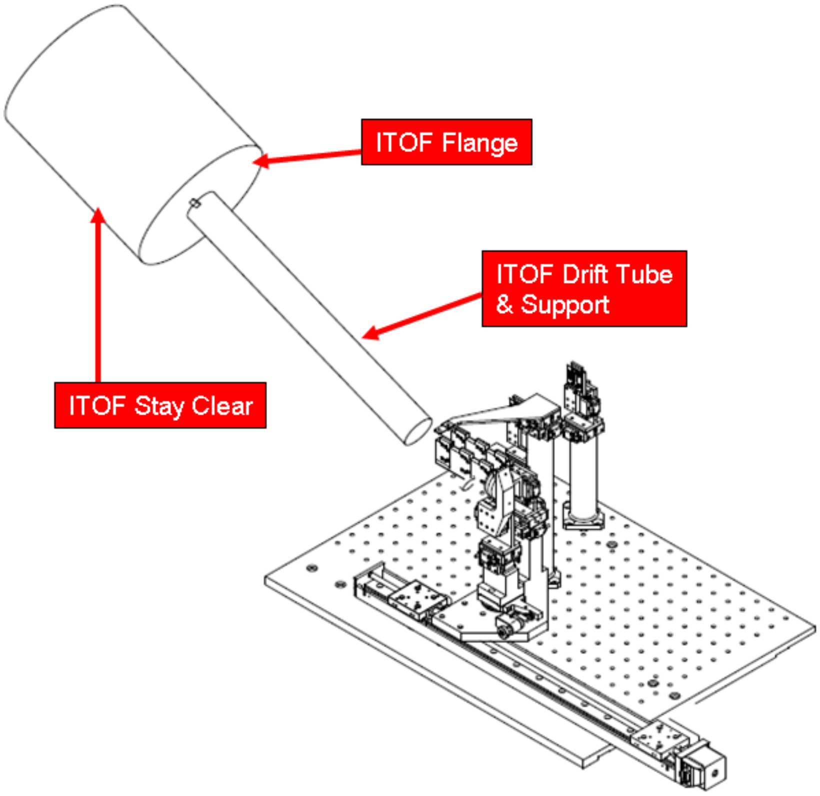

Figure 4: Cartoon of the Ion TOF and the inner components of the CXI 1 micron Sample Chamber.

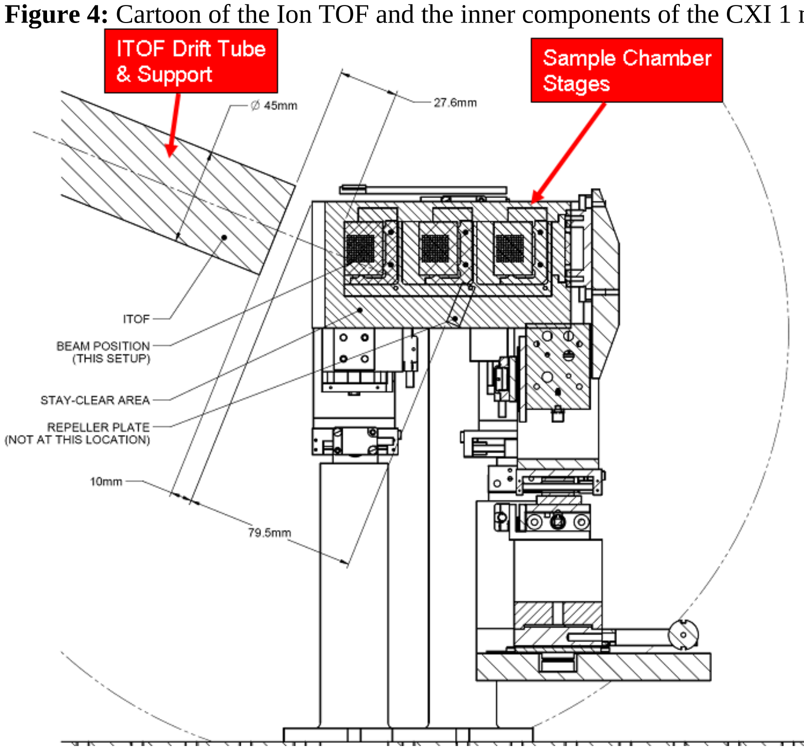

Figure 5: Representation of the interface between the CXI Sample Chamber components and the Ion TOF.

8. Materials

8.1. All parts and materials for the device shall be new and compatible with the performance requirements of this specification. Mil source certifications, including heat number, chemical analysis for all materials used in the manufacturing of the device shall be furnished. The device will be used in a radiation environment. Use of Teflon is specifically prohibited.

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

9. Kinematics/Supports

9.1. The position and alignment of the Ion TOF is fully dictated by the 8" CF flange it mounts to. Therefore no kinematics or supports are required.

10. Alignment/Fiducialization and Positioning

10.1. The long axis of the ion TOF shall be pointed directly at the interaction region to within ±3 degrees in pitch and yaw.

> The orientation of the long axis of the Ion TOF will be fully dictated by the interface to the 8" CF flange of the CXI Sample Chambers. The ±3 degree accuracy requirement of the pitch and yaw of the CXI Ion TOF shall be achieved with machining tolerances on the Ion TOF and the Sample Chambers.

10.2. There is no requirement on the roll angle of the long axis of the Ion TOF.

10.3. The surface normal of the repeller electrode shall be parallel to the axis of the drift tube to within ±2 degrees.

> This shall be achieved with machining tolerances.

11. Size Requirements

11.1. The ion TOF mechanical components and electrical feedthroughs shall all be attached to a single flange no larger than 8" O.D.

> This will allow the Ion TOF to be mounted or unmounted from the Sample Chambers with a single operation.

11.2. The ion TOF shall consist of a drift tube of 40 ±5 mm inner diameter.

> This tube shall be as large as possible without invading the ±45 degree angle from the interaction region to the 2D X-ray Detector.

11.3. An electrode grid shall be positioned at the entrance of the drift tube.

11.4. The closest point of approach of the ion TOF drift tube from the interaction region shall be 25 ±2 mm.

> This value is dependent on the diameter of the drift tube.

11.5. The drift tube of the ion TOF shall be at least 200 ±25 mm long. Interface issues with the sample chamber may preclude the drift tube from being this long and 200 mm shall be the design goal.

A longer tube improved the resolution of the Ion TOF.

11.6. A repeller electrode shall be located on the opposite side of the interaction region from the drift tube. This electrode shall be circular and of the same diameter as the drift tube.

The design goal is for the electrode to be of the same diameter as the drift tube. This may not be possible due to interferences with the sample stage in the Sample Chambers. The repeller electrode shall be as large as possible and shall also be removable.

11.7. The repeller electrode shall be located 25 ±2 mm away from the interaction region.

This value depends on the diameter of the electrode.

12. Vacuum Requirements

12.1. The ion TOF shall operate with a 10^{-7} Torr pressure environment or better under all operating conditions and the appropriate vacuum practice for the design, manufacturing, and installation of the system components shall be implemented.

12.2. All lubricants, cutting fluids, etc., used in manufacturing shall be "sulfur-free". SLAC document No. SC-700-866-47 is a compendium of SLAC approved lubricants. The use of sanding discs, abrasive paper or grinding wheels is typically prohibited. In special circumstances good vacuum practices should be followed when grinding and polishing is required. This process shall be reviewed and approved by the engineer for its vacuum compatibility.

12.3. All parts and subassemblies shall be cleaned for UHV. Once parts are cleaned for vacuum, handle only with clean latex or nitrile gloves in/on a clean room/surface. This includes all subassemblies. For storage or transportation, place in clean sealed vacuum grade plastic bag that has been back-filled with nitrogen.

13. Electrical Requirements

13.1. All electrical vacuum feedthroughs shall be included on a single 8" CF flange.

13.2. It shall be possible to apply voltages up to 5 kV (with either polarity) on the repeller electrode as well as on the drift tube and the entrance grid to the drift tube.

13.3. The components inside the Sample Chambers shall be precluded under all circumstances to come into contact with the electrodes of the ion TOF in order to prevent electrical discharges.

> The design of the Ion TOF shall keep in completely out of a stay-clear area where the internal chamber components can be placed. Software interlocks on the Sample Chamber components shall prevent collisions.

13.4. The electric field at the interaction region shall have lines parallel to the axis of the drift tube to within ±2 degrees.

> This will be achieved with machining tolerances to align the repeller electrode and the axis of the drift tube to with the required accuracy.

13.5. Acquisition of unique, device specific controllers, when required, will be the responsibility of CXI; all other power supplies and control cables shall be provided by the Controls/Data Acquisition Group.

13.6. The interface from the control racks to the CXI Ion TOF (cable trays and routing, connector supports, etc.) will be determined jointly with the Controls/Data Acquisition Group.

13.7. To comply with OSHA/DOE regulations, all electronics will have certification either through a National Recognized Testing Laboratory (NRTL) or the Authority Having Jurisdiction (AHJ) as per the SLAC Electrical Equipment Inspection Program

14. Controls Requirements

The controls and data acquisition associated with the CXI Ion TOF shall be consistent with the requirements outlined in the documents PRD SP-391-000-03, *Physics Requirements for the LUSI*

Controls and Data System and PRD SP-391-000-06, *Physics Requirements for the LUSI Data Management. Requirements* specific to the Particle Injector System are described below.

14.1. The voltage on up to 8 channels shall be controlled remotely via the instrument control system.

14.2. The voltages on up to two of the previously mentioned eight channels shall be pulsed at 120 Hz with synchronization to the LCLS pulse to within 100 picoseconds.

14.3. It shall be possible to delay the voltage pulse with respect to the LCLS by up to 1 μsec with 0.1 nsec resolution.

14.4. The instrument control system shall display all controls and status of the high voltage supplies.

14.5. It shall be possible to lock the settings of the high voltage supplies with password protection.

14.6. It shall be possible to record every voltage and pulsing parameters in the scientific metadata for every LCLS pulse for which scientific data is recorded.

14.7. The users of the instrument shall select from a list of parameters which ones they wish to record in the metadata for a given run.

14.8. Every controlled parameter included in the list that can be saved shall also be displayed on the control station at the request of the users with a refresh rate of 1 Hz.

15. Data Acquisition Requirements

The particle injector itself has no data acquisition requirements. However the charge detectors do have requirements related to data acquisition.

15.1. The analog signal produced by the ions impinging on the TOF detector shall be digitized at a rate of 1 GHz or faster.

15.2. It shall be possible to digitize and record up to 100,000 samples for every LCLS pulse, at 120 Hz, at the digitization rate of Requirement 15.1.

> An Acquiris digitizer, approved by the LUSI Controls Group shall be used to meet the previous 2 requirements.

15.3. It shall be possible for the user to set a trigger level on the digitized signal. This trigger shall be used to select which diffraction images will be saved by the system.

> This trigger level will look for signature peaks above the background level in the spectrum.

15.4. It shall be possible to set the trigger level on a limited window of the digitized waveform as well as on multiple independent windows.

> Some specific peaks, corresponding to ions with only a specific arrival time will be selected are requested by the users.

15.5. The trigger shall be used as a particle hit counter by counting the number of trigger events per user defined time window.

15.6. The particle hit counter shall be used as a detector when aligning the particle injector.

> This particle hit counter shall be included in a list of available detectors for the instrument. The users will then be able to scan any parameter of the instrument and plot the particle hit rate as a function of the scan parameter.

15.7. The hit rate averaged over a desired time window shall be displayed at the control console at a refresh rate of 1 second.

> A box on the instrument control panel shall display the instantaneous count rate in hits/sec.

15.8. The Ion TOF hit rate shall be recorded in the experimental metadata if desired by the users.

15.9. The digitized waveforms shall be displayed on the instrument console at a rate of 5 Hz when desired by the users.

> If the trigger rate is higher than 5 Hz, then only a fraction of the detected pulses will be displayed.

15.10. The average waveform shall be updated at a rate of 5 Hz and reset at the discretion of the users.

> There shall be a reset button for the Ion TOF average waveform that when pressed by the user will clear the average waveform from memory and start displaying the average from the moment the button was pressed.

15.11. It shall be possible to record each individual waveforms coming from ions being detected by the Ion TOF or to record an average waveform over multiple LCLS pulses, with this number set by the users via the instrument control system.

15.12. It shall be possible for the users to identify up to 50 peak positions and the height of each peak shall be calculated for each LCLS pulse that triggers the Ion TOF.

15.13. The height of each peak shall be displayed at a rate of 5 Hz, along with the displayed waveform discussed in Requirement 15.9.

15.14. The peak heights shall be recorded in the instrument metadata if desired by the users.

15.15. The time average peak height shall be displayed at a rate of 5 Hz and reset when desired by the users.

15.16. The time average peak height shall be recorded in the instrument metadata if desired by the users.

16. Environmental Safety and Health Requirements

16.1. Earthquake

SLAC National Accelerator Laboratory (SLAC) is situated in an active seismic zone. All hardware exceeding a weight of 400 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 2007 version of the California Building Code (CBC) and SLAC ES&H Division document SLAC-I-720-0A24E-001-R002: "Seismic Design Specification for Buildings, Structures, Equipment, and Systems".

16.2. Radiation Physics

No supplemental X-ray radiation shielding will be required for the Detector Stage since it shall be located in a radiation hutch.

16.3. Pressure Vessel/Vacuum Vessel

The CXI Ion TOF shall be designed for use in a High Vacuum environment with the appropriate safety factors.

Pressure relief safe guards will be provided on the Sample Chambers, where appropriate, to ensure compliance with all applicable guidelines/regulations, i.e. 10CFR851. No pressure relief is necessary on the Ion TOF itself.

16.4. Electrical Safety

The vacuum system of the sample chamber on which the ion TOF is attached shall be interlocked with the high voltage power supplies of the ion TOF so that the system is not energized when the pressure is above 10-4 Torr.

The pressure level at which the interlock is triggered shall be user-modifiable with password protection.

All SLAC electrical safety requirements associated with the high voltages required for the Ion TOF shall be observed in the design, fabrication and operation of this device.