CXI

Coherent X-ray Imaging

CXI Overview

The Coherent X-Ray Imaging (CXI) instrument will make use of the unique brilliant hard X-ray pulses from LCLS to image single sub-micron particles. The full transverse coherence of the LCLS laser will allow single particles to be imaged at high resolution while the short pulse duration will limit radiation damage during the measurement. The instrument will allow imaging of biological samples beyond the damage limit that cannot be overcome with synchrotron sources. Samples can be introduced to the x-ray beam either fixed on targets or using a particle injector that will deliver free-standing particles to the beam. High quality focusing optics will generate three foci (10 µm, 1 µm and 100 nm) and this will allow imaging of single nanoparticles of various sizes, with the hope of pushing the limit down to single biomolecules. The CXI instrument, while primarily designed to perform Coherent Diffractive Imaging experiments, will offer a flexible set of instrumentation suitable for a variety of experiments not limited to imaging. The CXI instrument is located in Hutch 5 of the Far Experimental Hall of LCLS. The hutch is 20 m long by 7 m wide. The CXI instrument is location 440 m away from the LCLS source.

Main Contacts

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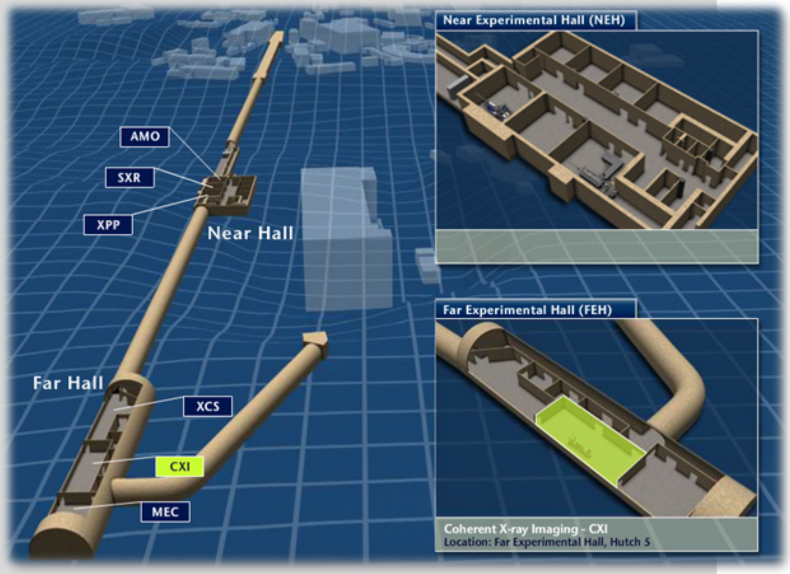

Scientific Goals

X-ray diffraction has long been used to determine atomic structures of biomolecules. The X-ray dose needed to achieve a given resolution for a particular sample can be calculated. It can be shown that the dose required to image a single biological molecule is much larger than the dose required to completely destroy the molecule through radiation damage processes. X-ray crystallographers mitigate this problem by spreading the damage over billions of molecules in a single crystal, greatly enhancing the diffraction signal. Since the molecules are all identical and precisely aligned in the crystal, the X-ray scattering information is preserved and the structure can be determined.

LCLS offers another way around the damage problem. Since the FEL X-ray pulse is very intense and very short, it is possible in principle to deliver the required dose to a nano-scale sample and record the scattered X-ray information before the damage processes have time to destroy the sample. In other words, an LCLS X-ray pulse could be focused onto a single molecule, which would be destroyed – but not before the scattered X-rays are already on their way to the detector carrying the information needed to deduce the image. The Coherent X-ray Imaging (CXI) Instrument will offer the possibility of determining structures at resolution beyond the damage limit for samples which do not form crystals, including important classes of biological macromolecules.

Scientific Programs

Imaging of reproducible biomolecules

Only a two-dimensional diffraction pattern will be collected from a single biomolecule before it is destroyed by the LCLS beam. Such a two-dimensional pattern encodes information about a projection image of the object onto a plane parallel to the detector. Three-dimensional structural information about highly-reproducible molecules such as viruses, large proteins or molecular complexes could be derived if a series of the molecules were delivered into the LCLS beam one after the other. Each molecule would have a different orientation and a full 3D diffraction data set could be obtained from a large number of identical copies of the sample. In theory, it could be possible to obtain high resolution structures for difficult to crystallize biomolecules. Research and development is required is required to demonstrate this capability.

Protein Nanocrystallography

It is often the case that large crystals of a certain protein cannot be grown but a large number of very small crystals can readily be obtained. These sub-micron crystals do not scatter enough X-rays to yield an atomic structure using conventional protein crystallography techniques. The high flux of LCLS could allow these to be used for structure determination. Assuming all the nanocrystals possess the same crystal symmetry, a series of nanocrystals could be illuminated by LCLS X-ray pulses and the diffraction patterns recorded. The variations in alignment of the crystal axes from sample to sample can be determined from the indexing of the Bragg peaks in the diffraction patterns. A full 3D set similar to conventional protein crystallography could be built up phasing methods could yield the protein structure. It will be possible to deliver these nanocrystals directly into the CXI beam without a substrate.

Scientific Programs

Imaging of nanoparticles

LCLS will make it possible to obtain two-dimensional projections of any non-reproducible nanoparticle and three-dimensional images of reproducible objects. Furthermore, the LCLS beam could be attenuated to a level slightly below the damage threshold of an inorganic nanoparticle and a full 3D reconstruction could be obtained from a single particle using multi-image tomographic techniques. The transverse coherence length of the LCLS will allow small particles to be imaged in 3D at high resolution.

Imaging of hydrated living cells

Living cells are all unique at the atomic level. It will therefore not be feasible to obtain a full three-dimensional image of a cell at atomic resolution at LCLS since damage would occur to the single cell with a single exposure. However, LCLS will offer the capability to study fully hydrated cells beyond the damage limit in two dimensions. The cells can be injected sequentially into the X-ray beam and a 2D diffraction pattern can be collected from each LCLS shot. The rapid injection of the cell into vacuum would prevent it from drying out and it would remain fully hydrated during the measurement. The high peak flux of LCLS will make this measurement possible.

Scientific Programs

X-ray-matter interactions

The LCLS source will produce hard X-ray fields of unprecedented high intensity. It will allow for the first time tests of radiation damage models under such extreme conditions. These models are directly relevant to atomic-resolution imaging since the damage suffered during a pulse must be limited or the image reconstruction will suffer. The interaction of the powerful LCLS pulses with solid matter can be studied using the CXI instrument under unique extreme conditions.

Pump-probe imaging

It would be possible, with the use of an optical pump laser, to image photo-induced changes in non-crystalline samples with sub-picosecond time resolution. Currently, no pump laser is provided in the CXI instrument but may become available in the future. These pump-probe experiments are possible with a user-supplied laser system.

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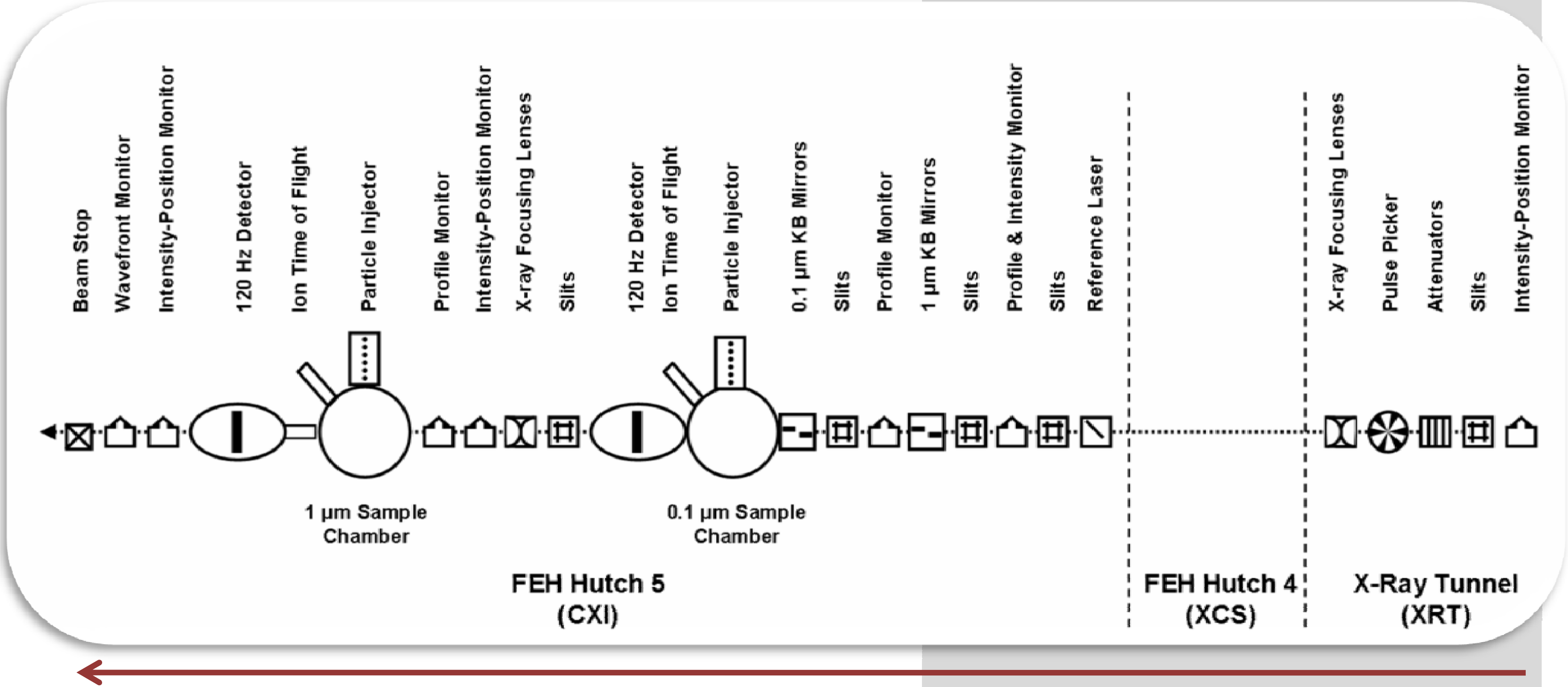
CXI Beamline Schematic



LCLS Beam Direction

CXI Capabilities

Scientific Capabilities

Scientific Applications	Coherent X-ray imaging on sub-micron particles
	X-ray interactions with matter
	Macromolecular Crystallography
	High fluence X-ray interactions with matter
	Time-resolved imaging and scattering with hard x-rays
Techniques and Scattering Geometries	Forward scattering on target-mounted samples and free-standing injected particles
	Back-scattering
	Ion time-of-flight

CXI Parameters

Source Parameters

Photon Energy	**4-10 keV for 1st harmonic***
	Up to 25 keV for 2nd and 3rd harmonic
Source Size	**60 x 60 μm^2 (HxV) FWHM @ 8.3 keV**
	78 x 78 μm^2 (HxV) FWHM @ 2 keV
Source Divergence	**2 x 2 μrad^2 (HxV) FWHM @ 8.3 keV**
	7 x 7 μrad^2 (HxV) FWHM @ 2 keV
Repetition Rate	**120 , 60, 30, 10 Hz**
Pulse Duration	**70 - 300 fs (high charge mode)**
	<10 fs (low charge mode)
Pulse Energy	**1-3 mJ (high charge mode)**
	~ 0.2 mJ (low charge mode)
Photons per Pulse	**~1 x 10^{12} (high charge mode @ 8.3 keV)**
	~1 x 10^{11} (low charge mode @ 8.3 keV)

[*] Energies below 4 keV are in principle usable but the beam size at the end station is large leading to poor focusing performance and reduced flux

CXI Capabilities and Parameters

Photon Beam Properties

Focusing Capability	KB1 mirrors (1 μm focus) available in early 2011
	KB01 mirrors (0.1 μm focus) available in Fall 2011
	Beryllium Lenses in XRT (10 μm focus)
	Beryllium Lenses in Hutch 5 (~1 μm focus)
Beam Size at Sample (Calculated for perfect optics) (8 keV)	1.3 x 1.3 μm^2 FWHM with 1st KB pair (KB1)
	90 x 150 nm^2 FWHM (V x H) with 2nd KB pair (KB01)
	10 x 10 μm^2 FWHM with XRT Be Lenses
	~1 x 1 μm^2 FWHM with Hutch 5 Be Lenses
	750 x 750 μm^2 FWHM unfocused beam
Beam Size at Sample (2 keV)	4 x 4 μm^2 FWHM with 1st KB pair (KB1)
	300 x 450 nm^2 FWHM (V x H) with 2nd KB pair (KB01)
	Unusable with XRT Be Lenses
	Unusable with Hutch 5 Be Lenses
	3000 x 3000 μm^2 FWHM unfocused beam
Energy Range	2-10 keV (1st harmonic)
	10-25 keV (2nd and 3rd harmonic)
Energy Resolution ΔE/E	~0.2% (bandwidth of the LCLS beam) No monochromator currently

CXI Capabilities and Parameters

Sample Environment and Detector

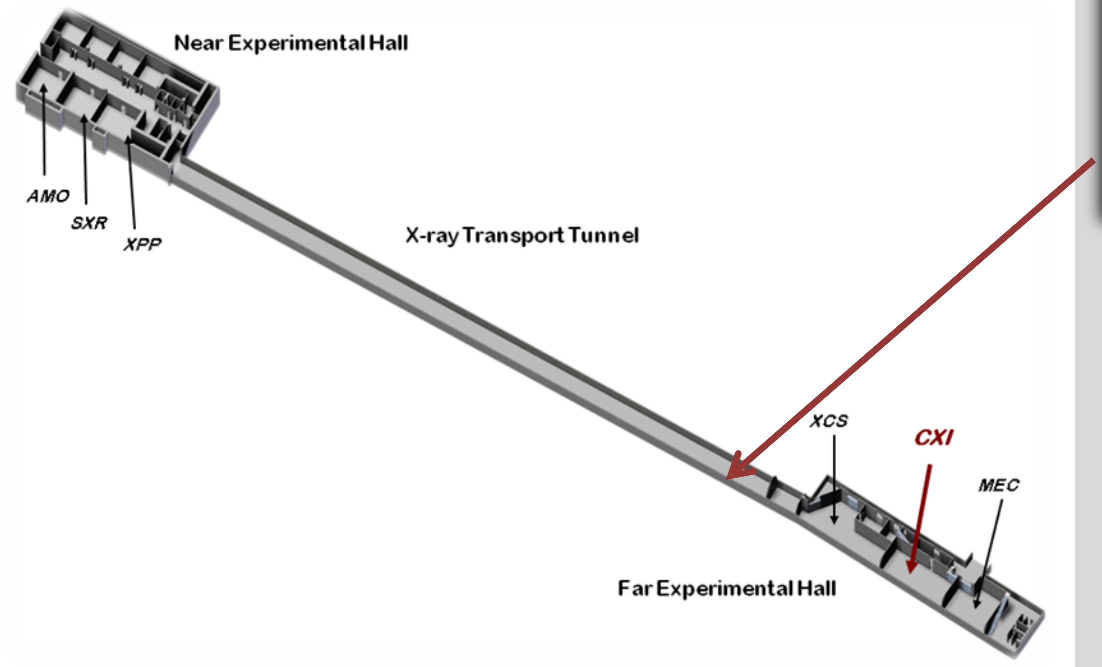
Sample Environment	**High vacuum: $\sim 10^{-7}$ Torr**
	Fixed sample on grids at room temperature
	Possible to operate at atmospheric pressure with limitations on use of some CXI equipment
Particle Injector	**Free-standing nanoparticles delivered to the beam using an aerodynamic lens particle injector**
	User-provided injectors can be integrated into the system
Detector	**2-Dimensional pixel array detector, 110 x 110 μm^2 pixel size**
	Single photon sensitivity, 10^3 dynamic range at 8.3 keV
	760 x 760 pixels (minimum available in early 2011) 1520 x 1520 pixels (expected Spring in 2011)
	120 Hz operation

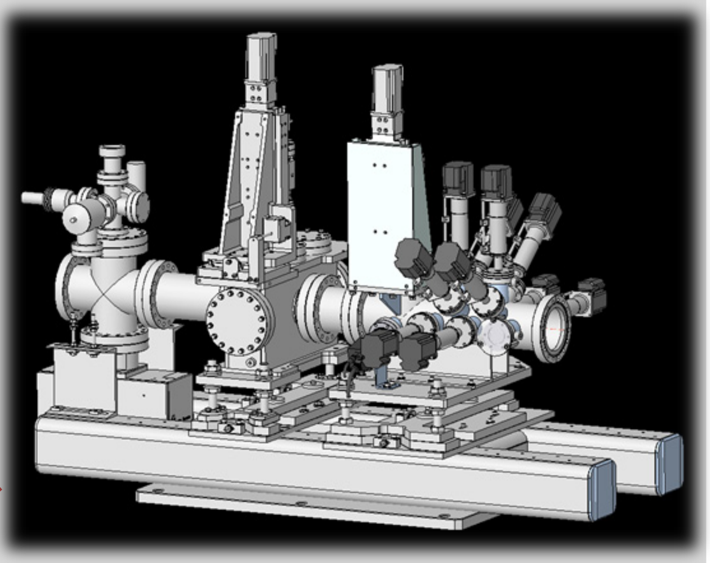
Other Equipment

Ion Time-of-flight	**Provide trigger signal when a particle is hit**
	Identify good hits
	User-supplied spectrometers can be integrated into the system

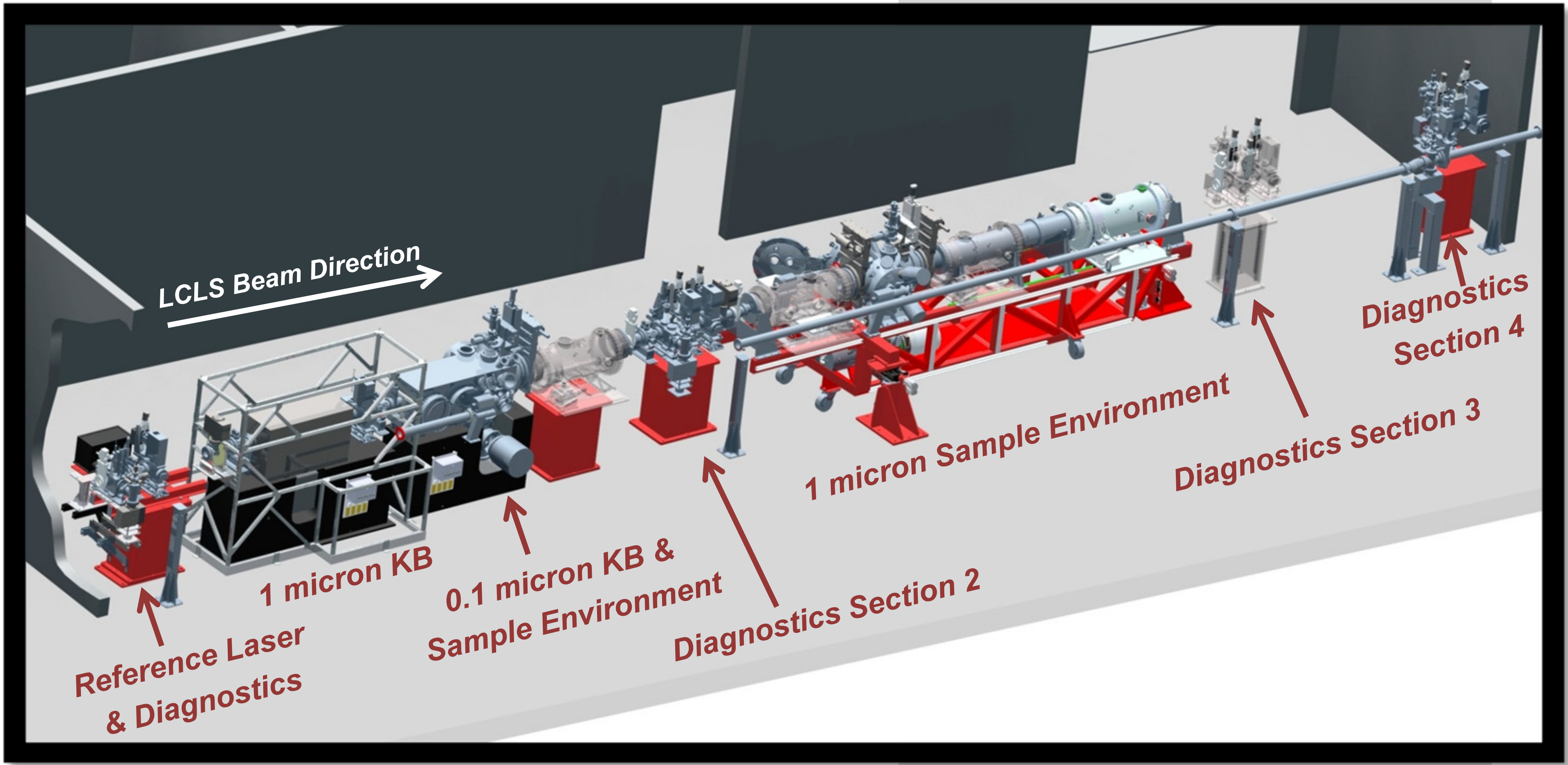
CXI Diagnostics and Optics in X-Ray Tunnel

The beam is shown travelling from right to left. The attenuator system with 10 individually actuated filters is the first component upstream, followed by the Pulse Picker and the X-ray Focusing Lenses. Most downstream is a pumping system. The X-ray Focusing Lenses are located 60 m upstream of the CXI Sample Chamber in order to produce a 10 µm FWHM focal spot.





CXI Complete System in Hutch 5



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Optics

LUSI Pulse Picker

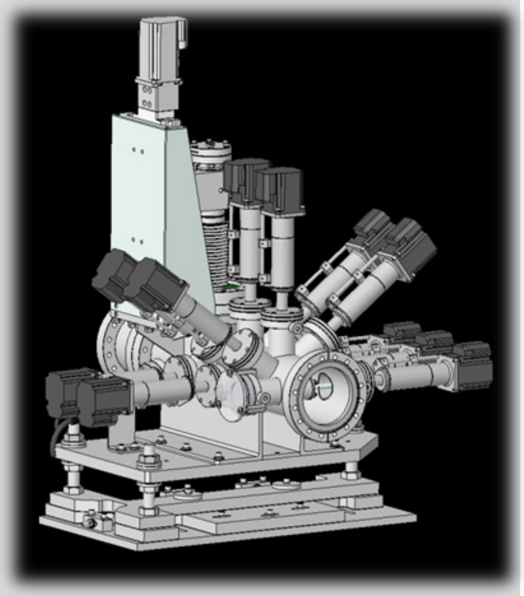
A single pulse shutter can be used to allow only a single FEL pulse to pass through to the experimental chambers. A millisecond shutter from azsol GmbH will be incorporated into a vacuum chamber on a translation stage to allow insertion into the beam. It can be operated up to 10 Hz.

LUSI Attenuators

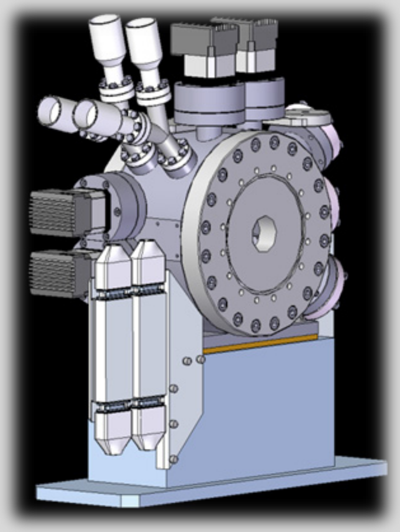
A set of silicon foils of varying thicknesses will be used to tailor the intensity of the LCLS beam. Multiple attenuation factors will be possible by introducing any desired combination of foils into the LCLS beam path. Ten foils of different thicknesses will be provided and can be used in any combination.

LUSI Guard Slits

Cylinders of 3 mm diameter made of silicon nitride (Si_3N_4) will be used to slit the beam. Silicon nitride will not get damaged by the LCLS beam downstream of the Near Experimental Hall. In the case of the CXI instrument, the slits will primarily be used to remove unwanted light around the central FEL beam.



Attenuator/Pulse Picker Assembly



Slits

Diagnostics

LUSI Pop-in Profile Monitors

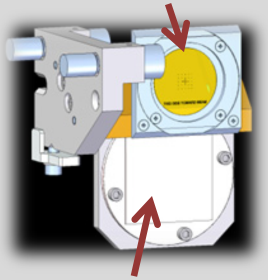
The spatial profile of the LCLS beam will be measured at various locations along the CXI beamline using a scintillating screen and a high resolution camera-lens combination. The screen will be mounted on a translation stage to allow insertion into the beam. The beam profile measurement will be destructive of the beam and will be used for alignment and troubleshooting procedures.

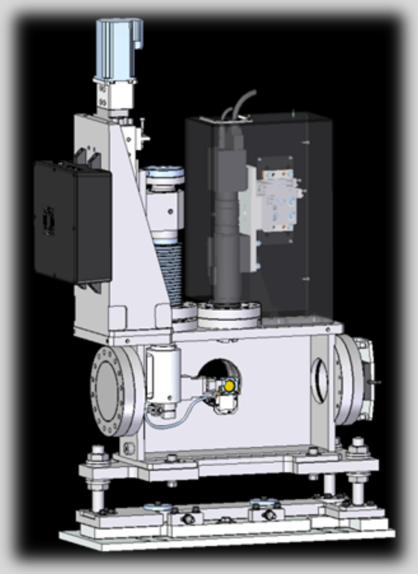
LUSI Pop-in Intensity Monitor

The integrated intensity of the LCLS beam will be measured at various locations along the CXI beamline using a photodide which will be mounted on a translation stage to allow insertion into the beam. The intensity measurement will be destructive of the beam and will be used for alignment and troubleshooting procedures.

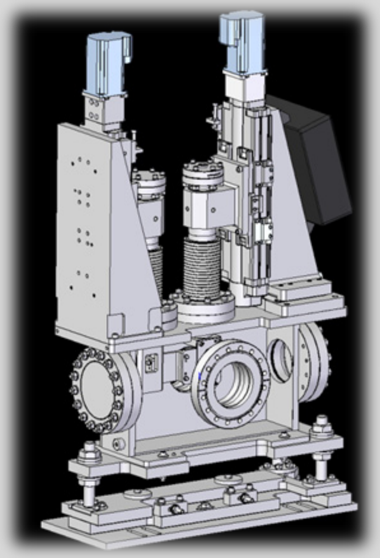
LUSI Intensity-Position Monitor

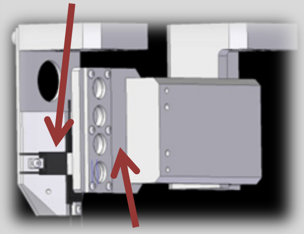
A thin foil allowing most of the beam to be transmitted will be used to measure the LCLS pulse energy on a shot-to-shot basis. Compton back-scattering from the thin foil will be measured using a set of diodes located upstream of the foil. The sensing area of the diodes will be facing the foil and they will be place in a tiled arrangement leaving a hole in the middle. The integrated intensity of all the diodes will provide a measurement of the beam intensity on every pulse. The relative signal from each tile will be used to get a measurement of the beam position.





Profile/Intensity Monitor Combo





Intensity/Position Monitor

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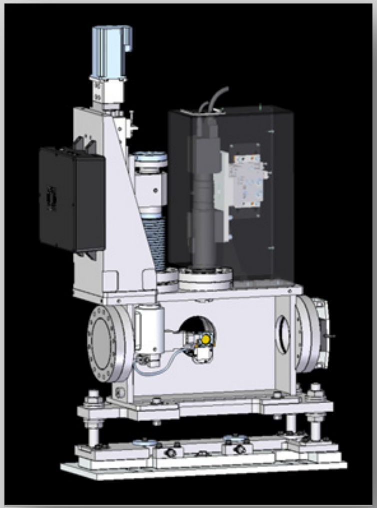
Diagnostics

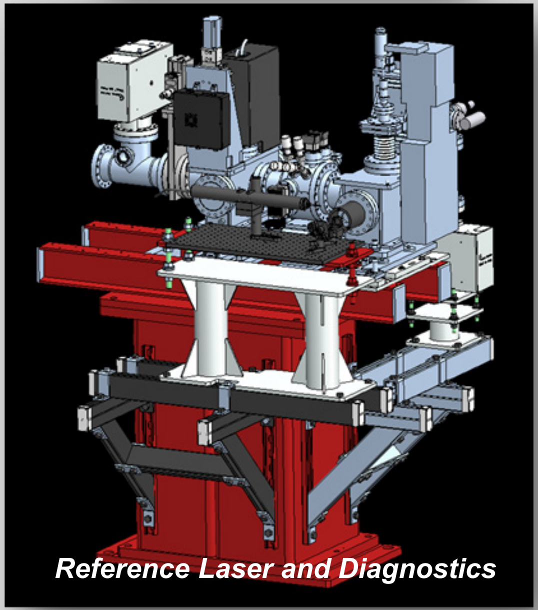
LUSI Wavefront Monitor

The Wavefront Monitor will use a scintillating screen and a high resolution camera-lens combination. The screen will be mounted on a 2-axis translation stage to allow insertion into the beam and potentially centering of a beam stop or attenuator right in front of the screen. The beam profile will be measured after the experiment and can be used to measure low angle scattering or potentially algorithms could be used to recover the wavefront from the measured beam profile downstream of the focus.



CXI Reference Laser

While the LCLS beam is unavailable to the CXI instrument either during machine studies or because the beam is being used by a different instrument, it will be possible to align the CXI experiment using a laser beam collinear with the LCLS beam. The red laser beam will be introduced into the vacuum beamline using a vacuum window and an in-vacuum mirror. Window valves will be provided downstream of the Reference Laser System to allow the laser beam to be used with any part of the beamline vented to air.



Reference Laser and Diagnostics

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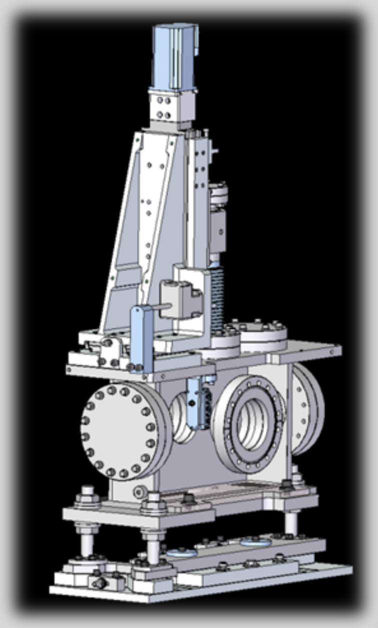
Focusing Optics

LUSI X-ray Focusing Lenses (10 μm focus)

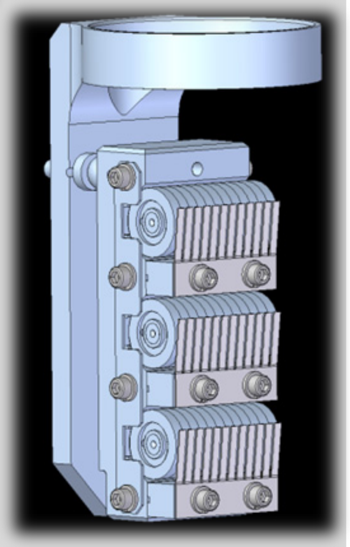
Compound refractive lenses made of Beryllium will be used to produce a 10 μm focus in the CXI main Sample Chamber. An translation stage will allow one of three stacks of lenses to be selected which will allow certain ranges of photon energies to be focused. Not all photon energies will be focused by the lenses since the are chromatic optics. These lenses will be installed in the X-Ray Tunnel 60 m upstream of the CXI Sample Chamber which will utilize this beam. The lenses will only be usable for photon energies above 4 keV due to the high absorption below this energy.

LUSI X-ray Focusing Lenses (refocus)

A second set lenses will be installed inside the CXI hutch roughly 3 m upstream of the Sample Chamber on Diagnostics Section 2. These lenses will allow the 0.1 micron beam focus by the KB mirrors to be refocused into the 1 micron Sample Chamber to run experiments in series simultaneously. These lenses can also be used as the primary focusing optics and should produce a focus on the order of 1 μm in this case.



X-ray Focusing Lens System



Lens Stacks

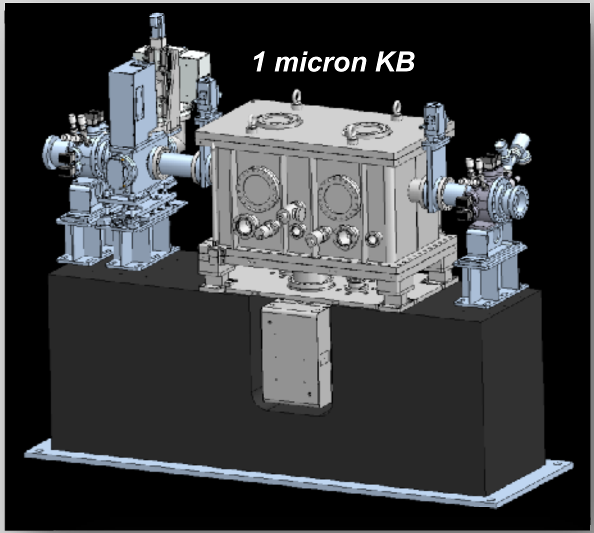
Focusing Optics

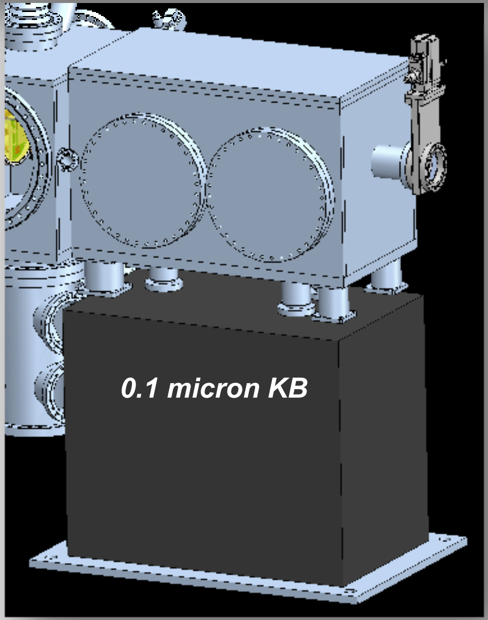
CXI 1 micron Kirkpatrick-Baez Mirror System

A pair of elliptical mirrors will be used in a Kirpatrick-Baez configuration to produce a diffraction limited spot of roughly 1 micron at the interaction region of the CXI instrument (inside the 1 micron Sample Environment). The midpoint between the KB pair will be located 8.5 meters upstream of the focus and this will produce a round focal spot between 1 and 4 microns FWHM, depending on the photon energy.

CXI 0.1 micron Kirkpatrick-Baez Mirror System

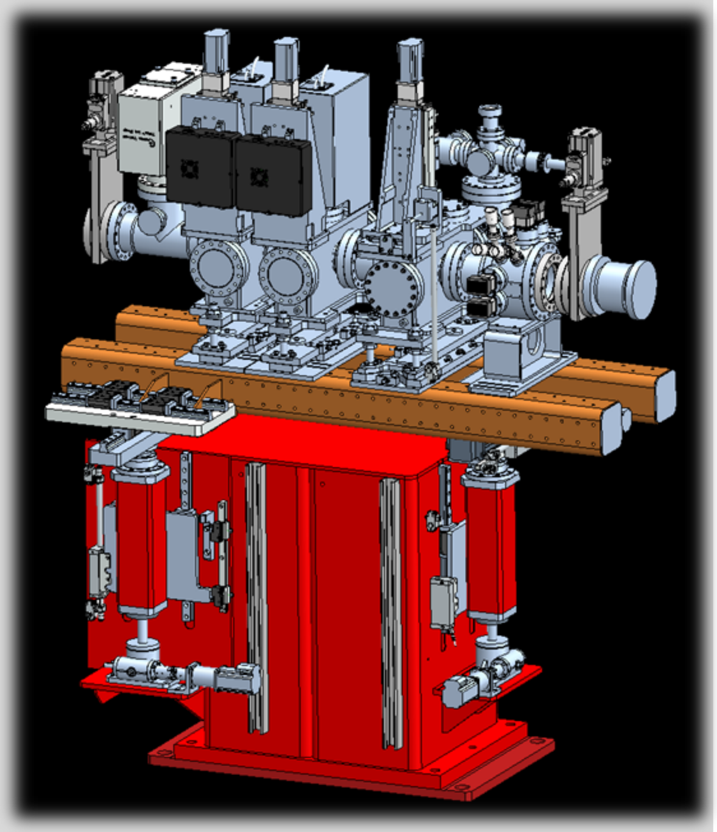
A pair of elliptical mirrors will be used in a Kirpatrick-Baez configuration to produce a diffraction limited spot of roughly 0.1 micron at the interaction region of the CXI instrument (inside the 0.1 micron Sample Environment). The midpoint between the KB pair will be located 0.7 meters upstream of the focus and this will produce an elliptical focal spot of roughly 90x 150 nm^2 FWHM at 8.3 keV. The spot size will vary with photon energy since the source size varies with photon energy and the mirrors aperture the beam a lower photon energy. The focal spot is expected to be on the order of 300 nm at 2 keV.





Diagnostics Section 2

Beam is shown travelling from right to left. A gate valve is followed by Slits, and then X-ray Focusing Lenses. An Intensity-Position Monitor will allow the beam intensity to be measured and will be followed by a beam Profile Monitor. A differential pumping system is placed just before the downstream gate valve. This downstream gate valve is the last “permanently installed” CXI component. Every component downstream of it can be removed (only if a given experiment absolutely requires it) and a user-provided experimental system can be installed to use the CXI beam.



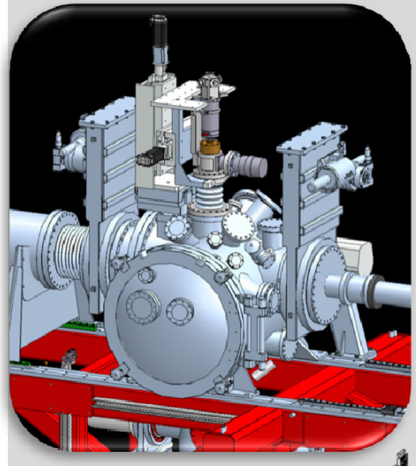
CXI Sample Chambers

1 micron Sample Chamber

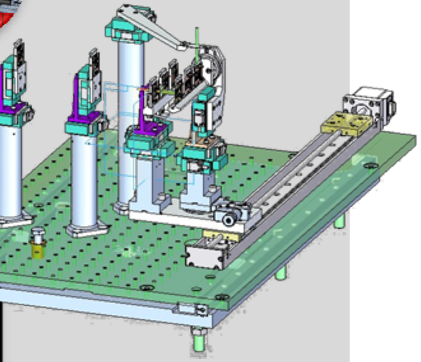
A large vacuum chamber capable of supporting various experimental configurations will be used to control the environment of the sample. The pressure inside the chamber will be on the order of 10^{-7} Torr but could potentially be higher if needed. Inside the chamber will be a 5-axis sample stage and three aperture stages. Sample mounted on thin supports will be positioned accurately into the LCLS beam using a long range microscope with on-axis viewing of the sample. The sample environment will also allow samples to be delivered to the LCLS beam without a substrate, in the gas phase by interfacing with the CXI particle injector or any other sampel delivery system that can connect to a 6 inch Conflat flange. The 1 micron Sample Chamber will be the main sample Chamber for CXI and can be used with the 1 μm KB focus, the beam focus with either sets of X-ray Focusing Lenses or with the unfocused beam.

0.1 micron Sample Chamber

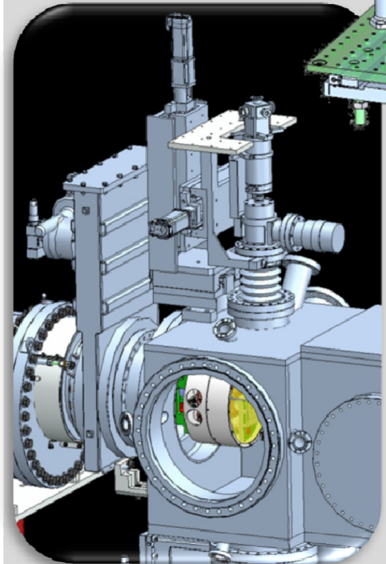
The 0.1 micron Sample Environment will have all the functionality of the 1 micron Sample Environment except that this Sample Chamber will only be usable with the 100 nm KB focus.



1 micron Sample Chamber



Sample Chamber Internal Components



0.1 micron Sample Chamber

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Sample Delivery

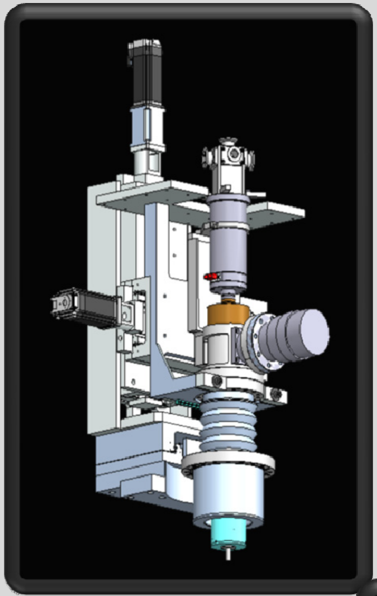
CXI Particle Injector

A single particle injector will be used to transfer particles from the gas phase at atmospheric pressure into the high vacuum of either Sample Environments. A tightly focused beam of particles will be delivered and the Particle Injector will be mounted on translation stages allowing the beam to be steered into the interaction region. These translation stages can be used with any other sample delivery system which interfaces to a 6 inch Conflat flange. The injector provided by CXI requires highly concentrated samples to provide a high hit rate due to the random arrival time of the particles at the interaction region.

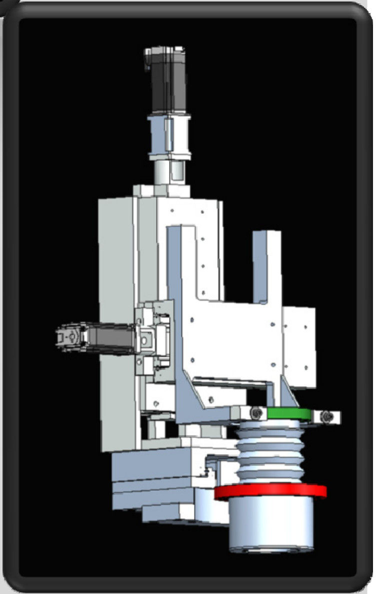
Sample Diagnostics

CXI Ion TOF

A small ion time-of-flight mass spectrometer will be used to detect the creation of ions at the interaction region. These ions produced by the Coulomb explosion of the sample when hit by an LCLS pulse will be accelerated away from the interaction region and their arrival time will be detected. This will provide a trigger signal when an injected particle was hit and also provide some information on the chemical composition of the particle that was hit.



CXI Particle Injector



CXI Particle Injector
3-axes Stage

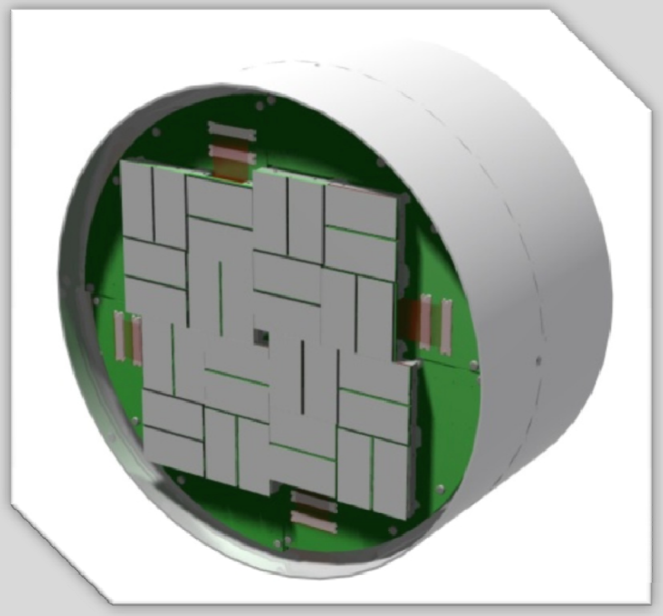
2D Detector System

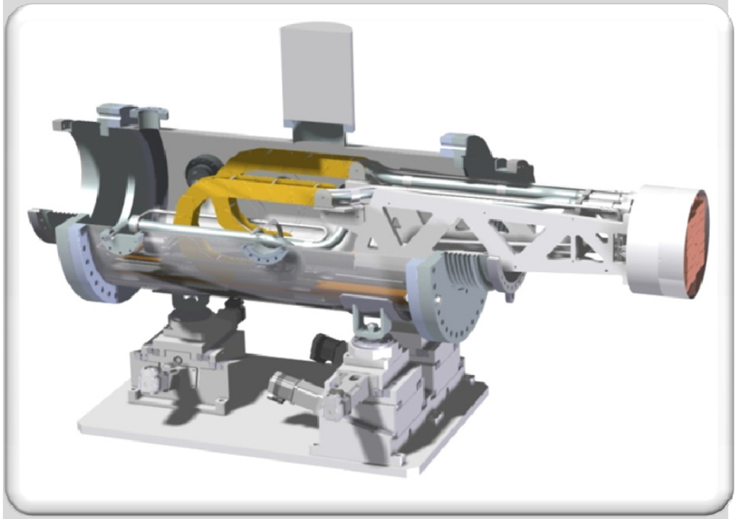
CXI/Cornell Detector

A 2D X-ray pixel array detector will be used to measure the scattered x-rays. The detector is made of several tiles arranged so that a central hole is present. The central hole size can be varied from 1.5 to 9.4 mm. Each quadrant of the detector moves as a solid unit. Initially, the detector will have 760x760 pixels but the tiled nature of it will allow the number of pixels to be increased to 1520x1520. It is hoped that the full detector will be available in early 2011.

CXI Detector Stage

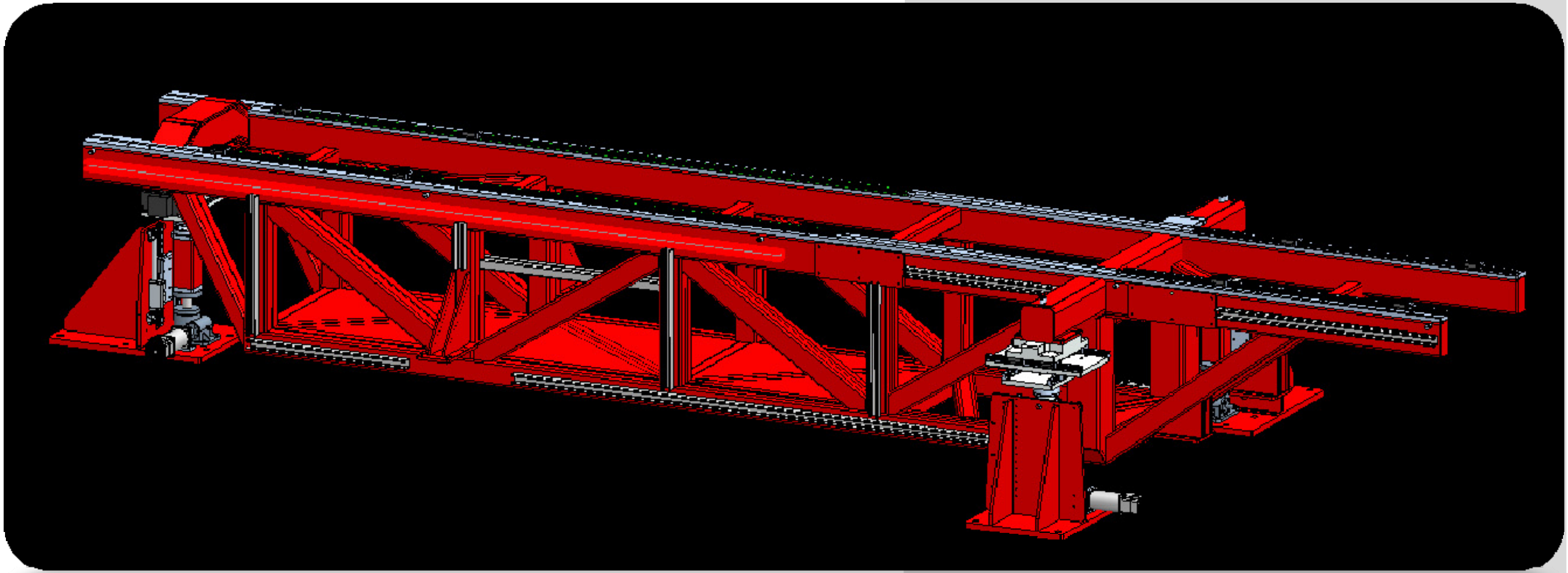
The 2D X-ray detector will be mounted in vacuum and it will be accurately positioned relative to the interaction region and the LCLS beam direction. It will be possible to vary the sample to detector distance from 50 mm to 2600 mm. The Detector Stage will position the detector transverse to the LCLS beam so that the direct beam passes through the central hole in the detector. There will be a 500 mm stage in-vacuum that will allow continuous variation of the detector distance over that range without breaking vacuum. The full positioning range can be accessed by disconnecting the system and moving it to a different position, requiring venting of the system.



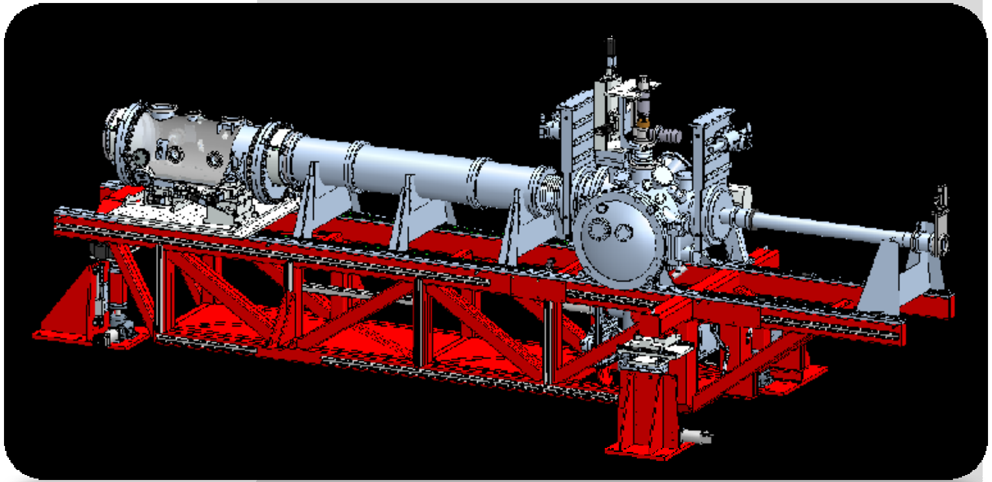


CXI Precision Instrument Stand

The 1 micron Sample Environment will be mounted on a large frame with 6-axis positioning. This frame is almost 6 m long and capable of supporting many tons and can be used to attach user supplied equipment. If a user experiment requires it, the entire CXI Sample Environment can be removed and a user supplied experimental system can be mounted on this stand in its place, given that this user supplied equipment can fit within the 447 mm distance from the top of the frame to the beam height. The CXI Precision Stand provides a very flexible platform for user needs.

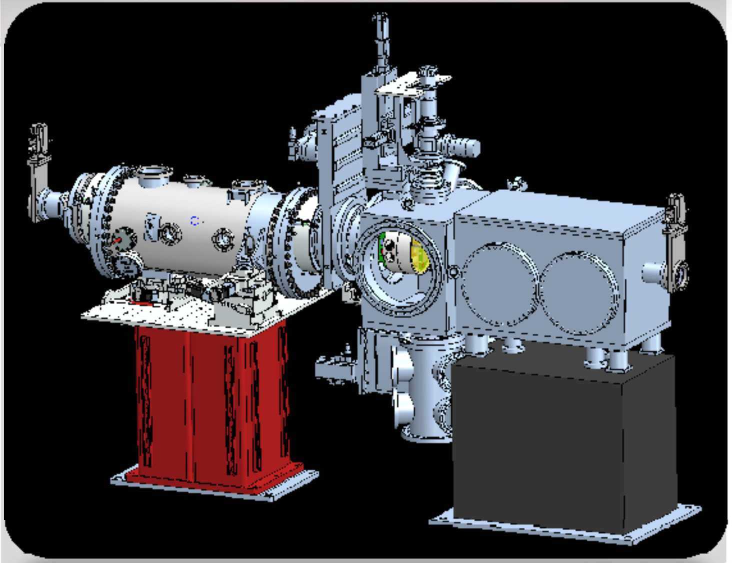


CXI Sample Environments



1 micron Sample Environment

The 1 micron Sample Environment includes the 1 micron Sample Chamber, the Particle Injector and the Detector Stage which can be mounted at multiple locations.



0.1 micron Sample Environment

The 0.1 micron Sample Environment will have all the functionality of the 1 micron Sample Environment except that this Sample Environment will only be usable with the 100 nm KB focus. The detector distance will be limited to 50-550 mm for this setup.

CXI Equipment Availability

Available for Spring 2011 (For April 1 2010 Call for proposals)	Available in Fall 2011
Pulse Picker	CXI Particle Injector*
Attenuators	CXI Ion Time-of-Flight
All Slits	CXI 0.1 micron KB Mirrors
All Pop-in Profile Monitors	CXI 0.1 micron Sample Environment
All Pop-in Intensity Monitors	
All Intensity-Position Monitors	
Wavefront Monitor	
CXI Reference Laser	
CXI 1 micron KB Mirrors	
X-ray Focusing Lenses in XRT for 10 µm focus	
X-ray Focusing Lenses in CXI Hutch for ~1 µm focus	
CXI 1 micron Sample Environment	
CXI 2D Detector with minimum of 760 x 760 pixels**	CXI 2D Detector with 1520x 1520 pixels
CXI Detector Stage	
CXI Precision Instrument Stand	

* The CXI particle injector system cannot be guaranteed to be available for the Spring 2011 run but could be available in time. Should it not be available, arrangements can be made with collaborators to have an existing system made available to users willing to collaborate with external groups. Users are also welcome to propose experiments using their own sample delivery systems.

** The CXI 2D detector cannot be guaranteed to have all 1520x1520 pixels for the Spring 2011 run but the full detector could potentially be available by then.