This document is derived from the SXR Technical Design Report, July 2008, prepared for the LCLS by the SXR consortium. Sections 1 to 4 are the same. Section 5 has been revised to represent the current status of the design. Section 6+ the end station requirements and interfaces still to be revised.
# OUTLINE  SXR - Summary of the Technical Design:

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1. INTRODUCTION

The Linac Coherent Light Sources (LCLS) is building the first x-ray Free Electron Laser (FEL) where light is scheduled to be delivered in August 2009. The facility will operate in the wave length range of 1.5 nm-0.15 nm (800 eV-8 KeV). The proposed soft x-ray imaging and pump-probe x-ray spectroscopy program on materials was approved by the LCLS Scientific Advisory Committee (SAC) in 2006, and space was allocated in the LCLS near hall for the accompanying instruments. Due to budget constraints, the materials soft x-ray program did not receive any instrumentation funding from LUSI. We here propose a plan to move forward with the soft x-ray program by constructing an instrument that contains a monochromator, refocusing optics and various locations where experimental endstations can utilize the beam in the soft x-ray energy regime.

In order to fund, design and construct the beam line we have formed a consortium with members from the Stanford Institute of Material and Energy Sciences (SIMES), the Advanced Light Source (ALS), University of Hamburg-DESY, Center for Free Electron Lasers (CFEL) in Hamburg and BESSY in Berlin. The consortium will serve as a central hub for a broader scientific community with interest in utilizing the unique capabilities of the LCLS in the soft x-ray regime. The consortium and various collaborators will also bring different endstations and detectors to the instrument for the experimental program that can also be utilized by the general users.

Since LCLS will be delivering light at longer wave length in its early operation and the completion of several LUSI instruments is delayed it is essential that instruments exists that can make use of the early LCLS beam. We therefore plan to move forward in a timely fashion with this effort with the goal to have an instrument ready in late summer of 2009. In the following we will describe the science, parameters, optical and technical design of the instrument. We will in the appendix include a short description of the various experimental endstations that will be brought to the instrument and letters of intent from the broader scientific community demonstrating their interest.
2. SCIENTIFIC PROGRAM

2.1 Pump-Probe Ultrafast Chemistry

The ultimate goal in chemistry and physical chemistry is to understand on a fundamental level how bonds break and reform during chemical reactions. In many cases we arrive at simple pictures of electron motion with respect to electron pair redistributions or electrostatic interactions along a reaction path. For many systems bonding can be understood in terms of molecular orbitals and reactivity in dynamical rearrangements of different molecular states. Such knowledge provides the basis for the understanding of chemical trends and prediction of chemical reactivity for chemical compounds. Since the excitation and probe steps with conventional optical lasers involve valence electrons that are delocalized over many atomic centers it is difficult to study complex systems. Unprecedented insight into chemical reaction dynamics would be gained by probing exactly the atomic site involved. X-ray spectroscopies can directly access molecular orbital changes associated with or even during chemical reactions. In particular, accessing core levels in the soft x-ray regime with spectroscopy opens up new prospects to study time-resolved changes in the electronic structure of complex systems containing the essential elements C, O and N or 3d-metal atoms. Detailed insight into surface reactions, catalysis, hydrogen-bonded systems and aqueous solutions can be expected.

![Schematic illustration of X-ray Spectroscopy](image)

**Figure 0-1.** Schematic illustration of X-ray Spectroscopy. Here, the radiative decay of a core-hole in N$_2$ adsorbed on a Ni surface by x-ray emission spectroscopy is shown. In addition to elemental sensitivity the method provides specificity to different chemical sites as shown in this example.

X-ray spectroscopy has the unique ability to provide an atom-specific probe of the electronic structure. In x-ray emission spectroscopy (XES) the atomic or elemental sensitivity arises from the filling of a core hole by valence electrons from the same atomic site. In addition, core-level energy shifts (often denoted chemical shifts) connected with different environments allow for selective probing of chemically non-equivalent atoms (Figur 0-1). The final state of the x-ray emission process is a valence-hole state similar to the final state in valence band photoemission with the unique feature that the valence electronic structure is projected onto a specific atom. Notably, selection rules of XES, and similarly of X-ray photoelectron spectroscopy (XPS), in conjunction with variation of polarization...
vector of the incident light or angle-resolved detection of electrons allows to access molecular orbital symmetry and associated bond geometry. In addition, XPS can be uniquely tuned to high surface sensitivity, which is particularly desirable when studying interfaces, including the aqueous/vacuum interface. Resonant excitation and Auger electron spectroscopy gives unique access to the electronic structure of atoms and molecules in the gas phase, on surfaces and in liquids and solids. Some of the projects planned here are described in further detail in the following:

**Surface Reactions and Catalysis:** The microscopic understanding of heterogeneous catalysis requires a detailed understanding of the dynamics of elementary processes at surfaces including adsorption, formation of different intermediates, and desorption. These can be initiated by an ultrashort (optical) laser pulse, and the evolving product can be uniquely probed with XES and XPS using FEL soft x-ray pulses at a given time delay. Charge and energy transfer processes, for instance between an adsorbate and the (catalytic) substrate, can thus be studied with high site-selectivity and high temporal resolution. Likewise, we expect to identify and to characterize chemical bonding in short-lived reaction intermediates by transient changes of the electronic structure, from which kinetic models with an unprecedented level of detail can be derived.

**Hydrogen Bonding, Radiation and Aqueous Solution Chemistry:** Water is the key species for our existence on earth, and it is involved in nearly all biological, geological, and chemical processes. Knowledge about the hydrogen-bonded network structure in liquid water is essential for understanding its unusual chemical and physical properties. Infrared and optical excitations will be used to induce changes in the hydrogen bonding network, and to initiate reactions of hydrated molecules. Moreover, on a practical level, radiation damage of concentrated electrolyte solutions, relevant for fuel storage, involves the anions interacting with ionizing radiation. To give another example, low-energy electrons created upon laser irradiation may attach to DNA bases in aqueous environment. Dissociative electron attachment is a major cause of strand breaks in DNA. Hydrogen-bond dynamics, solute-solvent interactions, and the interplay of electronic and nuclear dynamics during chemical reactions in solution will be accessible with time-resolved optical pump and x-ray probe spectroscopy. Techniques include XAS, XES, and XPS measurements; the latter will be performed in conjunction with the liquid microjet technique.

**Warm Dense Matter:** Warm Dense Matter refers to the region of the density-temperature phase-space between solids and plasmas, where the standard theories of condensed matter physics and/or plasma statistical physics are invalid. [x] These states of matter are of broad interest, as similar conditions of high temperatures and pressures exist in planetary interiors and in shock compressed matter. Further, there is an incomplete understanding of how materials damage under Free Electron Laser (FEL) irradiation. A femtosecond optical or FEL pulse will isochorically heat the sample. The x-ray emission will yield information about the occupied density of states. The objective is to develop a quantitative understanding of the electronic structure of materials at solid densities and temperatures of several 1000 °K.


### 2.2 Clusters as new Materials

Materials assembled atom by atom offer the chance to create new materials with controlled but as yet unprecedented new properties. In the nanometer size range, new electronic, optical, chemical, magnetic or even mechanical properties arise due to the effects of the quantized nature of the electronic interactions. Thus, as far as the development of the novel materials is concerned, the properties of these particles are not predictable by scaling laws. In this size range every atom counts, i.e. adding or removing just a single atom from the particle will result in different materials properties. One of the most prominent examples of this kind are the materials formed by condensing C<sub>60</sub> or related fullerenes into solids bound by van der Waals forces. These purely carbon based solids exhibit distinctly different properties from diamond or graphite, the other known solid carbon materials.

LCLS offers the unique opportunity to study both the electronic properties as well as the actual atomic structure of individual mass selected particles with an exactly defined number of atomic constituents. The pulse properties of
the LCLS source are required for these studies, since cluster production coupled with mass selection results in a highly diluted target density. The electronic properties will be accessible by studying the Auger spectrum following the creation of a core hole, whereas the atomic arrangement will be studied by core level photoemission (XPS) and (N)EXAFS, once the photon energy at LCLS can be readily tuned. For non-resonant Auger spectroscopy the exact photon energy does not need to be determined, as long as it is sufficiently high above the core electron absorption threshold. For XPS the monochromator running in spectrograph mode is required, since the photon energy and photon lineshape need to be recorded for each LCLS pulse individually together with the XPS spectrum.

Initially in these experiments we will concentrate on the characterization of particles with controlled magnetic and/or chemical properties.

Control of the magnetic properties of nanoparticles. The control of the properties of magnetic nanoparticles is crucial for applications ranging from data storage to cancer treatment. Under basic science aspects, it is intriguing to note that all atoms, except the rare gases, exhibit magnetism (Hund’s rule). Thus, in the form of well defined clusters, even elements such as Al form magnetic particles. As extended solids, on the contrary, only the latter part of the transition metals and the f-electron systems are magnetic. In general, the magnetic moments of clusters are larger than in the corresponding solids, whereas the temperature, below which magnetic order is stabilized, is lower. In summary, there are many degrees of freedom to design the magnetic properties of nanoparticles by controlling the exact size and composition, whereby not only metals, but also oxides are interesting candidates.

Control of the chemical properties of nanoparticles. Not only transition metals and their oxides are interesting candidates as catalysts, but also small Au and Ag clusters and their oxides exhibit quite a high catalytic activity, for example in various oxidation reactions. Again, the electronic structure of individual mass selected nanoparticles will be probed by (resonant) Auger spectroscopy and XPS to elucidate not only the particle properties but also the chemical bonding of adsorbates, while pump-probe spectroscopy will give insight into photo-chemical reaction cycles.

2.3 Magnetic Imaging

One of important topics of physics is the study of phase transitions, where structural, electronic, or magnetic properties undergo discontinuous or continuous changes. Powerful symmetry and statistical concepts have been developed to describe such phase transitions, and corresponding scattering and thermodynamic measurements have been used for experimental verifications. Such approaches are quite successful and satisfactory to many. Complementary and equally powerful, the conceptualization of a simple physical picture in the real space has played an important role in the formulation of physical understanding of many phenomena. This method of direct representation, however, has not received equal recognition perhaps due to the lack of corresponding experimental techniques until now. By combining the powerful Fourier Transform Holography (FTH) imaging technique with LCLS’ high brightness, short pulse structure, and fully transverse coherence, the dynamics of magnetic fluctuations and magnetization relaxation processes can be visualization at extremely fast time scales and at nm resolutions. This soon-to-be-established new capabilities will not only provide direct experimental proof of the symmetry and statistical concepts in magnetic phase transitions, but will also have far-reaching impact beyond magnetism in the studies of critical phenomenon such as other order/disorder transitions or the demixing of binary alloys.
The proposed experiments will be designed to investigate the critical fluctuations occurring at magnetic phase transitions. An initial LCLS experiment will demonstrate the existence of magnetic spin blocks by taking snapshot pictures on a time scale faster than the fluctuations. The next step will be to study the spin block dynamics by recording a series of such pictures at well-defined delay times. For imaging of the magnetic spin blocks a newly developed lensless imaging technique will be used. These experiments, however, would not be possible without the LCLS’ ultra-bright, ultra-short, and fully coherent x-ray pulses. Key properties and implications of the proposed experiment are:

**Single x-ray pulse imaging:** A single LCLS pulse will be sufficient to obtain an image of the instantaneous magnetic domain structure which is expected to be static on the time scale set by the ultra-short x-ray pulse length (230 fs), even close to the phase transition.

**50 nm spatial resolution or better:** It has been demonstrated that a 50 nm spatial resolution can be achieved with the newly developed lensless x-ray imaging technique which will take full advantage of the unprecedented full coherence of LCLS x-ray pulses. Subsequent phase retrieval may improve this to near-wavelength limited spatial resolution.

**Dynamics of critical fluctuations:** To image the fluctuation dynamics we will split the beam and produce consecutive x-ray pulses with a well defined time separation at the sample. From each pulse we will obtain an image of the magnetic domain structure, using a scheme discussed below, and thus resolve the dynamics occurring on a femtosecond to nanosecond time scale.

**Ultrafast, non-deterministic dynamics:** It is important to realize that the proposed experiments significantly differ from today’s ultrafast pump-probe experiments. Such experiments rely on reversibility of the sample to a well defined state before each pump-probe cycle. In contrast, the critical fluctuations that are the subject of our study are non-deterministic and their study requires complete images to be recorded in a single shot.

**Ultrafast relaxation dynamics:** It is clear that once we have demonstrated the feasibility of ultrafast single shot imaging a whole class of new experiments will become possible. Besides single shot imaging of spontaneously occurring fluctuations we also envision to study ultrafast relaxation dynamics in pump-probe experiments.
2.4 X-Ray Scattering Spectroscopy on Strongly Correlated Materials

Among the current research issues of condensed matter physics, the electronic structure of the strongly correlated materials is one of the most active topics. In this class of materials, the Coulomb interaction between electrons can not be ignored, which manifests itself as “strong correlations” acting as a “tuning parameter” to switch the ground state from one to the other. These collective ground states for different phases are known as “emergent” phenomena of many body systems, which can not be deduced from any perturbation theory and often involve novel forms of order.

X-Ray scattering experiments on strongly correlated materials have been performed to probe the charge ordering and elementary charge/magnetic excitations containing important information of the ground state properties. Recent theoretical developments show that resonance x-ray scattering can provide rich information on many-body wavefunctions. Soft x-ray, being sensitive to valence electrons and in the spectral range of important L edges of transition metals that often are key elements of correlated materials, provide special opportunity. However, so far most of these experiments were performed in the equilibrium state, which can not provide any information along the time axis regarding how the electrons form this particular ground state. The exciting opportunity provided by the SXR of LCLS is exactly this missing piece of information along the time axis. Using the high pulse intensity and ultra-short pulse length, it is possible to perform optical-pump-and-X-ray-probe experiments to study how the electronic states of strongly-correlated materials relax from an excited state to the ground state. The relaxation process is closely related to the correlation effect among the electrons and the electronic interactions to other degrees of freedom; therefore “snap shots” obtained from the pump-probe experiments provide important clues to construct a microscopic physics picture of the strongly-correlated systems. In addition, x-ray probe experiment also has some unique advantages, such as element specific information, bulk sensitive signal, and the dynamic structure factors, which are not accessible by the most common ultrafast optical pump-probe experiments in the visible light regime.

Figure 3 (a) A sketch of the momentum-resolved inelastic scattering experiment chamber. (b) The momentum transfer covered by different locations of the spectrograph at the Mn L edge. (c) The Fermi surface of La$_{1-x}$Sr$_{1+x}$MnO$_y$ and the region which can be covered by this spectrograph with the designed rotary sample stage. (d) The dispersion of orbital ordering of the La$_{1-x}$Sr$_{1+x}$MnO$_y$.

Three kinds of experiments were proposed for using LCLS to study the physics of the strongly correlated materials:

**Absorption experiment:** Absorption spectrum reveals the partial density of states of the unoccupied state of the materials. As a first step, it is important to understand how density of state change after the system been “pumped” by the optical Laser pulse. It is also an ideal initial experiment to do for the initial operation stage of the LCLS, since it is not an extremely photon hungry experiment, which can be done using with less powerful pulse and lower repetition rate. In addition, this absorption experiment would become a routine diagnosis experiment for the chamber alignment, sample damage assessment and a survey experiments for the resonant scattering experiments.
Resonant Elastic Scattering experiment: Charge, spin and orbital order is one of the interesting phenomena in many strongly correlated electron systems. These orderings, mostly incommensurate to the lattice constant, produce extra Bragg peaks in the elastic X-ray diffraction pattern. As these orders are often complex and thus relatively large in real space, making it possible for soft x-ray to have sufficient q to probe the extra Bragg peak. Using SXR pump-probe capability of LCLS, one could destroy the charge ordering by the optical pump Laser and probe by the LCLS X-ray pulse at different delay times after the pump as the system relaxes back to the charging ordering state. This experiment shall reveal important microscopic information of the charge ordering formation.

Resonant Inelastic X-ray Scattering (RIXS) Experiment: To probe the excitations of the ground state, it is necessary to record the energy loss of an inelastic scattering process. In addition, the information at different momentum transfers of the scattering process is also extremely important for the scattering experiments on solids as it is related to the momenta of these excitations. Time resolved pump-probe RIXS experiments can be used to measure time evolution of collective modes and thus, information about the dynamics involves in the many-body excitations that gave the collective modes. In addition, we will also use RIXS to obtain the wave function properties through various projections to its intermediate states. The pump-probe experiment using the SXR shall provide a description of the wave function evolution from the pumped exciting state to the ground state.

2.5 High-Resolution Ultrafast Coherent Imaging

X-ray microscopy at synchrotron sources is steadily progressing, with the nanofabrication of better zone-plate lenses and the development of lensless coherent imaging techniques. However, even with cryogenic sample cooling, radiation damage limits the achievable resolution to about 10 nm. Higher resolution is required to understand the structure and organization of living (unstained and unsectioned) cells, and would greatly complement real-time optical fluorescence microscopy to study cell processes, such as cell division, and full function of components such as the cytoskeleton. Coherent diffractive imaging with intense and ultrashort X-ray pulses could achieve the required resolution on living cells by recording the scattering information before any structural changes due to interaction with that pulse. This method of flash imaging has been verified at FLASH. In principle the resolution should only be limited by the wavelength of the radiation, given the appropriate pulse parameters and size of the focused pulse. The details of the matter–FEL interaction must be studied to gain an understanding of achievable resolution limits. Methods must also be developed for 3D imaging of reproducible samples, using streams of particles in the gas phase or in droplets. These delivery systems, first developed at FLASH, are required to quickly replenish the sample and allow time-resolved stroboscopic imaging of laser alignment of particles. Also the coherent diffractive method (with fixed or injected samples) enables the highest spatial resolution of ultrafast processes in non-periodic systems, such as the study of laser-induced phase transitions in materials. Experiments at FLASH demonstrated this technique on the study of phase separation in laser-ablation, but the shorter wavelengths of LCLS are required to achieve the necessary spatial resolution.

Imaging of biological cells beyond radiation damage limits: With the X-ray intensity provided by 5-micron focusing it will be possible to achieve a single-shot resolution of better than 5 nm. Imaging will be carried out on cells on thin membranes that can be placed into the beam as well as on cells injected into the LCLS beam.

FEL–matter interactions: Initial experiments will study the effects of damage by collecting coherent patterns of homogeneous samples (such as polystyrene spheres or nanocrystals) as a function of pulse fluence. In this case, the scattering pattern immediately gives the pulse-integrated size distribution of the particles, which can be compared with theory. Nanocrystals of biomolecular complexes (such as PS1) will give the high-resolution information about the damage of organic material as a function of resolution and pulse fluence.

Time-Delay Holography: This method, tested at FLASH, will be implemented to measure movies of the interaction and evolution of reproducible samples (such as virus particles) with FEL pulses. The apparatus will include a reflecting crystal, such as InSb, to direct the pulse back onto the sample. The detector will be placed in a
backscattering geometry. Samples will include layered spherical structures to test methodologies to prolong the onset of damage.

**Laser-matter interactions:** A synchronized optical pump pulse will be used for single-shot time-resolved imaging in materials and stroboscopic imaging of laser-particle interactions (such as laser alignment).
3. Science Driven Requirements:

In this section the basic science driven requirements of the beam line, optics and experimental stations for the SXR system are described. The proposal is for a monochromatic soft x-ray beam line with two positions for experimental stations.

3.1 Experimental stations:

The first experimental station shall be upstream of the monochromator in the unfocused beam. The second after the monochromator for focused beam.

3.1.1 Experimental station position 1:

It is important to allow for an experimental station at a position before the monochromator where x-ray interactions could be performed in a single shot mode. This is to be a simple chamber to allow transmission experiments on large samples, > 1mm in diameter. The requirement for absorption spectroscopy is a detector at the monochromator exit slit. A pump laser is required for pump probe experiments at this position. Ultra-high vacuum, <5x10⁻⁹ torr, is required in the first station.

3.1.2 Experimental station position 2:

Experimental position 2, or the end station, is to be a position that allows for highly diverse set of experimental configurations. This station, after the monochromator, will allow for either monochromatic or white beam that is either focused or unfocused at the sample. The beam line should be laid out in such a way to allow for the role-up of different end stations for various experimental programs. Below are the specific specifications of the LCLS delivered beam at this position. A pump laser is required for pump probe experiments at this position. Both ultra-high vacuum and high vacuum experiments shall be performed in these experimental stations. As the final optical elements should be maintained in a UHV environment differential pumping will be required for the non-UHV experiments. The SXR project is not building the experimental systems for the end station.

3.2 Monochromator:

Many of the experiments require a narrower band width than the inherent energy spread in the FEL pulse. A monochromator will be used to define the energy resolution for those experiments. It is also essential that the instrument can deliver the beam in a non-monochromatic mode. This will allow experiment to utilize higher intensities.

3.2.1 Energy range: 500 – 2000 eV.

The 500-2000 eV energy range covers several of the important K and L edges of the second and third row elements for resonant excitations. The lower part of this energy range is outside of the base specifications of what the LCLS will deliver. During the initial operations, the minimum energy will be 827 eV but, it has been suggested that at a later date it may be possible to decelerate the electron beam and access lower photon energies. Since several important experiments would be possible if resonant excitations could be performed at the O K (530 eV) and Mn L (630 eV) edges it is essential that the monochromator and optical system is designed to reach these energies.

3.2.2 Energy resolution: 0.2 eV at 1000 eV.

In monochromatic operation an energy resolution of E/ΔE of 5000 from 500 to 1000eV is required for the scientific program outline in section 1. Above 1000 eV the resolution can fall off to 2500 at 2000 eV.
3.2.3 Pulse stretching: <100 fs

This energy resolution will allow for selective excitation at specific x-ray absorption resonances with a broadening of the pulse length as delivered by LCLS. Though the nominal long wavelength FEL pulse duration is 320 fs fwhm it could be reduced in special operating modes. The monochromator should stretch the pulse by less than 100 fs. The monochromator should include an angular aperture in order to provide a choice of reduced x-ray pulse stretching at the expense of lower intensity and energy resolution.

3.2.4 Spectrometer detector

A position sensitive detector with sufficient spatial resolution to match the energy resolution will be required near the exit slit to allow the monochromator to be run in spectrograph mode with transmission samples in the first experimental station.

3.3 Focusing optics

The SOMS optics in the Front End Enclosure collimators, up stream of the SXR system, consist of three flat mirrors. These mirror along with their associated collimators are to filter out the spontaneous and Bremsstrahlung radiation and deflect the FEL beam horizontally. This horizontal deflection defines the space between the AMO, SXR hard x-ray beam lines. There are no focusing elements until the monochromator.

3.3.1 Focus: 10x10 μm at the second station

The experimental station focus requirement is kept at ≤10 x 10 μm, with a smaller focus of 3 x 3 μm tried on a best effort basis. The resolution of x-ray emission spectrometers without entrance slit would improve from a smaller focus in one dimension, generally the vertical. Coherent imaging of single molecules would profit from a smaller focus in both dimensions; for example 3 μm. The improved spot size for x-ray emission and coherent imaging could be provided by the non-monochromatic mode. For holographic imaging experiments the divergence should be < 1 mrad.

3.4 Diagnostics

3.4.1 Intensity monitor

A pulse by pulse intensity monitor is required after the exit slit for normalizing detector signals. The intensity measurement only needs to be relative, and have noise <0.1%.

3.4.6 Fast shutter:

A fast shutter is needed to quickly turn on or off the beam or to select individual LCLS x-ray pulses. It should close or open in <8 ms. The fast shutter should be up stream of the first experimental position.

3.5 Laser systems:

Two type of supporting laser systems are required at both experimental positions. A pump laser to excite samples and an alignment laser for positioning.
3.5.1 Pump Laser:

The pump laser should be capable of producing 2mJ/pulse at 120Hz. The pump laser system is defined in Physics Requirements for LCLS/NEH Laser System, Requirements Document # 1.6-010 rev 0 section 2, 3, 4, 6, 7 and 8. To summarize it should be capable of delivering 800nm with an energy of up to 3mJ in a pulse ≤50 fs at the sample. The pump laser shall be synchronized with the LCLS FEL at a repetition rate of 120Hz. The pulse laser should be synchronized to the LCLS RF with a jitter of ≤100 fs. The delay system should be capable of adjusting the laser timing by ±1ns with 10fs accuracy. There are some experiments that require 25 mJ/pulse at a 10Hz rate. The conversion to shorter and longer wave lengths is not required for initial experiments on the SXR (section 5 of the above mention document), but provision should be made to accommodate this at a later date.

3.5.2 Alignment Lasers:

A HeNe alignment laser beam shall be set up coaxial with the FEL beam to facilitate the positioning of samples in the FEL beam. This laser shall be class IIIa rating or less.
4. Optical Design

4.1 Optical layout

At synchrotron radiation sources, two of the most successful types of grating monochromators are the Varied-Line-Spacing grating monochromator (VLS) and the Plane Grating Monochromator (PGM). The VLS monochromator was developed by Underwood, Koike and coworkers at the Advanced Light Source (ALS). A spherical mirror produces a converging beam in the vertical plane and a varied-line-spacing grating diffracts the x-rays onto an exit slit. The variable period of the grating provides additional parameters to keep the focal distance constant as a function of photon energy and to compensate for aberrations of the mirror. The focal plane is erect, which is convenient for implementing the spectrometer mode. The photon energy is scanned by a single rotation of the grating.

The PGM monochromator was developed by Peterson, Follath and Senf at BESSY. In the PGM monochromator a plane mirror reflects the x-rays onto the grating and an elliptical or spherical mirror focuses the beam onto the exit slit. The plane mirror provides a variable included angle on the grating, which allows the grating efficiency to be optimized over a wide photon energy range. The photon energy is scanned by coordinated rotations of both the plane mirror and grating.

We have chosen the VLS monochromator type because of its simplicity. Only two optical elements are required, and only the grating rotates. The limited photon energy range of the SXR Instrument, 500 to 2000 eV, would not take advantage of the variable included angle of the PGM monochromator.

![Figure 4-1. Optical layout of the SXR Instrument.](image)

The optical layout of the SXR Instrument is shown in figure 1. Table 1 is a list of the optical elements and their parameters. The first component is experimental chamber 1, which is a location for samples in the unfocused non-monochromatic beam. Next, there is the M1 spherical mirror and G1 and G2 plane gratings of the VLS monochromator. In monochromator mode, an exit slit selects a narrow bandwidth. Alternatively in spectrometer mode, a detector will measure the dispersed x-ray absorption spectrum. The M2 plane elliptical mirror provides the horizontal focus in experimental chamber 2. The plane elliptical M3 mirror produces a vertical image of the exit slit at experimental chamber 2. The experimental chamber 2 provides the experimental environment for monochromatic and focused pink beam experiments. Endstation 1, the M1 mirror and gratings are in the first hutch of the LCLS Near Experimental Hall. The rest of the beamline from the exit slit and detector through the experimental chamber 2 are in the second hutch.

4.2 Optical elements

The design of the optical elements adopts characteristics of the LCLS soft x-ray offset mirrors in the Front End Enclosure. The incidence angle of the mirrors is 89.14° equivalent to a grazing angle of 15 mrad. The mirror substrates are single crystal silicon, and the preferred optical coating is B4C. Figure 2 shows the reflectivity of B4C in comparison with other coating materials. The reflectivity of B4C is excellent about 90% over the whole energy range.
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<th>Type</th>
<th>Coating and blank material</th>
<th>Dimensions l x w x t (mm)</th>
<th>Clear Aperture (mm)</th>
<th>Radius (m)</th>
<th>Figure error (μrad)</th>
<th>Roughness (nm)</th>
<th>Incidence angle(°)</th>
<th>Grating period order</th>
<th>Distance from source (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exp. Chamber 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M1</td>
<td>Spherical mirror</td>
<td>B₄C-coated silicon</td>
<td>250 x 30</td>
<td>175 x 10</td>
<td>943</td>
<td>0.3</td>
<td>0.4</td>
<td>89.14</td>
<td>-</td>
</tr>
<tr>
<td>G1, G2</td>
<td>Plane VLS grating</td>
<td>B₄C-coated silicon</td>
<td>220 x 50 x 23</td>
<td>170 x 24</td>
<td>∞</td>
<td>0.5</td>
<td>0.4</td>
<td>88.7-88.9</td>
<td>1/100, 1/200</td>
</tr>
<tr>
<td>Detector/Slit</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M2</td>
<td>Bent Elliptical mirror</td>
<td>B₄C-coated silicon</td>
<td>250 x 30</td>
<td>190 x 10</td>
<td>262.8</td>
<td>0.3</td>
<td>0.4</td>
<td>89.14</td>
<td>-</td>
</tr>
<tr>
<td>M3</td>
<td>Bent Elliptical mirror</td>
<td>B₄C-coated silicon</td>
<td>250 x 30</td>
<td>125 x 10</td>
<td>156</td>
<td>0.4</td>
<td>0.4</td>
<td>89.14</td>
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<td>Exp. chamber 2</td>
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<td></td>
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</tbody>
</table>

Table 4-1. The optical elements of the SXR instrument.
range of the SXR instrument. Boron and Carbon would also give acceptable performance. The incidence angle and coating materials maintain 2000 eV as the high photon energy limit. Silicon would limit the cut off to 1800 eV. The clear apertures are set to accept a 5 σ footprint of the x-ray beam including a tolerance of 0.5 μrad rms for the LCLS beam pointing stability. [4] The M1 mirror is polished as a sphere. On the other hand the M2 and M3 mirrors are polished as flats and then bent into their plane elliptical shapes. The M2 and M3 mirrors need an elliptical surface in order to eliminate the coma aberration. The coarse grating line densities, 100 and 200 l/mm, are a consequence of the included angle 2θ being close to 180°. It is planned to have both rulings placed on a single grating substrate. The gratings operate in the negative first diffracted order. The choice of negative order has two benefits. The larger grazing incidence angle reduces the required length of the grating. The grating in negative order has magnification, which eases the needed detector spatial resolution. For the distances of the optical elements, the source position is chosen as 10 m upstream from the end of the undulator. [5]

Figure 4-2. The reflectivity at 15 mrad grazing angle of B₄C, C, Si and B.

Figure 4-3a. The LCLS FEL source at 1000 eV.

Figure 4-3b. The x-ray beam at experimental chamber 1.
4.3 Raytracing, energy resolution and efficiency

Raytracing has been performed to confirm the optical design using the XOP software. Spot diagrams are displayed in figure 4. The LCLS FEL source at 1000 eV is predicted to be round with a diameter of 82 μm (fwhm) and a divergence of 8 μrad (fwhm). Compared with third generation synchrotron sources, the horizontal beam size and the divergence in both dimensions are significantly smaller. In experimental chamber 1 the unfocused x-ray beam is again round with a diameter of 1 mm (fwhm). The M1 mirror and VLS gratings G1 or G2 produce a vertical focus, 1.1 mm horizontal by 18 μm vertical (fwhm), at the exit slit or detector. The spot diagram (3c) shows three different energies 999.8, 1000 and 1000.2 eV at the exit slit. That these three photon energies are well resolved confirms that the resolution goal of 0.2 eV at 1000 eV is achieved. The M2 and M3 mirrors refocus the x-rays horizontally and vertically into experimental chamber 2. The predicted monochromatic focus in experimental chamber 2 is between 1 and 2 μm horizontal by 3 μm vertical (fwhm). In the case of the non-monochromatic beam, the vertical focusing is changed because now the grating has a magnification of unity. For the non-monochromatic beam the calculated focus in experimental chamber 2 is nearly round between 1 and 2 μm in diameter (fwhm). It should be noted that this ray tracing does not include optical fabrication errors.

The tolerances for FEL x-ray optics are quite demanding and beyond what is required for synchrotron radiation optics. This difficulty can be simply understood by the fact that the FEL and synchrotron source dimensions are similar but for FELs the first optic is roughly ten times further away; hence the allowable slope error is reduced by about an order of magnitude.

\[ 2 \Delta r r \leq \frac{s}{2}, \]

where \( \Delta r \) is the tangential slope error, \( r \) the source distance and \( s \) the source dimension. Preserving the source brightness of the LCLS is challenging.

Optical tolerances are included in table 1 for the slope error and roughness. The figure specifications for the M1 mirror and G1 and G2 gratings result from the energy resolution goal of 0.2 eV at 1000 eV. The figure tolerance for the M1 mirror is the most difficult because the image created by the M1 mirror is magnified by the grating. The figure specification of the M2 and M3 mirrors is derived from the required focus in experimental chamber 2, a 10 μm diameter. The B4C coatings place an upper limit on the roughness for spatial periods from 20 nm to 2 μm, the Atomic Force Microscope measurement range. With higher substrate roughness the B4C coating growth process changes. A specification from Fourier optics considerations will be added to the mirror and grating specifications.
The grating efficiency is the most important factor in determining the overall beamline efficiency. Efficiency calculations were performed with the GSolver code. [6] The optical constants for the B$_4$C coating were taken from the CXRO website. [7] For the laminar groove profiles, the groove depths and widths were varied to maximize the efficiency at single photon energies: 800 eV for the 100 line/mm grating and 1200 eV for the 200 line/mm grating. The optimal groove depths were found to be 19 nm for the 100 line/mm and 13 nm for the 200 line/mm grating. High peak efficiencies between 0.1 and 0.4 were calculated. These efficiencies should be related to the low groove densities and the high reflectivity of B$_4$C.

The average power in the LCLS FEL radiation is low, 0.2 W, because of the low repetition rate, 120 Hz. On the other hand, the peak power is quite high, 5 GW, as a result of the ultrashort pulses. Optical damage from the LCLS x-rays was modeled by London et al. [8] Their guideline is to stay below the melt fluence. The risk of optical damage is reduced by using small grazing angles and low Z coatings. Since the SXR mirrors employ the same incidence angle and coating as the LCLS soft x-ray offset mirrors, these mirrors should be safe from the damage calculations of these mirrors. An estimate of the absorbed energy for the M1 mirror is 0.04 eV/atom, well below melting dose of 0.62 eV/atom. The case of the gratings could be worse because of the larger grazing incidence angle and that a portion of the x-rays strike the leading edges of the lands at near-normal incidence. However, estimates of both these cases gave an acceptable dose of 0.05 eV/atom. These damage calculations were performed at 2000 eV, which is the most difficult case because of the reduced beam divergence. The optics of the SXR instrument should not damage from the FEL radiation.

The exit slit may be also damaged from the LCLS FEL beam, which is vertically focused at this location. Three cases must be considered: monochromatic beam, zero order and pink beam. For the monochromatic situation the dose is acceptable, 0.03 eV/atom, because the intensity is reduced by the dispersion of the different FEL wavelengths in negative first order. This damage consideration does require that the exit slit blades be made of B$_4$C or perhaps another low Z material. The zero order can be blocked at a small distance downstream of the gratings, where the x-ray beam is not focused. The final and most difficult case is the undispersed pink beam. Here the dose at the exit slit, 5 eV/atom, is not acceptable. One solution is to add an aperture upstream, where the FEL beam is large enough and the flux density below the damage limit. This aperture would need to be aligned to the exit slit and the exit slit would need to be openable to a larger width than the aperture. An aperture that opens to 2 mm would transit the dispersed spectrum to the detector for spectroscopy experiments.

Grating optics increase the x-ray pulse duration. This pulse stretching, $\Delta t$, results from the extra optical path, $m \lambda$, between groove n and groove n+1, where m is the order of diffraction and $\lambda$ the x-ray wavelength. It can be calculated from

$$\Delta t = \frac{Nm\lambda}{c},$$

here N is the number of illuminated grooves and c the speed of light. For 800 eV the estimated pulse stretching is 40 fs, which is well below the predicted LCLS pulse duration of 320 fs. For measurements with the sample in experimental chamber 1 or in experimental chamber 2 using pink beam, there is no optical pulse stretching. There are operating modes of the LCLS which will provide shorter pulses. [9] There should be an angular aperture in the SXR instrument in order that the pulse stretching can be reduced with a corresponding loss in intensity and in energy resolution.

There are existing mechanical designs for monochromators, bendable mirror assemblies and exit slits at the Advanced Light Source and other synchrotron facilities. It is planned to reuse existing mechanical designs with minimal modifications for the LCLS SXR instrument. Switching between monochromatic and pink beam may be accomplished in a convenient manner provided by the current,
“standard” ALS monochromator chamber design. The chamber is translated horizontally perpendicular to the beam propagation direction. If the grating surface has ruled and unruled areas, the grating can either diffract for monochromatic operation or reflect for pink beam operation.

References
1. P. Emma, private communication.
4. P. Stefan, private communication.
5. Y. Feng and H. D. Nuhn, private communications. The source distance depends upon the point along the undulator length where the FEL reaches saturation. 10 m from the downstream end of the undulator is the nominal saturation point for the LCLS start up parameters at 800 eV.
5. Instrument Layout:

In this section we will describe the constraints on the physical layout of the SXR systems and how we propose to meet the scientific requirements within those constraints. The proposal conforms to the new AMO experiment location in the first hutch of the Near Experimental Hall (NEH) on the 83 mrad line. The SXR systems are on the 28 mrad line, between the AMO line and the hard x-ray line, with a pre-monochromator sample position, M1 mirror and grating system in first hutch. The SXR exit slit, refocusing mirror and end station are in the second hutch.

In the Front End Enclosure (FEE) the M3-S1 or M3-S2 mirrors of the Soft x-ray Optics Mirror System (SOMS) direct the FEL beam down either the 83 mrad or the 28 mrad lines to the AMO and SXR experiments respectively. On each branch there are fixed collimators and insertable photon stoppers in the FEE that block the beam, so entry can be permitted into the first hutch. Just downstream of the first hutch wall there is an insertable beam position imaging system and an isolation valve. This terminates the SOMS vacuum system.

The basic optical layout is presented in section 3. There are several constraints on fitting this optical design into the NEH. The first is that it does not materially interfere with the program on the AMO experiment. Both requirements are physical, over space, and operationally for access during operations on each system. A second is the flux in the FEL beam. Though power is on average low, the flux density in the FEL beam will damage most materials. This is particularly critical where the beam is focused. The third requirement is the inclusion of a moderately high resolution monochromator, which essentially requires it span the first and second hutch.

The AMO group is locating their experiment in the first hutch of the NEH. The SXR beam will pass through the first hutch, horizontally between the AMO experiment and the hard x-ray beam line. The first experimental station and the monochromator would be located in the first hutch just upstream of the AMO focusing optics. These would have to be properly shielded for personnel to be in the first hutch while beam is passing through the SXR monochromator into the second hutch. These shielding requirements have not yet been defined. The controls on the shielding will follow SLAC personnel protection requirements. This shielding and controls will be required for the SXR experiment to run effectively. The hard x-ray beam line that also passes through the first hutch will be shielded.

The flux density in the FEL beam will damage most materials and is particularly critical where the beam is focused. Materials of low Z elements have the best properties for surviving in the beam [3]. Collimators and beam stops are to be fabricated from B$_4$C which should not damage in the unfocused FEL beam at this distance from the source. At approximately 0.12 eV/atom/pulse fatigue sets in and at 0.6 eV/atom/pulse single shot damage occurs in B$_4$C. The fatigue value sets a limit for optics and beam stops that are continuously or often in the beam. Collimator and apertures that will only see incidental beam strikes are limited at the higher single shot damage threshold. The monochromator proposed in section 3 focuses, in one dimension, both the monochromatic and the zero order, white, beam at the exit slit. All materials are likely to damage in the focused zero order beam at the exit slit. Thus the exit slit must be opened when zero order light is put through it to prevent damage to the slit blades. This does not substantially limit the ultimate focus at the second experimental station as the zero order focus is quite small, 1σ ~10μm. An aperture upstream of this zero order flux density 'stay clear' would contain the beam and prevent the focused zero order beam from striking the open exit slits.

5.1 Instrument Configuration:

The SXR proposal is predicated on the inclusion of a monochromator, which essentially requires the optical system to span the first and second hutch of the NEH. The basic layout is shown in figure 5.1. The transmission sample position and the monochromator focusing/grating system will be located in the first hutch along with, but up stream of, the AMO experiments. The SXR is laid out to make space for an extension of AMO experimental systems into the second hutch.
The hutches are roughly 10m in length, 10m in width and 4.5m high. Access is through interlocked doors. The hutches will also contain the optical tables for the pump and alignment lasers, electronics racks, electrical panels and other utilities. See figures 5.2 A & B. The first hutch is primarily dedicated to the AMO instrument on the 90mrad branch line (actually 83 mrad from the undulator center line). On the 30 mrad (23mrad) branch line is the SXR instrument. In the first hutch the single pulse shutter, the transmission sample chamber, the monochromator tank, collimators and drift tubes for the SXR will be located. On the 0 mrad line the XTOD, hard x-ray beam line, passes through both hutches 2m from the back wall. The nominal FEL beam height is 1.4m above the floor.

The SXR optical layout has the M1 mirror and grating system just up stream of the AMO experiment which puts the exit slit, 7.5m down beam, just inside the second hutch. The K-B pair of refocusing mirrors are in the middle of the hutch with the final focus 1.5m down stream of the center of the M3 mirror. See figure 5.2 A and B. The focus is 1.3m from the hard x-ray beam pipe and 3.3m to the back wall of the second hutch. The XTOD beam pipe is shown with a 0.1m beam pipe, but additional space will be required for valves, stands and shielding. The shielding requirements have not been defined at this time. The location of stands and valves is somewhat negotiable with the XTOD if done early on. The XPP experiment going into the third hutch requires space for a slit system in the second hutch. The proposed location is just up stream of the K-B mirrors. There will be electronics racks along the back wall of the hutch and access to these racks much be provided. A ~1m (36") access way around the end of the experimental system is shown.

From the focus there is ~2.4m down beam and ~1.2m on XTOD side available for experiment systems. The flange to the beam line is laid out at 0.5m before the focus. There is an optical bench for the pump laser near the center of the hutch. The pump laser beam is likely to be a bit lower than the FEL beam height and then introduced by directing it up into the vacuum system. The largest system proposed so fare, Down beam of the AMO experiment there is space marked out for a future extension of the AMO beam line. This station could be configured in several ways. This area should be kept clear of any permanent installations.
Figure 5.2 A: layout of AMO and SXR instruments in the first hutch.

Figure 5.2 B: Layout of SXR experiment in second hutch with potential third AMO experimental station.
5.2 Single Pulse Shutter System:

The first item in the SXR line is to be a Single Pulse Shutter (SPS) system. The system is to be a clone of the shutter system in development for the AMO experiment. The fast shutter system can close or open in less than 8 ms. The solenoid driven shutter will be triggered through the EPICs control system (see controls, sec 5.3). The position of the shutter will be adjusted with a motor driven manipulator and a camera will be mounted to observe the beam on the shutter’s upstream face for alignment. The shutter is essentially binary; it will be either in the beam or out of it.

5.3 Transmission Sample Station, Pre-Monochromator Position 1:

There will be an experimental station before the monochromator, experimental position 1, where samples can be introduced into the unfocused, ~1mm in diameter, beam. Several detection methods are potentially possible. The proposal is to concentrate on transmission through thin samples, using the monochromator in spectrograph mode, with a detector at the exit slit to measure absorption spectra.

The absorption experimental setup will be simple. A x-y manipulator will be provided to position the samples in the beam. Configuration of the sample holder and sample introduction system has yet to be defined. The sample holder will include a Ce doped YAG crystal for viewing and alignment of the FEL beam. There will be a camera to monitor sample position and to align the FEL, the pump laser into overlapping phase space at the sample position. The camera will be capable of 120Hz imaging and synchronized with the FEL pulse and time stamped. The spectrometer detector, at the exit slit, will fully instrumented and capable of operating at 120Hz with the data time stamped to each pulse.

The sample chamber will be isolated from the SOMS and the monochromator optics by a gate valve. The chamber will have an ion pump for UHV operation and a cold cathode gauge to monitor the pressure. The pressure in this system will have to be <5x10^-9 torr to be opened to either the monochromator or the SOMS system. Samples will have to be UHV compatible.

The shielding requirements for this sample system have not been determined, but it should be anticipated that samples cannot be run in this system unless personnel are excluded from the first hutch. Access to the first hutch with samples in the beam can only be permitted when proper shielding has been defined, implemented and qualified.

Figure 5.3 Conceptual layout of the Transmission Sample Station with the laser in-coupling mirror system. The input beam is from the left. The monochromator will be immediately downstream.
5.4 **Monochromator:**

The AMO systems occupy the later two thirds of the first hutch. This is to maximize the space between the 28 and 83 mrad beams. It opens up a limited area in the up stream end of the first hutch for an experimental position and the M1 mirror and grating system on the 28 mrad/ SXR line. See figure 5.1.

The first focusing element in the SXR beam is the M1 mirror. This mirror will have a fixed spherical radius. It will focus the beam at the exit slit of the monochromator. The angle incidence on the mirror can be adjusted to get the focus at the exit slit. The mirror pitch will be motorized and must have the range to both compensate for the as delivered radius of the mirror and correct for changes the virtual source distance as the FEL parameters are varied. The pitch motion will have limits and hard stops set so the beam can only strike the surfaces designed to take the FEL flux. The mirror will vertically deflect the beam upwards by 30 mrad.

The grating immediately follows the M1 mirror. It will be a Variable Line Space (VLS) type grating on a flat substrate. With this VLS grating the focal length of the monochromatic radiation is constant and at the same distance as the zero order, specularly reflected, radiation. The monochromator therefore has a fixed exit slit and can easily be operated as a spectrograph by placing a position sensitive detector at, or near, the exit slit. Both the M1 mirror and the grating will be fabricated from single crystal silicon and have B4C optical coatings [2]. The grating will vertically deflect the beam downwards with the output parallel to the input beam.

Monochromator mechanisms and optical elements are commercially available. The outline of such a commercial system, which meets the requirements of section 3, shown in figure 5.1.

The grating pitch and exit slit aperture will be interlocked to prevent damage to the exit slit blades. The pitch motion of both the M1 and gratings will have limits and hard stops set so the beam can only strike the surfaces designed to take the FEL flux.

5.5 **Zero Order Stop and Grating Aperture:**

Down stream of the grating there shall be a photon stop that will absorb the specularly reflected radiation from the grating when it is operating with diffracted beam going down through the exit slit. The monochromator is designed to only operate with out side orders, therefore the zero order stop will be on lower side of the transmitted beam. The zero order stop will extend passed the limits of beam travel when both the M1 and grating are at there maximum pitch. As there will be beam on the zero order stop when running in monochromatic or spectrographic mode the zero order stop will be either configured to be either, safe for indefinite exposure to the beam or back by a Burn Through Monitor.

Down stream of the zero order stop and up stream of the exit slit collimator will be an adjustable vertical aperture that can be used to limit the number of lines on the grating that can illuminate the exit slit. This will be used to limit the temporal stretching of the pulse, at the expence of flux and resolution. (See section 3.)

5.6 **Exit Slit Collimator:**

There will be an collimator between the zero order stop and the exit slit. This collimator has to be upstream of the zone in which the focused zero order beam can damage B4C. This collimator will have an aperture that is smaller than the exit slit when it is fully opened. This will prevent zero order beam from striking the exit slit, which is interlocked to the grating pitch as described below. The outer diameter of the collimator will be sufficiently large to contain the beam.
The SXR beam pipe will pass the AMO systems between the grating system and the exit slit. The only components in the SXR line adjacent to the AMO system would be apertures and diagnostics upstream of the zero order stay clear and these could be located so as not to interfere with AMO components. The collimator and beam pipe to the exit slit shall be shielded so personnel can work in the first hutch when beam is going through SXR monochromator.

5.7 Exit Slits:

The Exit Slit will be located just inside the second hutch as shown in figure 5.1. The exit slit shall open to a gap larger than the upstream collimator and close to <10 μm in the vertical direction. The horizontal aperture will be fixed. The slit blades will be B₄C, but the exit slit has will have to be open before the grating pitch can be moved to put zero order light down to the slit. The exit slit opening will be motorized and interlocked to the grating pitch angle. Basic interlock logic is outlined in table 5.1.6.

<table>
<thead>
<tr>
<th>Table 5.1: Zero Order/Exit Slit logic:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slit fully open</td>
</tr>
<tr>
<td>Grating pitch near zero order</td>
</tr>
<tr>
<td>Grating pitched for diffracted beam</td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

The grating scan motion shall have two sets of switches. One for limiting scanning in monochromatic mode. This sets the grating angle limits to allow only diffracted beam past the exit slit collimator, to the exit slits. A second switch will be activated as the grating is rotated past the first switch to put zero order beam through the exit slit collimator. If the exit slits are not fully opened, the second switch will generate an logic state that would generate a MPS fault if the up stream beam stoppers are open. This MPS fault would deflect the electron beam out of the undulator. If the slits are fully opened no fault will be generated. If exit slit is fully open and grating pitch is not in the safe monochromatic angle range the exit slit will not be permitted to close and would generate a fault if they come off the fully opened position.

The slit system shall be shielded to allow access to the second hutch with beam to the slits.

5.8 Spectrograph Detector:

At the exit slit an position sensitive detector is required for the monochromator to be run as a spectrograph. As noted in section 3 the imaging field is up right due to the VLSG design. Due to the long focal length of the mono the depth of field is large, on the order of 1m, so this detector can be either just up stream or down stream of the slits without appreciable loss of resolution. The detector selection has to be compatible with the required spectral resolution, the maximum pulse rate of 120Hz, and the high flux density even in the monochromatic beam. for example a Ce doped YAG crystal the same as or similar to the SOMS “POP” in monitors, with the appropriate camera will work.

The detector system shall be shielded to allow access to the second hutch with beam to the detector.

5.9 Photon Stoppers:

Photon stoppers are required if personnel are to work on SXR second experimental station while beam is in the first hutch. The hutch stoppers will be the standard LCLS Photon Stopper design [1]. The stoppers will have an associated collimator. This may be the exit slit collimator or a separate collimator.

The stopper system shall be shielded to allow access to the second hutch with beam to the stoppers.
5.10 Intensity Monitors:

The spectrum as well as the intensity of LCLS will fluctuate due to the SASE process. LCLS provides measurements of the number of photons on a shot by shot basis. As the spectrum of LCLS fluctuates beyond the spatial resolution of the monochromator, it is essential to measure the beam intensity after the slit assembly on a shot by shot basis to normalize measured spectra. The intensity monitor need only be relative and linear over a short energy range, on the order of 10 eV. A signal to noise ratio of 0.1% is needed.

A gas cell can exceed these requirements. Such a cell should be windowless to preserve the coherence of the FEL beam. Such a cell is complex to design and expensive construction and is not in the scope of the first experiments. Space between the slit assembly and the first focusing mirror tank should be kept clear as far as possible for future use by a future gas cell monitor.

The use of an in-vacuum photo diode to measure the fluorescent and scattered radiation from an optical element will be implemented inside the second focusing mirror tank. Similar intensity monitors have been implemented successfully at beam lines at SSRL. Scaling from the SSRL data and assuming $1 \times 10^{12}$ photons per pulse, there would be $0.5 \times 10^{6}$ photon per pulse in the diode, at 800 eV this would be $1 \times 10^{8}$ electrons per pulse which should approximately 0.15% signal to noise. For better statistics either the diode could be moved closer to the mirror, i.e. make detector more position sensitive, or use several diodes, to make it less position sensitive. As these detectors are only collecting scattered radiation from optics, they are non-destructive to the beam. Such detectors can configured specifically to be beam position monitors.

The photocurrent from a thin Aluminum foil has been implemented successfully at FLASH to be used as an intensity monitor for the fifth harmonic. The radiation after the monochromator is attenuated by two orders of magnitude and is not expected to destroy the foil. The aluminum foil assembly will be mounted on a motorized linear feed-through which allows one to insert and remove the assembly into / from the beam. A ring electrode at +1kV around the beam separated from the foil by 2mm is used to collect the photo electrons, avoiding non-linearity caused by space charge effects. The Al foil itself is connected to a charge sensitive amplifier through a coaxial cable and the detected signal is digitized at 120 Hz, synchronously to the repetition rate of LCLS. The Al foil will be 200nm thick (commercially available). Beryllium foils are also an option.

5.11 Refocusing Mirrors:

Refocusing optics are required that image the exit slit vertically, and the source horizontally at the second experimental position. The configuration from section 3 is to put these mirrors close to the final focus while being compatible with differential pumping and experimental chamber dimensions.

The proposed imaging system will be a K-B pair of elliptical cylinders. The elliptical cylinders will be generated by bending optical flats that have a profiled width and independent moments applied at each end. The mirror system shall be able to adjust from essentially unfocused to fully focused at the sample position. The mechanical design is to be very similar to that used for the AMO focusing mirrors with the exception that they do not need to be removed from the beam. The M2 and M3 mirrors are to be operated at essentially fixed angles of incidence. A fixed aperture will be located down beam of the M3 Mirror to contain the beam. Thus the components between the M3 and the focus can be fixed in space.

The K-B mirror system will be a clone of the AMO system with the exception that the profiles of the mirrors will be optimized for the focal lengths on the SXR beam line. The mirrors will be at a nominal grazing angle incidence of 13.85 mrad and fabricated from single crystal silicon with a B$_4$C optical coating.
5.12 Experimental End Station, Position 2:

Experimental position 2, the end station, is locate in the second hutch after the K-B refocusing mirrors. The experimental systems for this second station are not part of this proposal. The SXR proposal provides the basic requirements of:

- A focus of <10x10 μm.
- Compatibility with vacuum in the end stations from 10⁻⁶ to 10⁻¹⁰ torr.
- Introduction of coaxial pump and alignment laser beams.

The focal spot size requirement puts constrains on the space between the M3 and experimental systems. To get the <10x10 μm focus a 1.5m M3 to focus length is specified. The space shall include:

- Beam stop with aperture
- A differential pumping system.
- Coaxial in-coupling of the pump laser beam.
- Isolation valves
- Bellows
- Sample chamber.

In Figure 5.4 a preliminary layout is shown. The differential pumping is up stream of the pump laser introduction mirror because the pump laser beam is too large at this distance from the focus to put it through an effective differential pumping system. This layout allows 0.5m for the experimenters system.

Figure 5.4 Layout differential pump, laser in-coupling and isolation valves down stream of M3 mirror. The input beam is from the left.
5.13 Optical Pump Laser Transport, collinear in-coupling

Optical femto second Laser pulses to excite or probe ultra fast dynamical processes have be guided from the existing Near Experimental Hall optical laser facility (W. White) to the two sample interaction points, transmission sample chamber and end station. The pump laser will be transported to optical table adjacent to in-couple mirrors just up stream of each sample location. Focusing and pointing optics and feedback will be located out-of-vacuum. This allows for flexibility in bringing the laser beam in coaxially or near coaxially with the Hamburg in-coupling mirror system, described below, or though an off axis viewport. The nominal set up will have the laser bean brought in though the Hamburg in-coupling mirror with a \(\sim 1\text{nm}\) spot size at the transmission sample position and \(\geq 100\mu\text{m}\) spot at the end station.

The design is based on the Hamburg design used at the FLASH PG2 beam line. It has 2 inch diameter dielectric plane mirrors with a central bore to transmit the X-ray beam. For different wavelengths specific mirrors are mounted on a ball bearing stabilized manual translation stage. At 2 inch diameter and a central bore diameter of 2 mm minimum distortion of the optical wave front is ensured. In the initial stage 800 nm and 400 nm mirrors are used. The mirrors are in vacuum mounted in spring mounted holders, which allow bake out of the UHV system without putting mechanical stress onto the mirror surfaces. On the back of the mirrors matching fluorescence screens are mounted which allow rapid positioning of the X-ray beam through the central bore.

In this implementation the mirror chamber is fixed with the pointing feed back done out of vacuum. In the case of the transmission sample position, with the large spot size the pointing stability is not critical so the in-coupling mirror and the pointing feed back loops are supported separately. At the end station with the potentially small spot size the in-coupling mirror and the feedback loops and focusing optics will be mounted on the same optical table.

Figure 5.5  The operational design at the PG2 beam line at the Free Electron Laser at Hamburg (FLASH) facility.
Appendix C: Descriptions experimental systems groups propose to bring. Scheduling of chambers will depend on the interest of the community and rankings of the review panel.
Dear SXR representative,

This letter describes the intention to install, operate and support a fully equipped endstation at the Soft X-ray for Material Science (SXRF) beamline at LCLS. The endstation will comply with the requirements outlined in chapter 5 of the SXRF Technical Design Report and be available for extended periods of time (months) per year at the SXRF beamline for experiments conducted within the experimental group of A. Nilsson, by other SXRF collaborators as well as by outside users via LCLS experiment proposals.

The UHV endstation, outlined in the figure below, is designed for soft x-ray photoelectron spectroscopy (PES), x-ray emission spectroscopy (XES) and x-ray adsorption spectroscopy (XAS) of surface and solid state samples of up to 10mm in diameter having ultra-high vacuum compatibility. The endstation is equipped with an electron spectrometer (R3000, VG-Scienta) for PES, partial electron yield detector for XAS, and a soft x-ray emission spectrometer housing 2 gratings for photon energies from about 220 eV to 630 eV with a maximum resolving power of about 2000. A horizontally mounted manipulator (VG Omnix) allows transfer of the sample(s) between the preparation chamber and the analysis chamber. Sputtering facilities, evaporation sources, mass spectrometer and LEED optics are available in the preparation chamber. A pulsed gas delivery system allows an accurate deposition of gases in a reproducible manner.

The sample setup, illustrated in the figure below, is optimized for studies of adsorbate systems prepared on single crystal surfaces. A single crystal is mounted onto a Cu block via a pair of Ta (or W) wires. The Cu plate is electrically isolated from the sample holder by a sapphire spacer and thus a voltage can be applied. Temperatures between 30 and 1500 K can be achieved through cooling with liquid N2 (He) and heating performed by electron bombardment (with or without a bias). Temperature is measured by thermocouples spot welded onto the sample or via Ta foil.

This endstation is currently installed and commissioned at BL 13-2 at SSRL, and fully equipped for experiments at synchrotron radiation sources. To accommodate LCLS experiments a number of minor modifications will be installed. Of particular importance is the integration of fast cameras with the electron spectrometer and x-ray emission spectrometer. Since both of these instruments have a similar detection system (MCP + phosphor plate and a camera mounted on the outside of vacuum), we intend to use the same solution for both spectrometers.
Dear SXR representative,

This letter describes the intention to install, operate and support two fully equipped endstations at the Soft X-ray for Material Science (SXR) beamline at LCLS. The endstations will comply with the requirements outlined in chapter 5 of the SXR Technical Design Report and be available for extended periods of time (months) per year at the SXR beamline for experiments conducted within the experimental group of Z. X. Shen and Zahid Hussain, by other SXR collaborators as well as by outside users via LCLS experiment proposals. The capabilities of these two endstations are described in the following:

**Resonant X-ray Scattering Endstation:**

The photos of the actual chamber are shown in the following figure. This endstation is in an ultra-high vacuum (UHV) environment capable of maintaining a base pressure better than $10^{-9}$ Torr. A UHV compatible sample loading/transfer system is installed for the solid state samples. A motorized sample stage allows the sample to be rotated azimuthally about its surface normal. This sample stage (also shown in the following figure) is thermally contacted to a temperature control system, which consists of a liquid Helium cryostat and a heater, allowing the sample temperature to change from 15 K to 400 K. The sample also has three translational degrees of freedom (through manipulator) and two rotational degrees of freedom (through differentially pumped rotary seal).

This endstation equips with three different types of detectors, including a channeltron, a photodiode, and a multi-channel-plate. These detectors are mounted inside the vacuum chamber on a fully motorized detector stage, which allows those detectors to move in both horizontal (360 degrees) & vertical (45 degrees) scattering planes. Such capability can be used to efficiently search the superlattice reflections in a wide range of reciprocal space. X-ray absorption (XAS) can also be performed by measuring the total fluorescent yield and total electron yield (sample-to-ground current).

This endstation has been assembled and utilized at the Advanced Light Source (ALS), Lawrence Berkeley National Laboratory, and fully equipped for experiments at synchrotron radiation sources. To accommodate LCLS experiments a number of modifications will be carried out. The modifications include the installation of in-vacuum fast parallel readout fast CCD camera for recording the image on pulse by pulse basis, a motorized six-strut system for remote chamber alignment and an additional 7 Tesla YBCO puck underneath the sample for field-dependence studies.
Resonant X-ray Inelastic Scattering Endstation:

An illustration of the chamber and a photo of the actual endstation are shown in the panel (a) of the following figure. This endstation is in an ultra-high vacuum (UHV) environment capable of maintaining a base pressure better than $5 \times 10^{-10}$ Torr. A UHV compatible sample transfer system is designed for the solid state samples. A motorized sample stage is designed to rotate the sample azimuthally about its surface normal. This sample stage is thermally contacted to a temperature control system, which consists of a liquid Helium cryostat and a heater, allowing the sample temperature to change from 15 K to 400 K.

The endstation will be equipped with an emission spectrograph with a maximum resolving power of 2200 (~1400 for a source image of 10 μm x 10 μm, the focus beam spot of SXR beamline). The emission spectrograph will be supported by a guide rail and can be mounted on five possible mounting ports with an angular interval of 30 degrees in the horizontal scattering plane. The rotary stage underneath the experimental chamber can rotate both the chamber and emission spectrograph by +/- 15 degrees with respect to the incoming x-ray beam. This design allows the users to probe a wide range of momentum transfer (for instance, see panel (b) of the following figure which is calculated at Mn L edge). The spectrograph is necessary for the time-resolved pump-probe inelastic scattering experiment, as it can record a spectrum across a range of energy loss simultaneously. This endstation is also equipped with a photodiode for measuring the total fluorescence yield. The sample stage is electrically isolated from ground such that the total electron yield can be recorded.

This endstation has been currently assembled and tested at the Advanced Light Source (ALS), Lawrence Berkeley National Laboratory, and fully equipped for experiments at synchrotron radiation sources. To accommodate LCLS experiments a number of modifications will be implemented. These include a shutter system, a motorized six-strut system for remote chamber alignment, and fast parallel readout fast CCD camera for recording the image on pulse by pulse basis.
Dear SXR representative,

This letter describes the intention to install, operate and support a fully equipped endstation for photon-ion and photon-electron coincidence measurements at the Soft X-ray (SXR) beamline at LCLS. The endstation will comply with the requirements outlined in chapter 5 of the SXR Technical Design Report and will be available for extended periods of time (months) per year at the SXR beamline for experiments conducted within the CFEL experimental group, by other SXR collaborators as well as by outside users via LCLS experiment proposals.

The endstation, outlined in the figure below, is designed to explore the interaction of intense soft x-ray radiation with various targets of increasing complexity and size, ranging from atoms and (laser-aligned) molecules to nano-particles such as clusters and biological targets, which can be injected by a supersonic atomic, molecular or cluster jet or a particle injector. The endstation is equipped with two large-area, single-photon counting pnCCD detectors, which collect scattered or fluorescent photons with an energy resolution of 40 to 200 eV between 100 eV and > 10 keV at a frame read-out rate up to 120 Hz. A variable-sized hole in the center of the first CCD allows the direct FEL beam (and a high-power pump laser, if applicable) to pass through the detector, while the small-angle scattering signal within the area of the hole can be detected on the second CCD. A specially-designed ion and electron spectrometer (“reaction microscope”) mounted perpendicular to the FEL beam direction detects ions and/or electrons created by the interaction of the intense soft x-rays with the sample with a large solid angle, and allows measuring their kinetic energies and emission directions. In order to account for different operation modes, the reaction microscope is equipped with a delay-line anode for single particle detection as well as a phosphor screen/CCD camera for applications where several hundred or thousand electrons or ions are created by each FEL pulse.

The unique combination of large-area, single-photon counting pnCCD detector and advanced reaction microscope thus allows, for the first time, fluorescence-photoion and/or fluorescence-photoelectron coincidence experiments on atoms, molecules, clusters, and nano-particles. Additionally, the endstation is fully equipped for coherent diffractive imaging experiments on biological and other targets beyond the radiation damage limits. Coulomb explosion and damage processes can hence be studied directly via the correlated measurement of the fragment ions as well as with respect to their influence on the diffraction patterns. The whole set-up is constructed highly modular and flexible: the entire reaction microscope can be easily removed, various gas-jet, droplet-jets, aerodynamic lenses as well as fixed targets or specific types of detection devices such as a Thomson parabola spectrometer for instance can be inserted in a straightforward manner.

The endstation is currently being designed at CFEL and will be tested at FLASH early next year prior to its use at LCLS, which is envisioned as early as mid-2009.

*side view (cut):*
Dear SXR representative,

this letter describes the long-term intention to install, operate and support a fully equipped endstation dedicated to the investigation of the interaction of light with dilute clouds of highly charged ions (HCI), trapped in an Electron Beam Ion Trap (EBIT). A significant fraction of this research is concerned with energies up to 2 keV and requires a monochromatized photon beam such that the Soft X-ray (SRX) beamline at LCLS is an ideal and presently the only suitable location. While experiments are anticipated to be performed initially with an existing machine which was already successfully operated at the FLASH the collaboration intents to apply for a dedicated LCLS-based user endstation available for a broad community. Its potential applications cover experiments in the fields of astrophysics, in the physics of plasmas, nuclei and to the tests of fundamental forces and symmetries. The envisioned definitive, dedicated endstation will comply with the requirements outlined in chapter 5 of the SRX Technical Design Report and will be available for extended periods of time (months) per year at the SRX beamline for experiments conducted within the CFEL experimental group, by other SRX collaborators as well as by outside users via LCLS experiment proposals.

The EBIT endstation, outlined in the figures below, is especially designed to explore the interaction of photons with highly charged ions in any desired charge state. Scientific goals include: The determination of photoionization and photoabsorption cross sections, both of utmost importance for astrophysics; the production, trapping and investigation of photoionized samples of strongly correlated warm, dense plasmas, this point representing one of the forefront topics of present plasma physics research; the direct photoexcitation of low-lying nuclear levels, which would imply a significant advance in nuclear physics. Finally, precision measurements on the electronic level structure of HCIs shall be performed to test fundamental theories (QED) and parity non-conservation in the neutral currents sector. The endstation consists of a fully operational EBIT. It is equipped with various spectrometers for visible, VUV, X-ray or fluorescence photon detection. Eight ports transverse to the photon beam propagation direction give access for intense lasers into the trap region as well as for injecting clusters, droplets or any other gaseous targets. One axial port permits ion extraction and charge analysis along the trap axis. The complete endstation needs about 2.5 x 1.5 m$^2$ floor space and weighs about 1.5 tons. It is further equipped with diagnostic tools to guarantee the overlap between the LCLS beam with the ion cloud and to measure the photon beam energy in a pulse-by-pulse mode.

The present transportable EBIT endstation operates routinely at FLASH as well as at the BESSY synchrotron. It is therefore ready to be transferred to the SRX beamline at any time in the year 2009. Provided that the LCLS management and Proposal Review Committee supports the general EBIT user endstation, the collaboration would start seeking money within 2008 in order to commission a new, dedicated user endstation by the year 2010.
Left: Cross section of the EBIT with the FEL beam entering into the trap region axially, through the electron beam dump along the magnetic field lines from the left. Fluorescence or any other radiation can be detected through either one of the eight transverse ports as indicated. Right: Picture of the EBIT during successful operation in a recent beamtime at FLASH.
Dear SXR representative,

This letter describes the intention to install, operate and support a fully equipped endstation at the Soft X-ray for Material Science (SXR) beamline at LCLS. The endstation will comply with the requirements outlined in chapter 5 of the SXR Technical Design Report and will be available for extended periods of time (months) per year at the SXR beamline for experiments conducted within the experimental collaboration between S. Techert (MPI for biophysical chemistry, Göttingen), A. Föhlisch (Institute for Experimental Physics, Hamburg University), F. Hennies (Max-Lab, Lund University), by other SXR collaborators, in particular A. Nilsson and K. Gaffney (Stanford University) and P. Wernet (Bessy, Berlin) as well as by outside users via LCLS experiment proposals.

The experimental station to study chemical dynamics in the liquid phase is based on a differentially pumped liquid jet system, developed at the MPI of biophysical chemistry. With a Rowland-type soft X-ray spectrometer (Grace 3) X-ray emission spectroscopy is conducted using three gratings, effectively covering the energy range between 50eV< hv < 1500 eV. Thus detailed investigations of the valence electronic structure and the chemical state for chemically and biologically relevant molecular dynamics are accessible both with resonant and non-resonant X-ray emission spectroscopy. In particular the local valence electronic structure of carbon, nitrogen and oxygen, as well as transition and rare earth metals can be investigated. Femtosecond temporal resolution to study photoinduced dynamics will be achieved in an optical-pump/X-ray-probe set-up, using the collinear optical incoupling and the tools for X-ray/optical cross-correlation developed at Hamburg University. Additionally, X-ray induced radiation chemistry can be investigated through femtosecond time resolved X-ray-pump/optical-probe spectroscopy.

The liquid beam set-up is shown below with schematic illustrations of prototypical chemical dynamics that will become accessible with this facility. This station will be thoroughly tested at the Free-Electron LASer at Hamburg FLASH and the X-ray spectrometer and associated diagnostics will be characterized at Max-Lab Sweden. In particular we will develop the hardware and software, which we currently employ at FLASH further and optimize for the operating conditions at LCLS.
Dear SXR representative,

This letter describes the intention to install, operate and support a fully equipped endstation at the Soft X-ray for Material Science (SXR) beamline at LCLS. The endstation will comply with the requirements outlined in chapter 5 of the SXR Technical Design Report and be available for extended periods of time (months) per year at the SXR beamline for experiments conducted within the experimental group of J. Stohr, by other SXR collaborators as well as by outside users via LCLS experiment proposals.

The endstation is in design for soft x-ray resonant single-shot imaging and small angle resonant scattering with focus on magnetization dynamics and phase transitions. The system will run under HV conditions (~10^{-8} Torr). The endstation will be designed to accommodate the two large-area, single-photon counting pnCCD detectors from the CFEL endstation, which collect scattered or fluorescent photons with an energy resolution of 40 to 200 eV between 100 eV and > 10 keV at a frame read-out rate up to 120 Hz. A variable-sized hole in the center of the first CCD allows the direct FEL beam (and a high-power pump laser, if applicable) to pass through the detector, while the small-angle scattering signal within the area of the hole can be detected on the second CCD. Optional an in-vacuum CCD with center beam stop for low fluence (monochromatic) experiments will be integrated.

Compatible to the design of the existing soft x-ray coherent imaging endstation at SSRL beamline 13-3, see figure below, the main chamber will have an Omniax manipulator with cryostat providing a temperature range of 30-400K. Removable pole pieces of an ex-situ electromagnet will provide magnetic fields (~1 Tesla) applied along the x-ray beam path. Sample transfer will be possible without breaking vacuum through a load lock chamber containing several sample holders.

The differential pump section between the beamline and endstation will be equipped with beam diagnostics, magnetic filter (for circular polarized x-rays) and fast beam shutter.

Figure: Existing endstation at SSRL beamline 13-3 for Coherent X-ray Imaging.