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Impact of a Vertically Polarized Undulator on LCLS Hard X-ray Experiments

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1 Introduction

The LCLS-II project will install two variable gap, horizontally polarized undulators into the LCLS undulator hall. One undulator is designed to produce soft x-rays spanning an energy range of 200-1250 eV (SXU) while the other is designed for the hard spectral range of 1-25 keV (HXU). The hard x-ray LCLS instruments (X-ray Pump-Probe [XPP], X-ray correlation Spectroscopy [XCS], Coherent X-ray Imaging [CXI], Matter in Extreme Conditions [MEC]) will be repurposed to operate on the HXU line while two new soft x-ray beamlines will be created for the SXU line.

An alternate HXU undulator design is being considered that could provide advantages over the present design choice. In particular, the project team is collaborating with Argonne National Laboratory to develop a vertically polarized undulator (VPU). A 1-m prototype VPU device was successfully constructed this year and a full size prototype is in process. A decision to alter the project baseline, which is the construction of a horizontally polarized device, must be made in the coming weeks to not impact the present project schedule. Please note that a change to the soft x-ray undulator is not under discussion at the moment.

The rotation of the hard x-ray polarization to a vertical orientation impacts the performance of certain LCLS x-ray optics as well as the signal-to-background level for some experiments. In addition, there are sample environment impacts due to the preferential geometries of particular experimental setups. These considerations will be analyzed in this document following sections.

2 X-ray Optics Considerations

The hard x-ray optics used at the LCLS can be categorized into four types: mirrors, refractive lenses, channel-cut monochromators (CCM), large offset double crystal monochromators (LODCM) and hard x-ray self seeding (HXRSS) monochromator.

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2.1 Mirrors [XPP, XCS, CXI, MEC]

X-ray mirrors are widely used on the HXU line to distribute the beam to the instruments, focus the beam (CXI), and reject harmonic radiation (XPP, XCS, MEC). X-ray mirrors operate under the principle of total external reflection. In this regime, the reflectance of s-polarized light is the same as for p-polarized light. As such, the polarization choice of the HXU undulator has negligible impact on the performance of mirror optics.

2.2 Refractive Lenses [XPP, XCS, CXI, MEC]

Compound refractive lenses are used on all hard x-ray instruments at LCLS to focus the beam. These systems use the slight change in the x-ray index of refraction in a medium to impart a phase shift across the wavefront [1]. By placing many parabolic-shaped lenses in series, focal lengths of a few meters [micron scale spot sizes] are readily achieved with good transmission efficiency.

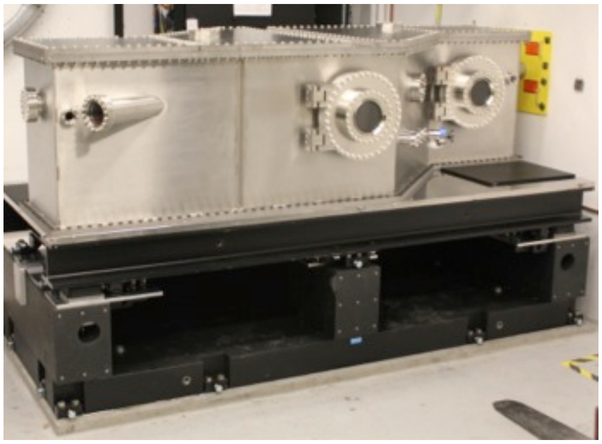
2.3 Channel-cut Monochromators [XPP, XCS]

The XPP and XCS instruments use artificial channel-cut monochromators. The CCM systems are based on a design developed at the Advanced Photon Source [2]. These systems are capable of very high precision motion and are proven to be stable and reliable in LCLS operation. Presently, the CCM systems operate in a vertical diffraction geometry to avoid polarization loses with the present horizontally polarized beam. However, these systems are designed with the option of rotating their orientation to diffract in the horizontal plane. As such, a change in polarization with the implementation of a VPU undulator will not impact the performance of the CCM systems.

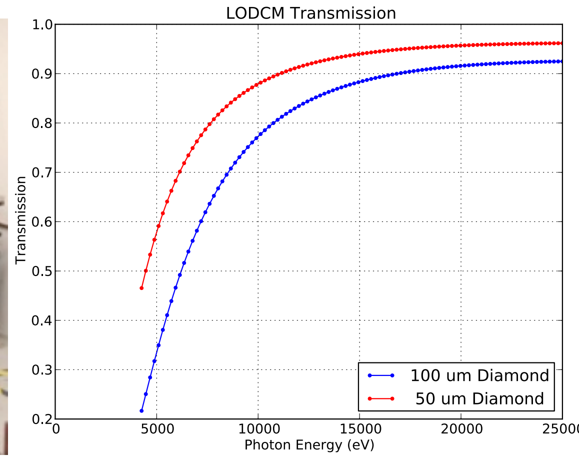
2.4 Large Offset Monochromators [XPP, XCS]

Large offset double crystal monochromators are installed on the XPP and XCS instruments (see Figure 1a). These devices are used to create monochromatic beamline branches that are horizontally displaced from the direct LCLS beam by 600 mm. These systems use symmetric Bragg reflections from perfect single diamond and silicon crystals, and can accommodate scattering angles ($2\theta_B$), where θ_B is the Bragg angle, between 9^o and 90^o. An image of the XPP LODCM is shown in Figure 1a.

Recently, thin (111) oriented diamond crystals ($100\,\mu$m) were developed and installed in the XPP LODCM (see Ref. [3]). These crystals efficiently reflect a monochromatic slice of the LCLS beam while while transmitting the majority of the remaining FEL spectrum that falls outside of the narrow energy acceptance window of the Bragg reflection. The transmitted photons can then be used to perform a second experiment simultaneous with monochromatic XPP operation. Beam sharing in this manner has



(a)



(b)

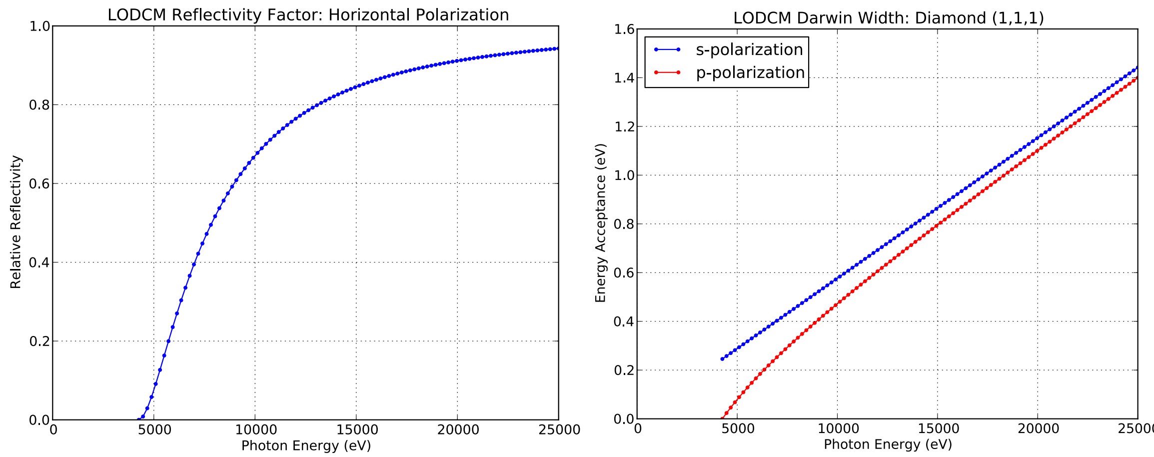
Figure 1: (a) Image of the XPP large offset double crystal monochromator. (b) LODCM transmission as a function of photon energy for a 50 and 100 micron diamond crystal in the (111) orientation.

led to a 20% increase in user beamtime at LCLS and is expected to increase the experiment capacity even more in the future. There is an ongoing effort to further reduce the thickness of the diamond crystal to 50 μm, which would transmit greater than $\sim 60\%$ of the LCLS beam above 5 keV. The transmission of the LODCM thin diamond crystal (50 μm and 100 μm), when angled to meet the Bragg condition, as a function of photon energy is displayed in Figure 1b.

There are significant polarization losses experienced with current LODCM operation conditions. The horizontal polarization of the LCLS beam represents a p-polarization with the LODCM diffraction geometry. From perfect crystal diffraction theory, a $cos\, 2\theta_B$ polarization factor loss is experienced for each crystal reflection and thus there is a total factor of $cos^2\, 2\theta_B$. Figure 2a displays this relative reflectivity of a p-polarized beam with respect to an s-polarized beam.

In addition to the polarization factor reduction, the total throughput of the monochromatic beamline is affected by the narrowed energy acceptance of the Bragg reflection for p-polarized x-rays with respect to s-polarized. This reduction in energy acceptance is proportional to $cos^2\, 2\theta_B$. The energy acceptance of a diamond (111) reflection is plotted in Figure 2b for both polarization states.

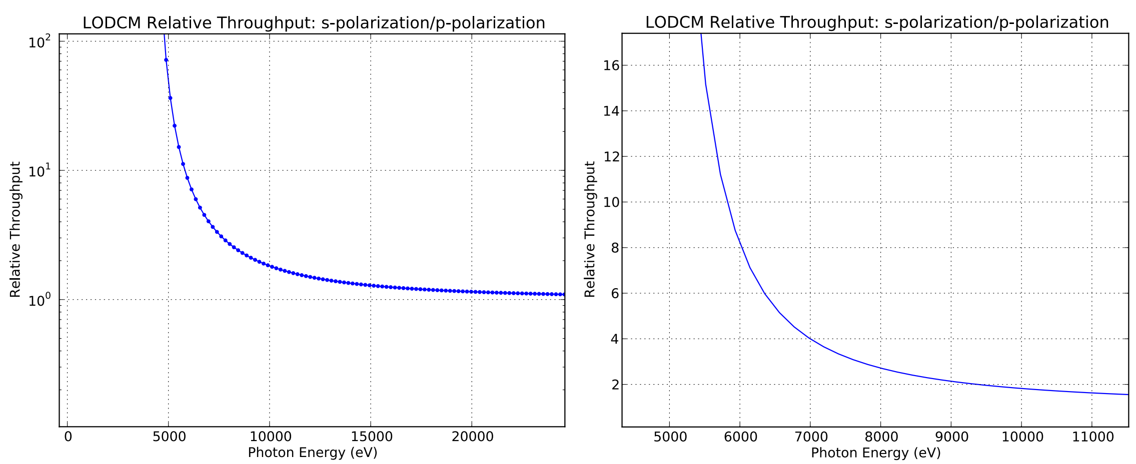
The total relative throughput enhancement realized with a vertically polarized beam, normalized to the horizontally polarized beam, for the LODCM monochromatic branches is displayed in Figure 3. These calculations include both the reflectivity loss as well as



(a) (b)

Figure 2: (a) LODCM polarization loss factor for horizontal polarization (p-polarization). (b) Energy Darwin width of diamond (111) for s and p polarization.

the narrowing of the energy acceptance of the Bragg reflection. Diamond (111) Bragg reflectors are assumed since this is the configuration used for the beam sharing operating mode, which is expected to be the dominant operating mode. As can be seen in the graphs, the throughput gain is significant and becomes very significant at photon energies below 7 keV (50x at 5 keV, 8x at 6 keV, 4x at 7 keV).



(a) (b)

Figure 3: (a) LODCM throughput gain with vertical polarization (s-polarization) as a function of photon energy. (b) Expanded view of (a) in linear scale.

2.5 Hard X-ray Self-Seeding Monochromator

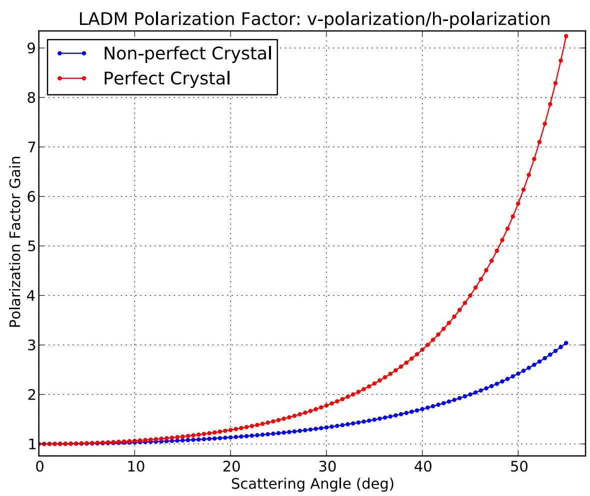
A hard x-ray self seeding technique proposed by Geloni, Kocharyanb and Saldin [4] was implemented successfully at the LCLS in 2012 [5]. This scheme uses a diamond crystal monochromator in Bragg-transmission geometry for seed pulse generation. This monochromator diffracts in the vertical plane to optimize the amplitude of the seed pulse with the present polarization state of the beam. This monochromator must be rotated to accommodate a VPU device. This monochromator can be rotated with relatively minor changes to the mechanical design.

3 Instrument Specific Considerations

3.1 XCS Large Angle Detector Mover

The XCS instrument uses an 8 meter detector arm to position an x-ray area detector, which is used to resolve speckle patterns created from coherent illumination of inhomogeneous samples. The large angle detector mover (LADM) operates in the horizontal plane and covers a scattering angle range between 0^{o} and 55^{o}. Polarization losses are experienced with the present horizontal polarization of the existing LCLS undulator when measuring coherent scattering patterns. The losses are proportional to $cos\,2\theta$ and $cos^2\,2\theta$, where 2θ is the scattering angle, for perfect and non-perfect crystals (i.e. all other samples) respectively. An image of the LADM and a plot of the vertical polarization gain factor, for both perfect and non-perfect crystals, are shown in Figure 4. As can be deduced from the graph, a VPU device provides a significant benefit to the XCS instrument where the vast majority of samples study do not fall into the perfect crystal category.

(a)



(b)

Figure 4: (a) Image of the XCS large angle detector mover. (b) Vertical polarization scattering factor increase of the XCS large angle detector mover for a perfect and non-perfect crystal.

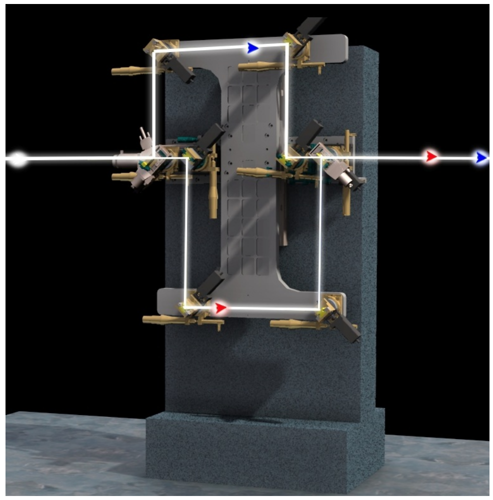


Figure 5: Schematic drawing of DESY hard x-ray split and delay system presently installed on the XCS beamline (see Ref. [6]).

3.2 XCS Split and Delay System

A hard x-ray split and delay device is presently installed on the XCS instrument. This device was designed and constructed at DESY and operates at fixed energy using 90^o crystal reflections (see Ref. [6] for details). A thin silicon Bragg reflector is used to divide the amplitude of the FEL beam into two beamline branches. Each branch goes through 3 successive 90^o reflections before the pulses are combined with a second thin silicon reflector. The time delay between the two pulses is achieved by varying the optical path length of the beamline branches. A 0 to 3 ns temporal range is achieved with this device, permitting ultrafast x-ray photon correlation spectroscopy (XPCS) studies in this time regime. A design image of the split and delay device is shown in Figure 5.

The present split and delay device is challenging to align and operate, which has impeded achievement of the science objectives. The overall mechanical stability of the device, as well as the use of high order reflections, has played a role in the experienced operational difficulties. A design that uses lower order reflections, which improves the bandwidth and eases the angular tolerances, is under consideration. However, such a design would deviate from the 90^o scattering geometry and potential significantly increase the device footprint. Constructing such a device with the required mechanical stability is a formidable challenge. This challenge is compounded by the need to operate in a vertical scattering plane to avoid polarization losses in the many crystal reflections. A vertically polarized beam would permit this entire device to operate in the horizontal plane, greatly reducing the mechanical difficulty to realize such a device. It is thus highly beneficial to the goal of performing ultrafast XPCS studies at LCLS to move to a VPU.

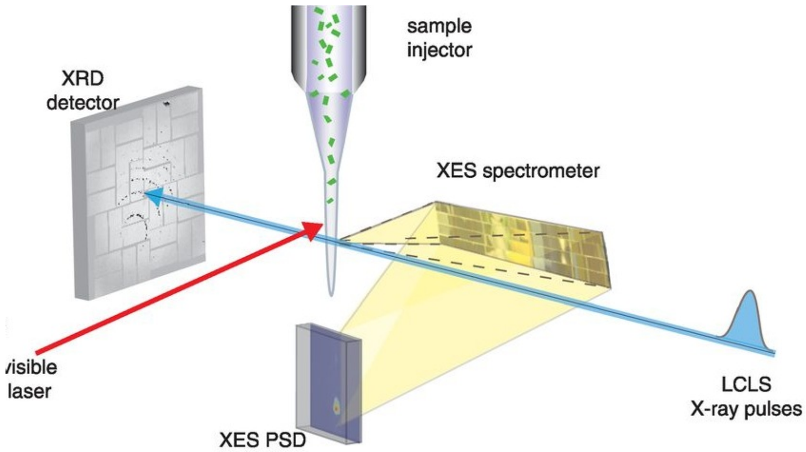


Figure 6: Schematic drawing of a simultaneous nanocrystal diffraction and emission spectroscopy measurement. Adapted from Ref. [7]

3.3 Emission Spectrometers

X-ray emission spectroscopy is a powerful tool for probing the element specific electronic states of atoms and molecules. Typically, energy dispersive x-ray spectrometers are used to isolate the emission line of interest with sufficient energy resolution to measure subtle spectral changes. X-ray emission is not directional and is emitted equally in the entire 4π solid angle. Due to the non-directionality and relatively low emission cross-section on dilute samples, sources of background noise must be carefully considered and in particular elastic scattering. Elastic scattering can emanate from the sample, gas surrounding the sample, windows, or anything else that is in the beam. This radiation can then be elastically scattered from the dispersive optic of the emission spectrometer (crystal or grating). A portion of this radiation will be redirected to the x-ray area detector, increasing the background level of the measurement. In order to minimize the elastic background, emission spectrometer optics are placed along the direction of polarization to the extent possible. For current LCLS experiments, emission spectrometers are placed perpendicular to the x-ray beam trajectory in the horizontal plane.

A hard x-ray emission spectrometer was constructed for use at LCLS and SSRL(see Ref. [8] for more details). This system functions in the von Hamos configuration, has a relatively large collection solid angle, and was successfully used to measure time-resolved emission spectra on the XPP and CXI instruments . The placement of these spectrometers must be rotated 90^o about the beam propagation direction to maintain present performance levels. This configuration rotation is likely accommodated in the in-air experimental configurations but presents complications for the in-vacuum nanocrystallography setup in the CXI instrument. This complication stems from the physical dimensions of the CXI sample vacuum chamber as well as the orientation of

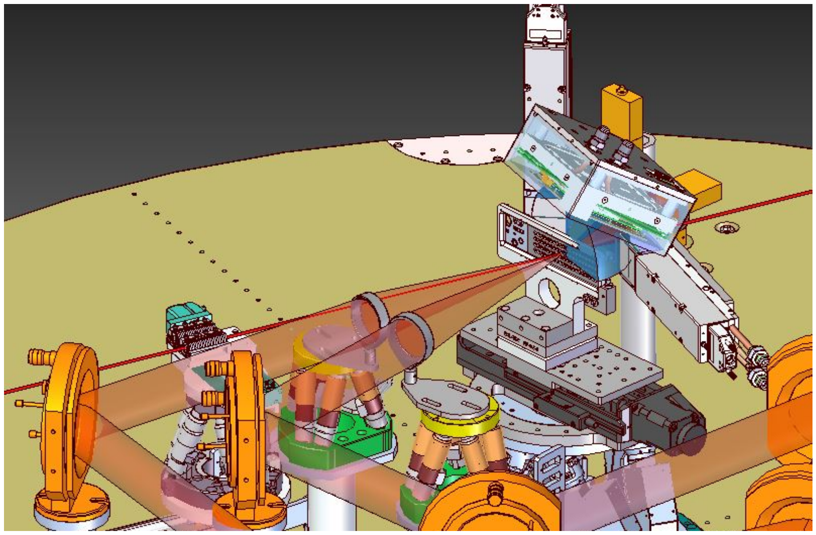


Figure 7: Design model of the MEC target chamber.

sample injector instrumentation, currently oriented in the vertical plane. A schematic of the current setup for simultaneous diffraction and emission spectroscopy is shown in Figure 6. A new CXI sample chamber must be constructed if the FEL polarization is changed to a vertical orientation to both minimize the XES background levels and to accommodate sample injector instrumentation. However, it must me noted that a feasible design has yet to be completed.

3.4 MEC Target Chamber

The Matter in Extreme Conditions instrument uses high power and high energy optical laser to generate extreme pressure and temperature states of matter. The present layout of the MEC target chamber constrains the optical path of these lasers to a horizontal plane at the same height as the LCLS FEL beam. A schematic model of a typical MEC experimental setup is shown in Figure 7. For diffraction and scattering measurements, x-ray detectors are placed in the vertical plane to avoid polarization losses. This geometry also has the advantage of avoiding interferences with the laser optics since the detector is placed above these components. The switch to a VPU would change the preference of the x-ray detector location to the horizontal plane, causing potential interferences with the laser optomechanics. The path of the optical lasers are generally biased towards one side of the target chamber and in many cases the other side of the setup is available to mount detectors in the horizontal plane without interference. However, this is not universally the case and in such instances the detector must be placed above the optomechanics resulting in some polarization losses (25% loss for 30^o angle).

4 X-ray Waveplates

An alternate approach to creating a vertically polarized beam is to use x-ray phase retarders rather than altering the undulator source [9]. X-ray phase retarders use diffraction from perfect crystals oriented with a Bragg diffraction plane rotated $45^{\,o}$ from the horizontal axis. A relative phase shift between the s and p polarization components over a narrow bandwidth of the transmitted x-ray beam is realized when the crystal optic is detuned slightly off the Bragg condition. Diamond based phase retarders have been widely used at synchrotron hard x-ray beamlines[10, 11, 12]. They were recently employed at the SACLA FEL to control the x-ray polarization, and this represents the first demonstration of such capability at a hard x-ray FEL [13]. While this demonstration shows that FEL polarization control can be realized with x-ray phase retarders, the practicality of using such a device in routine operations must be considered. In particular, the thickness and reflection plane used for the phase retarders must be tuned to cover the full spectral range of interest. The SACLA device was designed with 3 separate diamond crystals (0.1 mm, 0.5 mm and 1.5 mm thickness) to span a 5-20 keV energy range. The x-ray transmission through these crystals varies as a function of photon energy but is calculated to be 50-80% over the designed energy range. In addition, the degree of vertical polarization achieved in the SACLA demonstrated was estimated to be 67% and thus full polarization rotation was not achieved. In principle, a simliar sequence of phase retarding crystals could be used upbeam of the LODCM to rotate the polarization over a bandwidth matched to that of the LODCM. In this scenario one might ideally achieve only ∼50% to ∼70% of the benefit indicated in Fig. 3 (i.e. ∼25x at 5 keV and 2.8x at 7 keV). X-ray phase retarders are mosed effective at higher photon energies, where there is diminishing enhancement in the LODCM throughput from vertical polarization. Conversely, x-ray phase retarders are much less effective near 5 keV, where there is significant benefit in the LODCM throughput from vertical polarization (see Fig. 3). Thus, a VPU source is preferred, particularly for lower photon energies.

5 Summary

The polarization of the LCLS hard x-ray beam strongly influences the performance of the large offset monocrhomator systems and scattering measurements made on the XCS large angle detector mover. A strong performance enhancement is realized with a vertically polarized beam for these systems. In addition a vertically polarized beam offers opportunities to construct a functional variable energy split and delay device. However, the installation of a VPU on the LCLS hard x-ray line would necessitate changes in the orientation of instrumentation used for emission spectroscopy and scattering measurements in the MEC target chamber. There are potential mechanical interferences with the present day setups that require careful consideration and study. In summary, the benefits of a vertically polarized beam are clear and the drawbacks appear to have tractable solutions. A VPU device is the preferred source for the LCLS hard x-ray line.

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