Physics Requirements for the XTOD/XES K-Measurement Monochromator System

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Brief Summary: This document provides general physics requirements for the XTOD/XES K-Measurement Monochromator System (K-Mono), a stable, narrow-band, high-transmission x-ray photon-energy filter and detector, which is one component required in a scheme for in situ alignment of the LCLS Undulator segments.

Change History Log

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<th>Rev Number</th>
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<td>000</td>
<td>2007/5/4</td>
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<td>Major revision for better focus on requirements, independent of concept. Addition of beam-center-finding function.</td>
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1. Introduction

The XTOD/XES K-Measurement Monochromator System (K-Mono) is one component required in a scheme for in situ alignment of the LCLS Undulator segments. This document details the requirements for that instrument.

1.1. Undulator Segment In Situ Alignment

To function as an effective, high-gain FEL radiation source, the 33 segments of the LCLS Undulator must properly operate together, over the entire ~ 130 m undulator length. An important parameter characterizing the electron motion within an undulator is the deflection parameter, K. All segments must have identical K, within a relative error of 0.015% rms [1], to assure the desired LCLS Undulator performance.

The primary plan to accomplish this alignment relies on precise, laboratory magnetic measurements made on each undulator segment, together with the degrees-of-freedom incorporated in the undulator segment mover structure. That is, for a given desired K, previously-recorded magnetic measurements determine the desired position for each segment relative to the predicted path of the electron beam. However, in addition to this primary plan, a backup plan was thought desirable. Rather than rely entirely on magnetic measurements, this plan would match the K of each undulator segment with every other on the basis of its emitted spectrum of photons. This emitted spectrum of photons from an undulator, a sharp fundamental peak and a series of higher-photon-energy harmonic peaks, is determined primarily by K, together with the electron beam energy and undulator magnetic period length. Therefore, quantitative measurements of the emitted photon spectrum can be related back to K.

Following considerable work at several laboratories, and the LCLS Beam Based Undulator K Measurement Workshop, of November 14, 2005, a detailed, in situ scheme was developed to achieve a precise, common K-parameter all along the LCLS Undulator, based on measurements of spontaneous undulator radiation. It is described in a paper by Jim Welch et al, in the proceedings of FEL 2006 [2], hereafter referred to simply as "the paper [2]". In addition to providing a conceptual and theoretical description of the approach, it also provides a detailed simulation, which demonstrates the feasibility of the approach, while tabulating the sources and magnitudes of uncertainties which influence the results. Many of the requirements for the K-Mono derive directly from the parameters and uncertainties described in the paper [2]. Although several instruments within the LCLS accelerator complex must be utilized together to execute the scheme, the K-Mono is a key component, a narrow-band photon-energy filter (a monochromator) and detector system.
1.2. The General Procedure

In general, the scheme from the paper [2] requires precise measurement of a specific spectral feature from the combined spontaneous radiation of two adjacent or near-adjacent undulator segments (the other 31 segments are withdrawn from the electron beam path for the measurement). This feature (illustrated in Figure 1, below) is denoted as the High-Photon-Energy Edge of the Fundamental peak, the "HPEEF".

![Single Undulator Spontaneous Spectrum: 0.2 nC Charge, (17.5 urad)^2 Aperture](image)

Figure 1: A pair of vertical lines marks the "HPEEF", i.e. the spectral region containing the High-Photon-Energy Edge of the Fundamental. The lines are separated by 1 eV, the approximate band pass of the K-Mono. Electron energy = 13.6 GeV.

The extreme value of the slope in the HPEEF is a strong function of the "matching" between the two undulator segments. If the two segments are tuned to produce precisely the same fundamental photon energy, they are "matched", and the steepest extreme slope is produced. Using one segment from the initial pair as a new reference, a third segment can be matched to the first pair, and so forth, until all 33 segments are matched.
Multiple pulses of spontaneous radiation will be used to make precise measurements of the HPEEF, as illustrated in Figure 2 above. For each HPEEF curve, the $K$-parameter for each of the two undulator segments is fixed. For each Linac pulse, the $K$-Mono, located in the Front End Enclosure (FEE), will measure the spontaneous radiation photon pulse intensity falling within its photon energy transmission bandwidth. By systematically varying the Linac electron beam kinetic energy, and utilizing the inherent Linac electron beam energy jitter, the HPEEF can be sampled through the transmission window of the $K$-Mono, to permit the entire spectral region to be traced-out. Although the electron beam energy and beam charge for each Linac pulse cannot be controlled precisely, and will vary considerably from shot-to-shot, the Linac electron diagnostics should allow these characteristics to be quantified on each shot, to a precision better than the general variation. Therefore the HPEEF can be reconstructed when the $K$-Mono intensity data is properly normalized and binned. This is illustrated in Figure 2, by the way the plotted points continue to follow the ideal, solid-line curves.
The series of HPEEF curves illustrated in Figure 2 will be acquired by making small step changes in the $K$-parameter for one of the undulator segments. Each curve is associated with a different step. Once a series of HPEEF curves has been acquired, the extreme slope associated with each can be calculated. This is illustrated using the curves from Figure 2, in Figure 3 below [2]. The best matching of the two undulator segments is obtained by the tuning that produces the slope at the bottom of the best-fit parabola. Note that a $K$-parameter mismatch of 0.1% between segments produces an extreme slope change of over 3%.

\[ \Delta K/K = -0.003\pm0.004\% \]

Figure 3: The blue points are extreme slope values calculated for the 9 HPEEF curves illustrated in Figure 2, as a function of $K$-parameter variation for one segment [2]. The simulated data points are used for the calculations. The red curve is a best-fit parabola. The additional scale on the right indicates the average slope change resulting from the four step increments in $K$-parameter. Note that a $K$-parameter change of 0.1% results in an extreme slope change of over 3%.
1.3. Details and the K-Mono

1.3.1. General
The K-Mono, with its monochromator and detector, requires a high-stability monochromator transmission function and constant central photon energy. The monochromator angular acceptance must be properly matched to the LCLS undulator source, with high transmission/detection efficiency, to enable precise photon pulse intensity measurements. Overall, it should achieve high signal/noise and good photon statistics.

The K-Mono will be located at an LCLS coordinate position of ~ 734.5 m, about 87.5 m from the downstream end of the undulator. This is downstream of the XTOD Fixed Mask, X-Ray Slit, and Attenuator, and upstream of both the Total Energy Measurement System and the Direct Imager. As such, the X-Ray Slit and Attenuator can be used with the K-Mono, if desired. The Direct Imager will be used with the K-Mono, to affect beam alignment, as described further in Section 1.3.1.3.1 below.

1.3.1.1. The Monochromator
In the fundamental photon energy range of the LCLS, between 830 eV and 8.3 keV, the experience of synchrotron radiation user facilities suggests that requirements such as those in 1.3.1 are best met with a monochromator using silicon perfect-crystals in Bragg diffraction, at the LCLS hard x-ray setting, 8.3 keV. This choice permits the monochromatic output beam to be positioned and directed as an extension of the incident beam, that is, the output beam follows the same path that would be taken by the incident beam if the K-Mono monochromator were withdrawn. This facilitates K-Mono alignment. Such an arrangement also permits incorporation of an incident beam stop, which can significantly improve signal/noise.

1.3.1.2. The Detector
Initial requirements for the K-Mono detector stem from the assumptions made in the paper [2]. It should respond linearly to the magnitude of the incident photon pulse, for intensities between approximately $10^6$ photons/pulse to $10^4$ photons/pulse, subject only to fluctuations due to photon statistics and an assumed detector subsystem noise level. The photon statistics fluctuation is assumed to be proportional to the square root of the number of photons per pulse [2]. The detector subsystem noise level is assumed to be equivalent to 100 photons/pulse [2].

1.3.1.3. The Measurement Procedure
For the K-Mono, the K-measurement procedure involves two major steps, alignment, and data taking.
1.3.1.3.1. Alignment

For alignment, the monochromator section of the K-Mono is inserted into the spontaneous radiation beam, but the K-Mono detector section remains withdrawn from the beam, so that the monochromatic beam is passed downstream. The Direct Imager is also inserted into the beam path, downstream of the K-Mono. A far, upstream single segment of the LCLS undulator is inserted into the electron beam path (it produces the maximum transverse beam size at the K-Mono position) and the electron beam energy of the LCLS Linac is adjusted to place the HPEEF into the photon energy band pass of the monochromator. An image of the monochromatic beam should be visible on the Direct Imager, if the monochromator alignment is near optimum. Remote alignment adjustments of the monochromator are then made to obtain/optimize the monochromatic beam image. At the same time, the centering of the beam on the monochromator crystals is noted from the image. If the beam is properly centered on the crystals, the Direct Imager may be withdrawn and the K-Mono detector inserted. Careful intensity optimization is now performed using the same remote alignment adjustments of the monochromator, to complete the alignment procedure.

1.3.1.3.2. Data Taking

For data taking, both the K-Mono monochromator and detector sections remain inserted into the spontaneous radiation beam. Now the precise measurements of the HPEEF are to be performed. The HPEEF is illustrated in Figure 2 for the LCLS hard x-ray setting (8.3 keV), with two undulator segments installed. As can be seen, it has a width of approximately 40 eV [2]. A monochromator utilizing Bragg diffraction and low-index planes in silicon will produce a photon energy band pass of ~ 1 eV at 8.3 keV. The two vertical lines shown in Figure 1 are separated by 1 eV, to illustrate this band pass. The vertical scale of the same figure indicates that several x 10^5 photons should be available within this band pass per Linac pulse. The pulse-to-pulse electron beam energy jitter from the LCLS Linac shifts the fundamental photon energy from the undulator segments by an rms value of about 17 eV from shot-to-shot, but the Linac diagnostics can quantify the shift within approximately 0.5 eV [2]. At the same time, the bunch charge jitter is expected to be approximately 2%, but can be quantified within 0.5% [2]. Approximately 100 Linac pulses will be needed to measure the HPEEF once. This measurement should require approximately 10 seconds, at a Linac repetition rate of 10 Hz. For each pair of undulator segments, this measurement will be repeated an additional eight times, with different tuning settings for one of the segments on each repeated measurement. Altogether, these measurements for a single segment pair should require about 4 minutes, including the tuning time [2]. Finally, all 33 undulator segments must be involved in a tuning "session" at least once. Therefore, the entire procedure should require something
over two hours to complete for all undulator segments. In addition to the data measurements, periodic checks/adjustment of the monochromator intensity optimization (Section 1.3.1.3.1) should probably also be made.

1.3.2. Spatial/Angular Acceptance

1.3.2.1. The Source Distribution

The spatial/angular distribution of radiation from a single LCLS undulator segment, or a pair of segments, drives significant requirements for the K-Mono. To obtain reliable data of the HPEEF, a minimum angular-acceptance is required of the K-Mono. B. X. Yang noted that the HPEEF region becomes "stable" for an angular integration exceeding approximately 25 µrad, about the on-axis emitted radiation [4], as can be seen in Figure 4, below. For smaller integration values, the peak amplitude is a function of the integration range. For integration values of 30 µrad, 35 µrad, and 160 µrad, the entire HPEEF region is unchanging.

![Figure 4: Single-undulator-segment spectrum in the HPEEF region, as observed through an on-axis square aperture of varying angular size. The HPEEF region becomes "stable" for an angular integration above approximately 20 µrad to 30 µrad [4]. This figure is copied from Reference 4.](image)

The radial intensity distribution of emitted photons changes significantly through the HPEEF region. This is illustrated in Figure 5. An HPEEF spectrum (e.g. Figure 4, and the left-hand panel in Figure 5) is obtained by integrating over a spatial region. However, if the transverse spatial intensity is viewed, it is anything but uniform.
Within the HPEEF, the distributions always exhibit strong cylindrical symmetry, but the radial intensity distributions only peak on-axis for photon energies corresponding to the lower integrated intensities. Near the peak of the HPEEF spectrum, the radial intensity distributions resemble "doughnuts", with their maximum intensities occurring significantly off-axis.

![Single Undulator Spontaneous Spectrum](image1)

![Radial Intensity Distribution](image2)

**Figure 5**: The radial intensity distribution of emitted photons changes significantly through the HPEEF region. The left-hand panel illustrates the spectrum of the HPEEF region, with photon-energy-marking points at the intensity peak, 85% peak, 50% peak, and 15% peak. The right-hand panel illustrates the radial intensity distributions at the same 4 photon energies. The distributions always exhibit strong cylindrical symmetry, but resemble "doughnuts" for the higher-intensity photon energies, and "normal", center-maximum distributions only for the lower-intensity photon energies. The right-hand panel also corroborates that the HPEEF region is "stable" for a total angular acceptance greater than ~ 25 µrad; in this spectral region, there is little radial emission outside that angular range.

An angular limit for emitted photons from the upstream segments of the LCLS undulator is set by the undulator vacuum beam tube, whose effective maximum dimensions are 5 mmV and 8 mmH. The entire undulator is approximately 131.6 m long. Therefore, the maximum angular beam width obtainable from the most-upstream undulator segment will be approximately 38 µrad vertical and 61 µrad horizontal.
1.3.2.2. The K-Mono Acceptance

From the source description developed above, the intrinsic angular acceptance of the Bragg diffraction crystals in the K-Mono should exceed 25 µrad. (Note that a symmetric Si(111) reflection at 8.3 keV has an intrinsic angular acceptance of ~ 32 µrad.)

In addition, the physical dimensions of the K-Mono crystals must be sized large enough to accept the worst-case transverse beam size, i.e. that from the most-upstream undulator segment. That is, 25 µrad*(131.6 m + 87.5 m) = 5.5 mm. However, there will be some advantage to sizing the K-Mono crystals even larger than this. If they were sized large enough to accept slightly more than 38 µrad vertical from the most-upstream undulator segment, the vertical-defining edges of the undulator beam tube could be located using the Direct Imager to view the photon output from the K-Mono. Once the center position between the limiting vertical edges has been located, all subsequent segment-pair measurements can have their photon beams steered to this same, central position. That would require > 38 µrad*(131.6 m + 87.5 m) > 8.3 mm. Taking all of this into account, the physical acceptance of the K-Mono crystals should be at least 9 mmV x 9 mmH.

Some characteristics for the K-Mono detector subsystem also follow from this. The detector transverse dimensions should exceed the horizontal and vertical acceptance dimensions of the K-Mono monochromator crystals. In addition, the detector should have good uniformity over its entire sensitive area, as a result of the substantial variation in the radial intensity profile expected from the HPEEF photon distribution.

1.3.3. Stability/Drift

As the HPEEF photon flux spectrum is acquired point-by-point, each point is subject to uncertainties both in intensity and photon energy, which stem from a variety of sources [2], some of which were mentioned in Section 1.3.1.3.2 above. Most of these are shot-to-shot fluctuations, inherent in the LCLS accelerator complex, but the K-Mono monochromator and photon detector will also make contributions to pulse-intensity and photon-energy uncertainties (generally on longer timescales), which should be limited and quantified. The drift components can be categorized as Transmission Drift and Photon Energy Drift.

1.3.3.1. Transmission Drift

The transmission of the K-Mono contributes to the pulse-intensity uncertainty. "Transmission" may include the reflectivity of the Bragg reflections used in the monochromator, the mutual alignment of the diffraction crystals, the alignment of the entire monochromator to the incident beam direction, and the performance of the K-Mono photon detector. Relevant performance aspects of the photon detector subsystem include its uniformity of spatial response, the uncertainty from photon
statistics, the subsystem noise, and the subsystem gain stability. Overall, then, the transmission is "photons detected/photons incident". The variation of transmission with time is the Transmission Drift.

According to the paper [2], the shot-to-shot intensity uncertainty tends to be dominated by the pulse-charge-measurement resolution, 0.5%, except when the number of photons per pulse is considerably less than $10^5$, in which case photon statistics and detector noise may also become significant. The $K$-Mono mechanical design must assure that the monochromator does not suffer instabilities on a millisecond timescale. However, longer timescales are also relevant, namely those involved in the $K$-measurement scheme.

From Figure 3 (the variation of extreme slope in the HPEEF as a function of one undulator segment $K$-parameter), the five data points located near the bottom of the parabolic fit only differ by a few percent. This suggests that a $K$-Mono transmission drift of a few percent during this data acquisition could be sufficient to scramble the data over several segment tuning steps in the proposed procedure.

The time required to collect the nine HPEEF curves for a pair of undulator segments is approximately 4 minutes [2]. A transmission drift of $\sim 1\%$ over this period of time could be detrimental. However, this level of drift may be acceptable over a period of approximately 10 times that, i.e. 40 minutes, over which time it is unlikely to disrupt the matching of any two undulator segments.

Requiring a transmission drift of $< 1\%$ over 40 minutes has implications for $K$-Mono monochromator crystal alignment stability and gain stability in the detector subsystem.

1.3.3.2. Photon-Energy Drift

Ideally, the $K$-Mono should have a constant central photon energy. Variation in the central photon energy is denoted as Photon-Energy Drift. A permissible variation is estimated as follows: From Figure 2, each tuning step of one undulator segment ($0.05\% \Delta K/K$ [2]) produces a photon energy shift in the HPEEF spectra of approximately 3.5 eV. Recall that each curve requires approximately 10 seconds to acquire. Therefore, a photon energy drift of about 3.5 eV in 10 seconds is likely to render the acquired data unusable, by seriously distorting the HPEEF region from which the extreme slope would be obtained. Over a 4-minute period, however, the time required to obtain the nine HPEEF spectra, a continuous photon-energy drift of this magnitude may be acceptable, since the distortion to a single curve should be small. That is, the distortion due to $K$-Mono photon-energy drift over the collection time for nine spectra should be limited to the photon energy separation of adjacent spectra, $\sim 4$ eV over 4 minutes.
1.3.4. Operational Modes

The K-Mono requires a "fully-open" mode and an "in-operation" mode. When "fully-open", the K-Mono monochromator, beam stop, and detector are fully withdrawn, and the "stay-clear" aperture, defined by projection from the XTOD Fixed Mask, is preserved.

When "in-operation", the K-Mono components can be inserted into the beam. As mentioned in Section 1.3.1.3.1, the monochromator and its beam stop should be separately insertable from the detector, to enable monochromator alignment using the Direct Imager. Therefore, while insertion of the K-Mono monochromator and beam stop could be either a manual operation or a remotely-controlled operation, the insertion of the detector must be remotely-controlled.

1.3.5. Beam-Center-Finding Function

When first attempts are made to produce FEL radiation at the LCLS, at the soft x-ray setting, ~830 eV, it may be desirable to accurately locate the axis of the undulator photon emission cone within the FEE. One method of doing this is by producing a monochromatized beam in the K-Mono monochromator at the high photon energy edge of the ninth harmonic of the soft x-ray setting and viewing that beam with the Direct Imager. The K-Mono design should accommodate this measurement.

As indicated in Section 1.3.2.1, the spatial distribution of a monochromatized output beam in the HPEEF photon energy region displays strong cylindrical symmetry, i.e. the beam center is easily identified. This behavior is characteristic not only of the HPEEF but also of the high photon energy edge of odd harmonics of the fundamental photon energy. For example, for the fundamental at the hard x-ray setting, ~8.3 keV, this behavior will also be observed at ~24.9 keV, 41.5 keV, etc.

In a similar way, considering the K-Mono monochromator, which is designed to pass a photon energy of ~8.3 keV, a cylindrically-symmetric output beam will be produced for the ~8.3 keV/3 = 2.8 keV setting of the LCLS undulator, i.e. the third harmonic produces the pass energy of the K-Mono monochromator. To locate the beam center at approximately the LCLS soft x-ray setting, the ninth harmonic is used, i.e. ~8.3 keV/9 = ~900 eV. Operating at this setting should require only a small adjustment of the Linac electron beam energy from the nominal soft x-ray setting, but will permit the beam center to be accurately located in the FEE.

Unlike the K-measurement procedure, this beam-center-finding function will probably be needed when more than two undulator segments, and perhaps all 33 undulator segments, are installed. Therefore, significant additional incident beam power may be dissipated in the first crystal of the K-Mono monochromator. This should be taken into account.
2. Fundamental Requirements


2.1.1. The Monochromator: Shall employ low-index silicon perfect crystals, symmetric or asymmetric cut, to produce a stable, high-transmission, narrow photon-energy bandwidth and narrow angular bandwidth x-ray optical system.

2.1.1.1. Output Beam: Shall be positioned and directed as an extension of the incident beam, to facilitate monochromator alignment.

2.1.1.2. An Incident Beam Stop shall be employed, to enhance signal/noise.

2.1.1.3. Fixed Photon Energy: within $8.0 \text{ keV} \leq h\nu \leq 8.5 \text{ keV}$.

2.1.1.4. Intrinsic Diffraction Angular Acceptance: > 25 $\mu$rad.

2.1.1.5. Transverse Physical Beam Acceptance: > 9 mmV x > 9 mmH

2.1.2. The Detector Subsystem: Should respond linearly to the magnitude of the incident photon pulse, independent of beam position, subject only to fluctuations due to photon statistics and an assumed detector subsystem noise level.

2.1.2.1. Pulse Intensity Range: ~ $10^6$ photons/pulse to ~ $10^4$ photons/pulse.

2.1.2.2. Photon Statistics Fluctuation: proportional to the square root of the number of photons per pulse.

2.1.2.3. Noise Level: < 100 photons/pulse.

2.1.2.4. Transverse Physical Beam Acceptance: Shall exceed that of 2.1.1.5.

2.1.2.5. Transverse Uniformity of Response: Must be consistent with 2.2 and estimated beam position variation.

2.2. Stability/Drift:

2.2.1. Millisecond Timescale Instabilities: must be insignificant

2.2.2. Permissible Transmission Drift: < 1% in 40 minutes

2.2.3. Permissible Photon-Energy Drift: < 4 eV in 4 minutes

2.3. “Fully Open” and “In-Operation” Modes:

2.3.1. "Fully-Open" mode: In this mode, the K-Mono monochromator, beam stop, and detector are fully withdrawn, and the "stay-clear" aperture, defined by projection from the XTOD Fixed Mask, is preserved.

2.3.2. "In-Operation" Mode: In this mode, the K-Mono monochromator, beam stop, and detector can be inserted into the beam.
2.3.2.1. Separate Insertion: The monochromator and its beam stop shall be separately insertable from the detector, to enable monochromator alignment using the Direct Imager.

2.4. Beam-Center-Finding Function: The K-Mono shall accommodate a beam-center-finding function, where odd harmonics of the undulator fundamental are matched to the photon pass energy of the K-Mono monochromator.

2.4.1. This function must be coordinated with the Direct Imager, which will be used to view the resulting output beam. The K-Mono detector will not be used.

2.4.2. This function may present a worst-case heat load situation for the K-Mono monochromator, since all 33 undulator segments may be employed to generate the incident beam. This must be considered in the system design, although relaxed system drift and stability requirements may be appropriate here.

3. Interface/Requirements with Other Systems

3.1. Direct Imager: Used for alignment of the K-Mono monochromator.

3.2. X-Ray Slit System: May be used to adjust the angular acceptance into the K-Mono, as a function of the undulator segments under test.

4. Other Requirements

4.1. Heat Load: Nearly all the incident spontaneous radiation power from the LCLS Undulator segments will be absorbed in the first silicon crystal plate of the K-Mono monochromator. Subsequent Bragg reflections absorb little. As a result, there is a potential for thermally-induced drift, due to un-even heating. This must be considered in the system design.

4.2. Initial K-Mono Alignment to the FEL Beam Axis: Only modest tolerances are required for initial alignment of the K-Mono to the FEL beam axis. These can be manual adjustments; remotely-controlled alignment is required for final alignment.

4.2.1. Positioning of the instrument optical center transverse to the beam location (combined X and Y) should be within 0.5 mm.

4.2.2. Initial angular alignment of the instrument axis to the FEL beam axis (combined Pitch and Yaw) should be within 200 µrad.

4.3. The design of the XTOD/XES K-Mono shall adhere to all elements of PRD 1.5-002, XTOD Mechanical-Vacuum Systems.
5. Controls:
   5.1. Remotely-Controllable Degrees-of-Freedom:
      5.1.1. Final Alignment Drives are required for the K-Mono monochromator.
      5.1.2. An Independent Insertion Drive is required for the K-Mono detector.

6. References:
   [1] LCLS Parameter Database: Undulator-Hall/Undulator-System, 
      http://www.bessy.de/fel2006/proceedings/PAPERS/THBAU05.PDF
   [3] Linda Ott, 2005/10/26 presentation at LCLS Week on FluxViewer software and spontaneous database files generated from calculations by Sven Reiche. Linda's talk, the FluxViewer software and the database files may be found at: http://www-ssrl.slac.stanford.edu/lcls/x-rayoptics/documents/
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