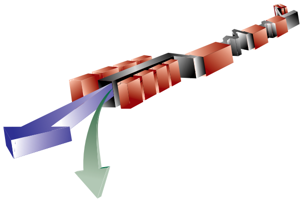
3 Scientific Basis for Optical Systems



TECHNICAL SYNOPSIS

The LCLS Scientific Advisory Committee (SAC) has recommended experiments in five scientific disciplines for the initial operation of the LCLS. These experiments cover a variety of scientific disciplines: atomic physics, plasma physics, chemistry, biology and materials science. The x-ray optics and detectors needed to verify the LCLS capability to address these five disciplines will be constructed and installed as part of the LCLS project. The experiments are described in detail in the document "LCLS: The First Experiments" referenced earlier.

Two classes of experiments are proposed for the LCLS. The first class consists of experiments where the x-ray beam is used to probe the sample, as is done in most experiments at current synchrotron sources. In the second class, the LCLS beam is used to induce non-linear photo-processes or create matter in extreme conditions. The same source can be used for both types of experiments by utilizing the six orders-of-magnitude change in photon flux density caused by focusing the LCLS beam, and by exploiting the strong dependence of the photo-absorption cross-section on photon energy and atomic number.

These experiments establish the basis for the designs of the x-ray optics to focus, monochromate, and manipulate the LCLS beam. In general, these designs are extensions of common practice at synchrotron sources today, but become demanding due to unprecedented peak powers, pulse lengths and coherence of the LCLS beam. These experiments also provide the requirements for a state of the art detector system for diffraction studies. Finally, the definition of the required synchronization of external lasers with the LCLS beam is derived from the experimental needs of these first five experiments.

3.1 Introduction

3.1.1 History of Scientific Interest in X-Ray Free Electron Lasers

The last thirty years have witnessed an exponential increase in the capability of x-ray sources, and x-ray physics has seen an explosion of new techniques and applications. The key to this huge change has been the development of synchrotron radiation sources from high-energy electron storage rings. The scientific capabilities of synchrotron radiation x-ray sources are reflected in the fact that in the US four such facilities are operated by DoE with a collective annual funding level of about $200 million (FY2001). In 2001, 6500 scientists made use of these facilities for their research programs, which range from fundamental physics to materials science to biology and medicine to environmental science [1]. Now, another type of high-energy accelerator has the capability to drive an x-ray source whose capabilities outshine those of a modern synchrotron source by nearly as much as the synchrotron does the 1960's laboratory source.

Advances in accelerator technology have been the driving force in the progress toward brighter synchrotron sources, with scientific applications developing in response to the availability of new sources. The rate of improvement in source capability has been tremendous: for thirty years x-ray source brightness has been increasing exponentially with a doubling time of about 10 months. A modern synchrotron radiation source is 11 orders of magnitude brighter than a 1960's laboratory x-ray source. Seldom, if ever, in history (perhaps only in the field of visible laser optics) has a scientific discipline seen its tools change so dramatically within the active life of a single generation of scientists. Such change makes it very difficult to predict the future. For example, no one foresaw the huge impact on biomedical research that has come in the last twenty years from synchrotron-based EXAFS and protein crystallography, even though those techniques had been developed many years previously using laboratory sources. The developing synchrotron source capability has made the techniques qualitatively and unexpectedly more powerful as scientific tools.

This history indicates that although it is very difficult to predict the eventual applications of the LCLS, a source that is more than 10 orders of magnitude brighter than today's synchrotron sources, it will make fundamental contributions to our understanding of the structure and dynamics of matter on the atomic scale. Over the past ten years there has been much consideration of the future development and applications of such new synchrotron radiation sources. A first workshop on "Fourth Generation Light Sources", at SLAC in 1992 [2], concentrated almost exclusively on accelerator technology rather than applications. This workshop served to alert the scientific community to the possibilities for x-ray FELs driven by linacs, including the SLAC linac. It is interesting to note that a workshop earlier in 1992 on "Applications of x-ray Lasers" [3] did not mention FEL sources at all; only chemical lasers were considered. The SLAC workshop directly stimulated the first workshops on scientific applications of x-ray FELs [4,5]. The next "Fourth Generation Light Sources" workshop, in 1996 at the ESRF [6], included sessions on both sources and applications. The discussions convinced nearly all the participants that linac based FELs would be the most effective machines for continuing to improve the performance of x-ray sources, and in particular, would provide the only viable route to a diffraction-limited hard x-ray source. Subsequent workshops at DESY in 1996 [7,8] and APS in 1997 [9] have assumed that future fourth generation x-ray user facilities will be based on linac FELs, and have attempted to foresee the new science that these sources will bring. These workshops, as well as more than 20 others, have firmly established the scientific opportunities that LCLS provides.

3.1.2 Unique Features of X-Ray FEL Radiation

Intrinsic to the short-wavelength FEL process are several features, which give unique and useful attributes to the radiation that is produced. Because of the difficulty of creating an optical cavity at x-ray wavelengths, a high-gain, single-pass FEL design is used, relying on the process of self-amplified spontaneous emission (SASE). This implies a very short, high-energy electron pulse producing a similarly short but very intense FEL radiation pulse. The radiation has a relatively short longitudinal coherence length, but complete transverse coherence. In addition to the FEL radiation, the SASE process produces a spontaneous radiation spectrum rich in higher harmonics. **Figure 3.1** shows a calculation of the LCLS radiation spectrum with FEL operation at 1.5 Å, and **Table 3.1** gives some descriptive parameters for the beam. Compared with existing x-ray sources, the radiation has three truly unique aspects:

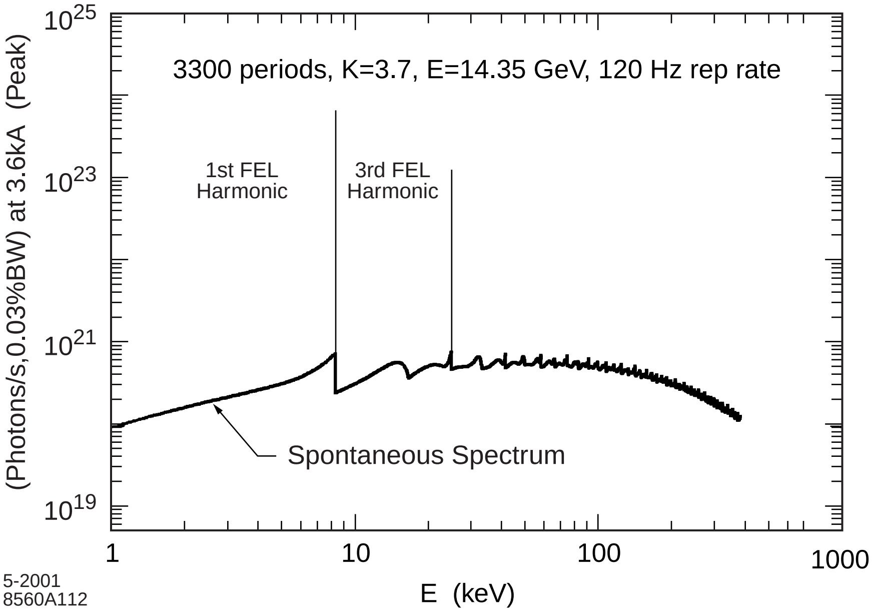


Figure 3.1 LCLS peak flux spectrum, with FEL radiation at 1.5 Å. The first harmonic FEL amplification is saturated. There is also some amplification of the third harmonic, but this is far from saturation, and is likely to be further reduced by magnet and beam errors.

The FEL peak intensity and peak brightness are both many orders of magnitude higher than can be produced by any other source (see **Figure 3.2**). Even the average brightness, though limited by the low repetition rate of the linac, is still orders of magnitude higher than the brightest synchrotron radiation.

The sub-picosecond pulse length is orders of magnitude shorter than can be achieved with a synchrotron. There exist x-ray sources with comparable pulse lengths (for example, plasma sources and inverse Compton scattering sources), but they have very much lower brightness.

Table 3.1 Calculated characteristics of the LCLS radiation at the short wavelenth end of the operational range.

FEL wavelength	1.5	Å
FEL bandwidth (*ΔE/E*)	0.003	
Pulse duration (FWHM)	230	fs
Pulse length (FWHM)	69	µm
Peak coherent power	8	GW
Peak coherent power density	1.1×10^{12}	W/mm^2
FEL energy/pulse	2.1	mJ
Peak brightness	1×10^{33}	flux/mm^2/mrad^2/0.1%BW
FEL photons/pulse	1.1×10^{12}	
FEL photons/second	1.3×10^{14}	
Degeneracy parameter	10^9	
Peak EM field (unfocused)	2.5×10^{10}	V/m
Average FEL power	0.25	W
Average FEL brightness	2.7×10^{22}	flux/mm^2/mrad^2/0.1%BW
Transverse size of FEL beam (FWHM)	70	µm
Divergence of FEL beam (FWHM)	1	µrad
Peak power of spontaneous radiation	92	GW

The FEL radiation has full transverse coherence (it is diffraction limited). In addition, the degeneracy parameter (photons per coherence volume in phase space) is many orders of magnitude greater than one. Only at the longest wavelengths can some synchrotron sources approach the diffraction limit, and no source has a degeneracy parameter much greater than one.

In addition to these features of the FEL radiation, the high-energy spontaneous radiation offers attractive characteristics. The spectrum of this radiation extends to nearly 1 MeV; above about 100 keV it is far brighter than any synchrotron radiation.

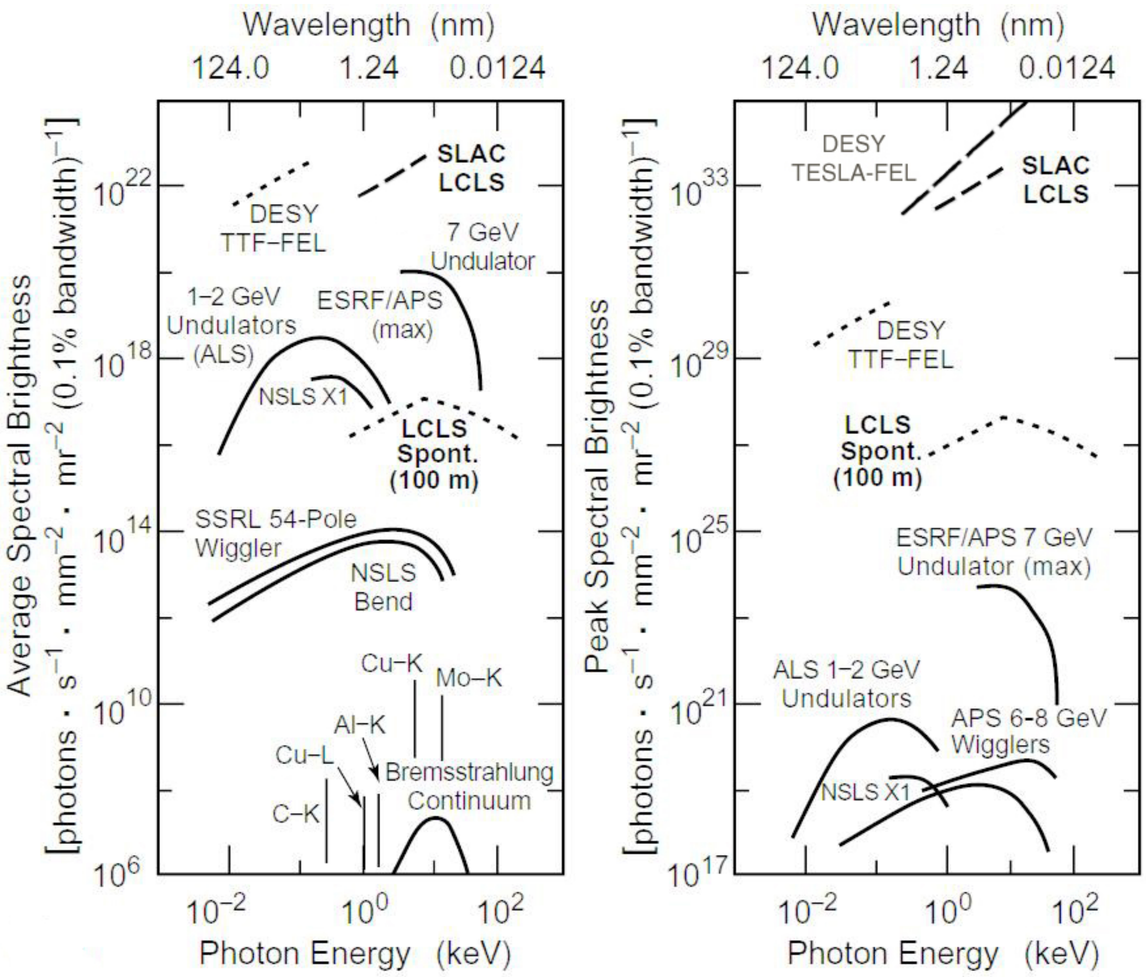


Figure 3.2 Average and peak brightness calculated for the LCLS and for other facilities operating or under construction. The data for the Average Spectral Brightness of the planned TESLA FEL facility are above the limit of the figure.

3.1.3 The Role of the LCLS

For the applications to be realized, much needs to be learned about the interaction between x-ray FEL radiation and matter. But today's radiation sources cannot fully address this issue. A recent workshop [10] concluded that all existing laser and synchrotron sources fail by at least 3 orders of magnitude in frequency or power density to duplicate the conditions of an x-ray FEL. The basic interactions between atoms and electromagnetic fields with the strength of the FEL radiation are not well understood. It is not known exactly what kind of damage this radiation will cause in solid samples, or how best to moderate its intensity.

Therefore, the first scientific contribution of the LCLS will be to provide an understanding of the interactions between very intense, very high frequency electromagnetic radiation and matter. In the process of gaining this understanding, many technical issues must be confronted, such as fast, high-dynamic-range detectors, high peak power optics, and precise synchronization with external probes. It is very likely that as experience with the LCLS grows, further advances in accelerator science will lead to greater control over the FEL radiation. It may become possible to produce even shorter x-ray pulses, energy-chirped pulses, or pulses with special polarization states. All of these will lead to new applications.

3.1.4 Science with X-Ray FELs

As mentioned above, there have been many international workshops called to discuss the scientific applications of FEL x-ray sources. The need to develop the scientific case for an XFEL in order to move forward with its design and construction was emphasized by the Leone report on Novel Coherent Light Sources [11]. In response to this need the LCLS Scientific Advisory Committee (SAC) put considerable effort into defining a small set of particularly exciting experiments that could be carried out with LCLS. This information is presented in great detail in the report, "LCLS: The First Experiments" [12] and has been accepted as the basis for going forward with the LCLS by the Basic Energy Sciences Advisory Committee. Many of the techniques mentioned are already in use, or at least proof-of-principle experiments have been done. An attempt has been made to try to project the impact of an FEL source on the future importance of these techniques. It is certain that, once it is available, the FEL source will stimulate the development of completely new techniques, the importance of which is extremely difficult to predict. In the section below we describe the optics requirements derived from the "LCLS: The First Experiments" [12]. It is important to note that the majority of these systems are similar to those now found at all synchrotron radiation facilities. They provide the generic means of manipulating the photon beam.

3.2 Optical and Experimental Challenges

3.2.1 Focusing

The LCLS x-ray beam has typical dimensions of 100 μm even with its extremely small divergence. In many applications this source dimension is more than sufficient and helps avoid sample damage issues for a wide variety of samples. In several experimental areas however there is the requirement to focus the beam to dimensions of order 0.1 μm or smaller. In the case of atomic physics for example in studies of multiphoton excitation, getting to 0.1 μm at the low energy end of the LCLS range (0.8 keV) is critical. For the bio-imaging similar spot sizes are required at the high energy end of LCLS performance (8.0 keV). Warm dense matter has less stringent requirements, 10 μm, but still requires focusing to achieve the needed energy density. Theses needs can be addressed with techniques developed at third generation synchrotron sources, refractive optics in the form of zone plates and reflective optics in the form of Kirkpatrick-Baez mirror systems. These methods will be carried over to the LCLS and demonstrated in the initial phase.

3.2.2 Monochromatization

The LCLS will have a natural bandwidth of 10^{-3} under normal conditions; however there is the possibility that the central wavelength may have pulse-to-pulse variations equal to its bandwidth. For some experiments this may not be a difficulty and the natural bandwidth is more than sufficient. However, for the warm dense matter experiments, when an external laser is used as the pump and the LCLS is used as the probe in Thomson scattering studies there will be a need to monochromatize the radiation. In the nanoscale dynamics experiment the bandwidth determines the longitudinal coherence length of the radiation and thus defines the coherent volume that is probed by the LCLS beam. To control the longitudinal coherence length the beam needs to be monochromatized as well. The techniques that are used routinely with both lab based x-ray sources and synchrotron radiation, Bragg diffraction from perfect crystals, will work as well at LCLS. The issue for LCLS is the damage threshold for these optics. By far the most widely used material is Si and calculations show that there are no damage issues in the far hall and there may be no difficulties in the near hall. Monochromators will be developed for both situations and early studies will address directly damage issues for these critical systems.

3.2.3 Harmonic Control

The LCLS radiation is dominated by its fundamental wavelength, but the spectrum contains higher harmonics as well. In general, the experiments described in the Report, "LCLS: The First Experiments" [12] are not sensitive to harmonic contamination on the expected percent level. However in the case of the atomic physics studies of multiphoton excitation it is critical that the highest degree of harmonic rejection be achieved. When looking for processes where the energy required is the sum of the energy from several photons contamination from higher harmonics makes the experiment impossible. This contamination can also be important for scattering experiments where the counting is based on the deposited energy and detectors cannot discriminate between three photons of energy E and a single photon of energy $3E$ present due to harmonic contamination. For these applications it will be critical to eliminate the harmonic contamination in the incident beam. The standard method of mirror reflection, with the mirror angle chosen to reflect the fundamental and not the higher harmonics, will be evaluated for the low energy end of the LCLS operating range for use in the laser-matter interaction studies.

3.2.4 Photon Pulse Manipulation

The LCLS, as an XFEL source, will require the development of x-ray analogues of many tools routinely used in conventional laser experiments. In particular for the study of nanoscale dynamics using x-ray photon correlation spectroscopy pulse manipulation methods are required. For UV, visible and IR lasers optical techniques permit pulse splitting and delay as well as recombination. These tools are not easily realized for x-ray radiation and this is a challenge for the LCLS. There are designs that use Bragg reflection optics. The LCLS performance puts stringent demands on these methods as one tries to split and delay pulses over the range of fractions of a picosecond up to perhaps a nanosecond while preserving the transverse coherence. The ability to develop the x-ray analogues of conventional optical methods will be important for the life of LCLS as the science evolves to make full use of the coherence of the LCLS beam.

3.2.5 Synchronization of an External Source (Laser Pump)

A wide range of experimental methods that have become routine in the ultrafast science community involve pump-probe techniques with the delay between pump and probe controlled to a small fraction of the pulse width. These techniques are inevitably based on a single laser source so that the setting and maintaining of the delay relies on mechanical stabilities that are no longer beyond the state of the art. The power of the LCLS as a probe for laser excited systems on the femtosecond time scale is unprecedented because LCLS can provide directly the atomic positions with Ångstrom resolution from diffraction studies. The difficulty is that the laser pump and x-ray probe must be synchronized with the same fractional precision as with femtosecond laser experiments. The present state of the art in synchrotron sources provides synchronization at perhaps the 1-ps level, a factor of 10-100 away from what LCLS will require. To address this critical need in femtochemistry, time resolved bio-imaging and other pump probe experiments one will first measure the jitter on the 10-100 fs time scale after phase locking the laser and x-ray beam. These techniques, developed to evaluate the jitter, will then be used as a means of tagging the data as it is acquired and providing the information to post process to derive the temporal dependences that are at the heart of the experiment.

3.2.6 Detectors

The power of the LCLS is that it will produce radiation at 8 keV, which is the standard for diffraction studies at atomic resolution. In synchrotrons around the world this power is already being exploited in the study of the structure of large macromolecules. The growth and success of these studies is based on the development of accurate, large-area, fast, 2-dimensional x-ray detectors. The technology for these conventional applications is now robust, but will not meet the demands for the LCLS. The bulk of the experiments using diffraction methods will require the acquisition of a full diffraction pattern from every LCLS pulse, an operating rate of 120 Hz. This readout rate is unprecedented in the synchrotron radiation field. Furthermore, these detectors will require very large dynamic range for scattering experiments in the area of biomolecules with intensities approaching per pulse what one gets per second form synchrotron radiation sources, today. The spatial resolution required will also be at the state of the art, 25 µm. There are exciting developments that are just beginning to be applied to synchrotron radiation experiments that borrow from high energy physics. These involve technologies for vertex detectors in colliding beam experiments called pixel array detectors. These developments have the capabilities, in principle, to provide the parameters that one desires for the LCLS and recent results [13] seem to be very promising. This is an area that has received too little attention in the past and will be important to the success of the LCLS over its lifetime for certain classes of experiments.

3.2.7 Summary

The success of the LCLS experimental program rests on the development of x-ray optics and detectors that can manipulate the incident radiation and measure the scattered beam. They will require exquisite control and/or knowledge of the temporal relationship between external laser and the LCLS beam for a variety of pump probe experiments. The first experiments described in the Report, “LCLS: The First Experiments” [12] provide guidance as to which tools one develops first in the LCLS project. These developments don’t end with the construction project completion. With the availability of first radiation one begins studying the interaction of the XFEL beam with matter and evaluating the performance of the optics that will be available. The developments during the life of the LCLS will be stimulated by, as well as stimulate, a rich variety of unique experimental methods that will add significantly to our understanding of the structure and dynamics of a wide range of physical systems.

3.3 References

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