

AN OSCILLATOR CONFIGURATION FOR FULL REALIZATION OF HARD X-RAY FREE ELECTRON LASER*

K.-J. Kim[†], T. Kolodziej, R.R. Lindberg, D. Shu, Y. Shvyd'ko, and S. Stoupin

Argonne National Laboratory, Argonne, IL, USA

T.J. Maxwell, Y. Ding, W.M. Fawley, J. Hastings, Z. Huang, J. Krzywinski, and G. Marcus

SLAC National Accelerator Laboratory, Menlo Park, CA, USA

W. Qin, Peking University, Beijing, China

N. Medvedev and J. Zemella, DESY, Hamburg, Germany

V. Blank and S. Terentyev, TISNCM, Moscow, Russia

Abstract

An x-ray free electron laser oscillator (XFEL) is feasible by employing an X-ray cavity with Bragg mirrors such as diamond crystals. An XFEL at the 5th harmonic frequency may be implemented at the LCLS II using its 4 GeV superconducting linac, producing stable, fully coherent, high-spectral-purity hard x-rays. In addition, its output can be a coherent seed to the LCLS amplifier for stable, high-power, femto-second x-ray pulses. We summarize the recent progress in various R&D efforts addressing critical issues for realizing an XFEL at LCLS II.

INTRODUCTION

The basic configuration of an XFEL is illustrated in Fig. 1, in which an x-ray pulse is trapped in an x-ray cavity. The pulse will then be repeatedly amplified in an undulator located in one of the straight paths in the cavity, and the pulse intensity starts to increase exponentially if the gain is larger than the round-trip loss. For hard x-rays, large-angle, low-loss reflection can be accomplished with Bragg crystals, as first proposed in 1983 [1]. It took more than two decades, after having witnessed the realization of a single pass x-ray amplifier, to theoretically demonstrate that an XFEL would be feasible within the achievable parameters of electron beam, undulator, and Bragg crystals [2]. With the zig-zag path shown in Fig. 1, the Bragg angle, and therefore the photon energy, is arbitrarily adjustable [3,4]. Another important advantage of the zig-zag path is that the choice of the Bragg crystal can be made from considerations other than the photon energy coverage. We chose diamond as having the most optimal optical and thermo-mechanical properties.

An LCLS II-based XFEL

The XFEL performance based on a 7 GeV superconducting electron linac in the range of 5 to 25 keV using fundamental harmonics has been studied and shown to be well-suited for hard x-ray photon sciences in areas complementary to self-amplified spontaneous emission [5]. It

was then pointed out that an XFEL can be run at harmonic frequencies. The electron energy can then be reduced, thereby also reducing the cost of the accelerator [6]. We have therefore studied a 5th harmonic XFEL based on the 4 GeV superconducting linac that will be built for the LCLS-II project [7]. A preliminary study found the XFEL performance satisfactory and also identified the ESA building to be a possible site at SLAC [8,9].

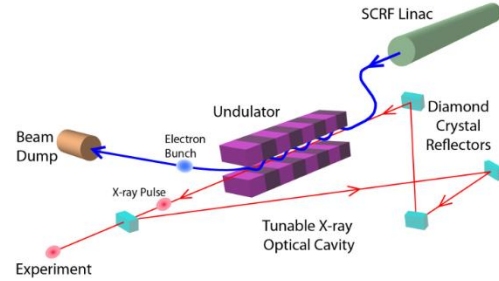
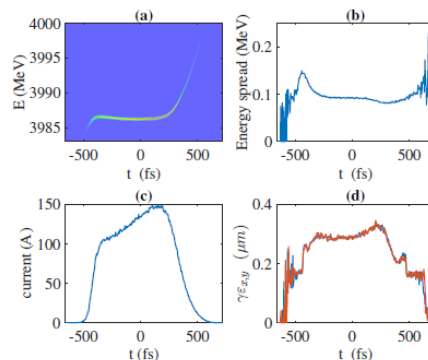


Figure 1: Layout of an XFEL facility

XFEL PERFORMANCE

An XFEL requires a low-emittance, small-energy-spread electron bunch. The bunch length should be sufficiently long to have a good overlap with narrow-band x-ray pulse. Optimization of the LCLS II injector and accelerator parameters has been performed, the main challenge being to maintain the flatness of the electron energy over the length of the electron bunch [10]. The result is shown in Fig. 2.



*The Argonne National Laboratory part of this work is supported under US Department of Energy contract DE-AC02-06CH11357 and the SLAC part under US Department of Energy contract DE-AC02-76SF00515

[†]email address: kwangje@aps.anl.gov

Figure 2: Electron beam optimized for flat energy distribution [10]

The XFEL performance at 14.4 keV using the electron beam distribution depicted above was simulated with GINGER, and the resulting spectral and temporal pulse shapes of output are shown in Fig. 3. A summary of the major parameters of an XFEL at LCLS-II are summarized in Table 1.

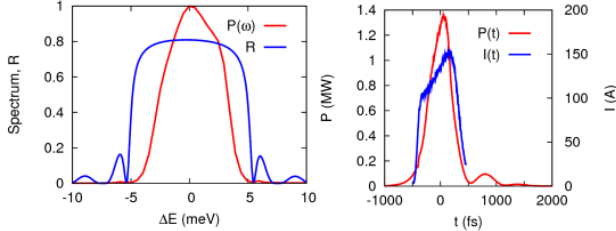


Figure 3: XFEL performance, spectral (left) and power (right) distribution

Table 1: Major parameters of an LCLS-II based XFEL

Parameter	Value	Units
Electron energy	4	GeV
Peak current	100-140	A
Bunch charge	100	pC
Bunch length	400	fs
Energy spread	0.1	MeV
Norm. emittance	0.3	μm
Photon energy@5 th harm.	14.4	keV
Round trip loss	15	%
Undulator period	2.6	cm
Undulator K	1.43	
# of undulator periods	1250	
# of photons/pulse	3	10^8
Spectral BW (FWHM)	5	meV

X-RAY OPTICS

Previous results

Working with several crystal manufacturers, we found that modern techniques can grow high-quality diamonds containing defect-free regions suitable for an XFEL. Experiments with 13.9-keV and 23.7-keV x-ray photons have established that the predicted reflectivity greater than 99% at near normal incidence is feasible [11, 12].

Temperature gradients that lead to gradients in the crystal lattice spacing can diminish the reflectivity. The simulation shows that the radiation heat load produced by an XFEL requires that the diamond crystal be cryogenically cooled to a temperature $T \leq 100\text{K}$. In this case, the diamond has sufficient time to conduct away the heat, so that the crystal temperature becomes homogeneous before the subsequent radiation pulse arrives. Low temperatures are favorable because diamond has an unmatched thermal

diffusivity and an extremely small coefficient of thermal expansion for $T < 100\text{K}$ [13].

The requirements to stabilize the crystals and the mirrors in the cavity are stringent—better than 10-nrad (rms) angular stability and 3- μm (rms) positional stability. The null-detection feedback technique employed at the Laser Interferometer Gravitational-Wave Observatory (LIGO) can stabilize several optical axes with a single detector, and therefore appears to be a promising approach. A pilot experiment with a high-resolution, six-crystal x-ray monochromator at the APS Sector 30 beamline succeeded in achieving an angular stability of 13 nrad (rms) [14]. We will need to improve the scheme to meet the XFEL requirements—a multiple-axis system with better than 10-nrad stability, and with a feedback BW of about 1 kHz.

Diamond resilience under high power exposure

The power density incident on diamond crystals in the XFEL cavity is 1-10 kW/mm², which is by one to two orders of magnitudes higher than that of the power density on the first crystals at undulator beamlines of third generation synchrotron radiation facilities. It is therefore of paramount importance to determine whether a diamond crystal can survive as an x-ray mirror for an XFEL. Theoretical estimates of various processes under intense x-ray exposure indicate that the damage threshold for the x-ray power density is several orders of magnitude higher than 10 kW/mm²[15].

A systematic experimental study of diamond resilience is in progress at the APS beamlines. The 35-ID beamline was used to produce a focused spot of 8 keV x-rays, roughly comparable in size and power density anticipated for an XFEL, 120×30 μm^2 and 8 kW/mm², respectively. A well-characterized, 100- μm thick diamond sample was irradiated at ten different positions for different duration—1/64, 1/32, 1/16, ..., 4, and 8 hours, as shown in Fig. 4 (left). The colour represents the rocking curve FWHM map of the irradiated crystal measured with 8 keV x-rays at the APS beamline 1BM-B, recording the FWHM of rocking curve peaks at each point on the surface. The fact that it is uniformly green implies that there is apparently no discernible change in the spectral responses when the diamond sample was exposed up to 4 hours (we disregard the 8-hour spot since there were some uncertainties for this exposure) within the relative accuracy of 10^{-6} of the topography set-up for this experiment. However, the image of the optical microscope revealed a darkening of the irradiated spots, indicating adsorption of impurity material, most probably carbon.

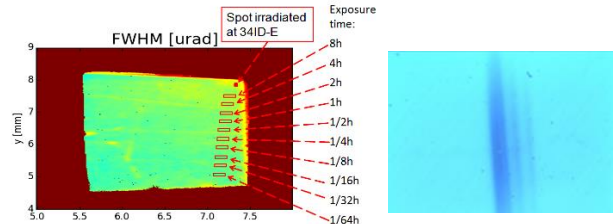


Fig. 4: The rocking curve FWHM map of the irradiated diamond surface where the irradiated rectangular areas are indicated with the exposure times (left) and the image of the optical microscope of the spot with 4-hr exposure (right).

Subsequent measurements with high resolution (10^{-8}) indicated possible shifts in the position of spectral peaks of the order of 1 meV in the irradiated area. Although this is a small effect that is probably correctable during an XFEL operation, we are planning a more detailed study about the physics behind the spectrum shift—is it possibly related to the impurity deposition on the surface, etc—by another round of x-ray exposure and precision topography.

XFEL focusing optics

In addition to high-reflectivity mirrors, an XFEL cavity requires focusing elements so that the transverse mode profiles can be controlled [5]. Grazing-incidence, curved mirrors, in particular those being perfected at JTEC [16], are an option. However, being large and heavy, these are challenging to operate, especially if the photon energy, and thus the incidence angle to the curved mirror, need to be tuned.

Another option is the compound refractive lens (CRL) made from Be with a parabolic surface profile [17]. One unit of a compound lens consists of two opposing parabolic faces. At synchrotron radiation beamlines, sets of more than ten units are used to create sub-micron spots.

The loss due to small angle scattering could be rather high, 40% or more. As a focusing element for an XFEL with 100-300 m roundtrip length, the focal length could be longer than 20-m [5]. A Be CRL composed of one or at most two compound units is then an attractive, compact option. The loss is small for IF-1 grade material. However, questions have been raised whether the surface of a parabolic Be CRL can be shaped sufficiently accurately and its roughness sufficiently controlled.

We purchased Be CRLs of radius of curvature $R = 100 \mu\text{m}$ and $50 \mu\text{m}$ from RXOPTICS. The surface profile measured at the APS metrology laboratory is shown in Fig. 5. The deviation of the surface from the ideal shape is less than $1 \mu\text{m}$.

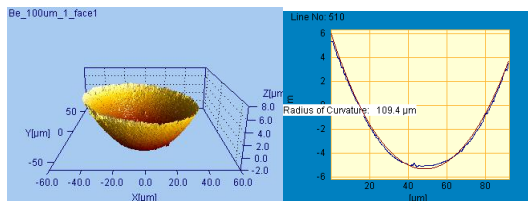


Figure 5: Surface metrology of a parabolic Be CRL

Figure 6 shows the phase and phase error of the image of the source formed by the CRL. The rms phase error measured to be 0.16 rad, from which the rms thickness

error of $0.75 \mu\text{m}$ can be deduced, is consistent with the metrology data. Thus, Be CRLs are an attractive candidate for XFEL focusing.

During the high-power irradiation of diamond, a $25\text{-}\mu\text{m}$ Be window was exposed to 3 kW/mm^2 of x-ray power density up to 8 hours without any apparent damage. Thus, the resilience of Be CRL is also demonstrated.

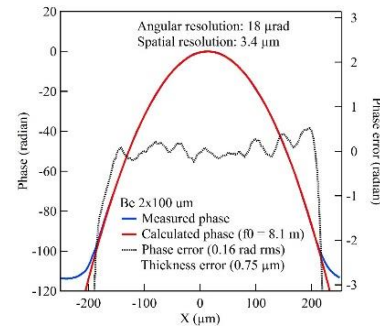


Figure 6: Phase and phase error of CRL imaging

CONCLUDING REMARKS

The results of the x-ray optics experiments on diamond resilience and Be-CRL performance are encouraging information for the feasibility of an XFEL. We have also demonstrated that the LCLS-II accelerator parameters can be optimized to implement a 5th harmonic XFEL, widening the scientific reach of LCLS II to areas that require intense, fully coherent, ultra-fine spectral resolution x-rays.

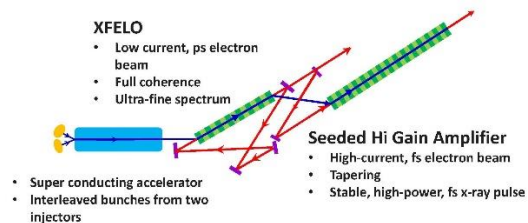


Figure 7: Concept for an ultimate XFEL Facility

We may further envision an XFEL facility consisting of both an XFEL and high-gain amplifiers. The XFEL output can serve as the seed for the amplifier. If the amplifier employs fs electron bunches, then only the fs portion of the seed will be amplified to provide stable, fully coherent, fs x-ray pulses. With full coherence, an efficient tapering section can be attached beyond saturation point, thus increasing the fs pulses to TW regime.

Harmonic generation starting from 10 keV coherent input could be a promising route to higher energy XFEL, perhaps to 50 keV or higher.

REFERENCES

- [1] R. Colella and A. Luccio, "Proposal for a free electron laser in the X-ray region," *Optics Comm.* **50**, 41 (1984).
- [2] K.-J. Kim, Y. Shvyd'ko, and S. Reiche, "A proposal for an x-ray free-electron laser with an energy-recovery linac" *Phys. Rev. Lett.* **100**, 244802 (2008).
- [3] R.M. J. Cotterill, "A universal planar x-ray resonator," *APL*, **403**, 133 (1968)
- [4] K.-J. Kim and Yu.V. Shvyd'ko, "Tunable optical cavity for an x-ray free-electron laser oscillator," *Phys. Rev. ST Accel. Beams* **12**, 030703 (2009).
- [5] R. R. Lindberg et al., "Performance of the free-electron laser oscillator with crystal cavity," *Phys. Rev. ST Accel. Beams* **14**, 010701 (2011).
- [6] J. Dai, H. Deng, and Z. Dai, "Proposal for an x-ray free-electron laser oscillator with intermediate energy electron beam" *PRL* **108**, 034802 (2012).
- [7] SLAC National Accelerator Laboratory, LCLS II Conceptual Design Report, SLAC-R-978 (2011).
- [8] T. J. Maxwell, et al., "Feasibility study for an x-ray FEL oscillator at the LCLS-II," IPAC 2015.
- [9] J. Zemella, et. al., "Time dependent study for an x-ray FEL oscillator at LCLS-II," FEL 2015.
- [10] W. Qin, et al, "Beam optimization study for an X-ray FEL oscillator at the LCLS II" this conference
- [11] Yu. V. Shvyd'ko et al., "High-reflectivity high-resolution x-ray crystal optics with diamonds" *Nature Physics* **6**, 196 (2010).
- [12] Yu. V. Shvyd'ko, S. Stoupin, V. Blank, and S. Terentyev, "Near-100% Bragg reflectivity of X-rays" *Nat. Photonics* **5**, 539 (2011).
- [13] S. Stoupin and Yu. V. Shvyd'ko, "Thermal Expansion of Diamond at Low Temperatures" *Phys. Rev. Lett.* **104**, 085901 (2010); S. Stoupin and Yu. V. Shvyd'ko, "Ultraprecise studies of the thermal expansion coefficient of diamond using backscattering x-ray diffraction" *Phys. Rev. B* **83**, 104102 (2011).
- [14] S. Stoupin et al., "Nanoradian angular stabilization of x-ray optical components" *Rev. Sci. Instrum.* **81**, 055108 (2010).
- [15] N. Medvedev, unpublished notes (2015).
- [16] H. Yumoto, et al., "Focusing of X-ray free-electron laser pulses with reflective optics" *Nature Photonics*, **7**, 43 (2012).
- [17] B. Lengeler, et al., "Imaging by parabolic refractive lenses in the hard x-ray range" *J. Synchrotron Rad.* **6**, 1153 (199).