Design and operation of a hard x-ray transmissive single-shot spectrometer at LCLS

D Zhu, M Cammarata, J Feldkamp, D M Fritz, J Hastings, S Lee, H T Lenke, A Robert, J Turner, Y Feng
Linac Coherent Light Source, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, California, USA
E-mail: yfeng@slac.stanford.edu

Abstract. We describe the design and operation of a transmissive single-shot spectrometer for the measurement of hard x-ray free electron laser (FEL) source spectrum at the Linac Coherent Light Source (LCLS). The spectrometer was built around a 10 µm thick near-perfect silicon single crystal that was cylindrically bent. Its energy range covered the full FEL bandwidth while its resolution was sufficient for resolving single spectral spikes characteristics of the FELs. Its application will not only greatly facilitate the understanding and optimization of the x-ray FEL sources, but can also serve as an invaluable inline diagnostic tool for experiments where the spectral content of the source plays an important role in data interpretation.

1. Introduction
The advent of the fourth generation x-ray FEL sources has opened up a broad range of new opportunities in scientific discoveries across multiple disciplines [1, 2]. Currently, the lasing process of x-ray FELs is based on the principle of self-amplified spontaneous emission (SASE) [3, 4], whose stochastic nature leads to statistical fluctuations in all beam properties. In particular, the spectral intensity profile is believed to consist of a large number of fluctuating spikes, posing a potential challenge for many experiments [5]. Single shot source spectral measurement was previously performed at FLASH and the SXR beamline at LCLS using grating based technique [6, 7]. However, it is difficult to extend the method into the hard x-ray regime, and even more difficult to adapt the scheme into an in-situ beam diagnostics. We describe in this paper an FEL source spectral diagnostic device for hard x-rays. It has an energy range that covers the full FEL source spectrum and sufficient resolution to resolve individual SASE spikes, and high transmission to allow the beam through for downstream experiments.

2. Spectrometer details
The dispersion geometry of the spectrometer is illustrated in figure 1(a). It was designed and built around a near-perfect ultra-thin silicon crystal that is bent to a cylindrical shape. Assuming a parallel incoming x-ray beam, over its footprint on the crystal the incidence angle varies. As a result, different wavelengths fulfill the Bragg conditions and are reflected into different directions. The dispersion relation in the measurement plane can be described by:

$$
\Delta x = 2 \tan \theta_B \left( \frac{R \sin \theta_B}{2} + L' \right) \frac{\Delta E}{E},
$$

(1)
where $\theta_B$ is the Bragg angle, $E$ the photon energy, $R$ the crystal radius of curvature, and $L'$ the distance between the crystal surface and the measurement plane. The term $R' = R \sin \theta_B / 2$ is a correction factor for the effective distance $L$ because for different photon energy the reflecting point shifts along the crystal. Given the radius of curvature, the spectral range of the spectrometer can be written as $\Delta E_{\text{max}} = \cot \theta_B \sin^{-1} \theta_B H \cdot E/R$, where $H$ is the size of the beam in the dispersion plane.

The thin crystal was fabricated in collaboration with Nordaca Inc. The process started from a silicon-on-insulator wafer, where the silicon crystal of the desired orientation was first bonded to a Si(100) substrate via a thermal oxide layer. The top silicon layer was then cut, grounded, and polished to the specified thickness, verified by ellipsometry. KOH etching was used to remove the substrate within a rectangular area to form the thin-layer-only silicon window, 5 mm by 15 mm in our case. Three edges of the window connected to the substrate were finally removed by optical lithography, forming the shape of a spring board. The small thickness allowed the crystal to be bent to very small radius of curvatures ($< 100$ mm) previously unattainable with thicker wafers used in traditional x-ray analyzers. We have implemented a crystal bender utilizing a precision actuator to translate the free end of the spring board to adjust the amount of bending, thus the energy range the spectrometer covers. The dispersed x-rays were converted to an optical spectrograph through a 100 µm thick Ce:YAG scintillator screen at a distance of 300 mm. A Navitar motorized zoom lens combined with an OPAL-1000 CCD detector were used to capture the spectrograph at the full beam rate of 120 Hz.

3. Experimental observations

Initial test of the spectrometer was performed at the X-ray Pump Probe instrument at LCLS. Two spectrometers were setup in tandem as shown in figure 1(b). The crystals were bent to radius of curvatures of about 300 mm for the Si(111) and 150 mm for Si(333). A FWHM beam size of 400 µm yielded for the two spectrometers energy ranges of 200 eV and 32 eV respectively. The spectrometers were calibrated using an upstream double crystal monochromator. The calibration data are fitted to equation 1 as shown in figure 2(a) with only the crystal curvature as the free parameter. The full spectrum of a typical LCLS pulse is shown in figure 2(b), measured using the Si(111) geometry. Si(333) produced higher resolution measurements within a reduced range, shown in figure 2(c). The two measurements agreed qualitatively over their common
energy range. The expected shot-to-shot fluctuation of the SASE spectrum was observed (see the animated GIF image in the supplementary material). In addition, we also observed the constantly shifting spectrum centroid over a 20 eV range (FWHM), a direct result of the electron beam energy jitter from the accelerator. Their strong correlation (see supplementary figure) indicates the mean photon energy jitter can be corrected for based on electron beam energy measurement to an accuracy of about 5 eV. The experimentally observed resolutions for Si(111) and Si(333), determined by the finest resolved features in the spectra, are 0.5 eV and 0.2 eV. More detailed discussion of the resolution function can be found in reference [8].

The information contained in the spectrograph can greatly facilitate the understanding and optimization of the FEL operation. The characteristic feature width in the spectra can be used to deduce the x-ray pulse width. Future upgrade of the FEL towards a transform limited x-ray source will also require high resolution spectral measurement. Another example is the observation of the spatial chirp. While one dimension of the spectrograph is the photon energy axis, the other follows the spatial dimension perpendicular to the dispersion direction. We observed that the spectrum could differ significantly at different horizontal locations under certain machine configurations as shown in figure 3. However, the difference is much less pronounced in the vertical direction in the spectrograph obtained with the Si(111) spectrometer in the horizontal reflection geometry. The chirp can be attributed to the horizontal dispersion elements in the electron optics in the accelerator and this was confirmed by its enhancement/suppression when adjusting the bunch compressor. Optimization based on reducing the chirp could ultimately improve the coherence properties of the beam.

**Figure 2.** (a). Spectrometer calibrations using the upstream monochromator. (b). The spectrum of a typical LCLS pulse measured by Si(111) spectrometer. The FEL was operating at 8.3 keV, using 150 pC bunch charge and normal compression. (c). A high resolution portion of the spectrum measured simultaneously using the Si(333) spectrometer (black) overlaid with the Si(111) measurement (blue).

**Figure 3.** (a). Partial FEL spectrum measured by the Si(333) spectrometer showing significant spatial chirp of the beam in the horizontal direction. (b). Spectrum lineout from different horizontal positions as indicated in the color arrows above.
4. Applications

![Figure 4](image)

Figure 4. Two examples of how the spectrometer can be adapted in experiments. (a). The coherent scattering/imaging scenario, with the spectrometer inserted before the final wavefront sensor. (b). Efficient X-ray absorption spectroscopy using the pink beam and shot-to-shot spectral normalization.

The thin silicon crystal offers very high x-ray transmission of the device. The Si(333) geometry let through 83% of the photon flux at 8.3 keV. Therefore the spectrometer can be used as an inline diagnostics in a variety of experimental scenarios. Two examples are shown in figure 4. In the case of coherent scattering and imaging experiments in general, where maintaining the maximum flux and a stable wavefront is of the utmost importance, the spectrometer can be inserted after the main detector while before the wave front sensor. For ultrafast x-ray absorption spectroscopy, having two spectrometers, one in front of, and another behind the sample, will allow shot-to-shot normalization of the fluctuating source spectral content, thus more efficient data collection compared to scanning a monochromator upstream.

5. Conclusion

In conclusion, a transmissive hard x-ray single shot spectrometer concept based on cylindrically bent ultra-thin silicon crystal was designed, built, and tested at LCLS. SASE spectrum measurements in the hard x-ray regime are presented. While the first demonstration described here used two complimentary setup for large range and high resolution applications, a more recent test using a Si(440) geometry with increased bending have shown that 100 eV energy range can be achieved with no apparent decrease of resolution. We believe with further optimization of the crystal curvature, thickness, as well as the detection distance, in combination with a higher resolution high-speed camera, we will be capable of capturing the full SASE spectrum while resolving single energy spikes at the same time.

Acknowledgement
This research were carried out at the LCLS at SLAC National Accelerator Laboratory. LCLS is an Office of Science User Facility operated for the U.S. Department of Energy Office of Science by Stanford University.

References
[1] Emma P, et al. 2010 Nat. Photonics 4 641
[2] Ishikawa T, et al. 2012 Nat. Photonics 6 540
[3] Bonifacio R, Pellegrini C and Narducci L M 1984 Opt. Commun. 50 373
[4] Saldin E I, Schneidmiller E A and Yurkov M V 1998 Nucl. Instrum. Meth. A 407 291
[5] Lee S, et al. 2012 Opt. Express 20 9790
[6] Martins M, et al. 2006 Rev. Sci. Instrum. 77 115108
[7] Schlotter W F, et al. 2012 Rev. Sci. Instrum. 83 043107
[8] Zhu D, et al. 2012 Appl. Phys. Lett. 101 034103