

# GENERATION OF DOUBLET SPECTRAL LINES AT SELF-SEEDED X-RAY FELS

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## Abstract

We extend our recently proposed single-crystal monochromatization setup to the case when two or more crystals are arranged in a series to spectrally filter the SASE radiation at two or more closely-spaced wavelengths within the FEL gain band. This allows for the production of doublet or multiplet spectral lines. We present simulation results for the LCLS baseline operating at two closely spaced wavelengths. We show that we can produce fully coherent radiation shared between two longitudinal modes. Mode spacing can be easily tuned within the FEL gain band. The proposed scheme allows for a modulation of the electron bunch at optical frequencies without a seed quantum laser. In fact, the XFEL output intensity contains an oscillating “mode-beat” component whose frequency is related to the frequency difference between the pair of longitudinal modes considered. At saturation one obtains FEL-induced optical modulations of energy loss and energy spread in the electron bunch, which can be converted into density modulation with a weak chicane behind the baseline undulator. Powerful coherent radiation, synchronized with the X-ray pulses, can then be generated with an OTR station. **More information and a detailed reference list is available in [1].**

## INTRODUCTION

LCLS began routine user operation with photon energy up to 10 keV. This success motivated the planning of a significant upgrade over the next several years. Plans for the near-term upgrade include self-seeding for hard X-rays.

Self-seeding options for the LCLS baseline were investigated using a scheme relying on a single-crystal monochromator in Bragg-transmission geometry. The Bragg crystal reflects a narrow band of X-rays, resulting in a ringing within the passband in the forward direction, which can be used to seed the second undulator. The chicane creates a transverse offset for the electrons, washes out previous electron-beam microbunching, and provides a tunable delay of the electron-bunch with respect to the radiation, so that the electron beam only interacts with the ringing tail of the X-ray pulse.

In this paper we extend our previous investigations to the case of a self-seeding scheme with a similar kind of monochromator, consisting of two or more crystals in the Bragg geometry arranged in a series. The impinging SASE radiation is therefore spectrally filtered at two or more

closely spaced wavelengths within the FEL gain band. This allows for generation of doublet spectral lines.

Simultaneous operation of a high-gain FEL at two separate wavelengths using narrow band seed lasers was previously studied elsewhere (see [1] for references). Applications of such mode of operation involve any process where there is a large change in cross section over a narrow wavelength range. Here we present simulation results for the LCLS baseline and we show that our method can produce a doublet structure in the LCLS hard X-ray FEL spectrum.

The XFEL-output intensity contains an oscillating “mode-beat” component whose frequency is related to the frequency difference between the pair of longitudinal modes considered. With the help of a weak chicane installed behind the baseline undulator a powerful, coherent pulse of radiation can then be generated with the help of an optical transition radiation (OTR) station. We briefly consider how the generation of doublet structures in the XFEL spectrum can be monitored by an optical spectrometer analyzing this OTR coherent pulse. Furthermore, we stress how the OTR coherent radiation pulse is naturally synchronized with the X-ray pulses, and can be used for timing the XFEL to high power conventional lasers with femtosecond accuracy for pump-probe applications.

## OPERATION OF THE LCLS HARD X-RAY FEL AT CLOSELY SPACED WAVELENGTHS

An overview of the proposed setup is sketched in Fig. 1. The reader may recognize similarities with the previously proposed schemes, except for the presence of two crystals, instead of one, located in the transverse offset provided by the magnetic chicane. As before, the first undulator in Fig. 1 operates in the linear high-gain regime starting from the shot-noise in the electron beam.

After the first undulator, the output SASE radiation passes through the monochromator, consisting of a series of two (or more) crystals in the Bragg transmission geometry. The monochromator setup is sketched in Fig. 2. According to our monochromator principle, the SASE pulse coming from the first undulator impinges on a set of two or more crystals in Bragg diffraction geometry. Then, the crystals operate as bandstop filters for the transmitted X-ray SASE radiation pulse, as shown in Fig. 3. Parameters used in the simulations for the short pulse mode of operation are presented in Table 1. In the plots we present a statistical analysis consisting of 100 runs.

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self-seeding scheme with wake monochromator for the LCLS baseline undulator

two-color operation of LCLS baseline at closely spaced wavelengths

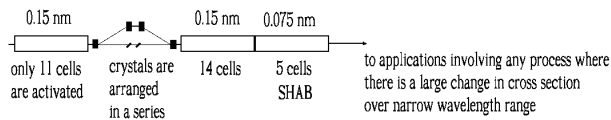


Figure 1: Design of the LCLS baseline undulator system for generation of doublet spectral lines.

operation of wake monochromator at two closely spaced wavelengths

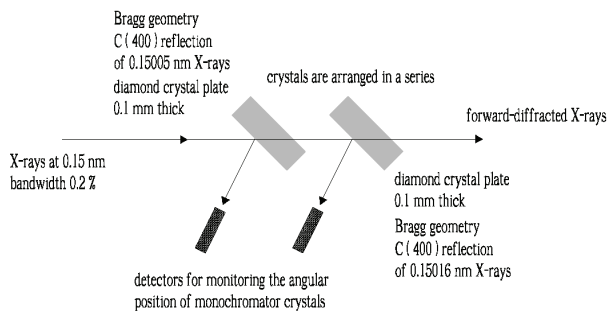


Figure 2: Forward diffraction in a series of crystals in Bragg geometry. The incident angles on the first and on the second crystal are different. Due to multiple scattering, the transmittance spectrum of the crystals shows doublet absorption lines. The temporal waveform of the transmitted radiation pulse is characterized by a long tail. The radiation power within such tail is shared between two harmonic waves with slightly different wavenumbers.

The incident angles of the first and of the second crystal are different, so that the Bragg condition is met for different frequencies within the SASE spectrum. The temporal waveform of the transmitted radiation pulse shows a long tail, whose duration is inversely proportional to the bandwidth of the absorption line in the transmittance spectrum. This tail can be used for seeding the electron bunch after the chicane. It should be noted here that the ringing tail does not depend on the distance between the crystals, and that such distance has no influence on the output characteristics of the radiation, Fig. 4. At variance with previously considered schemes relying on a single crystal, here two bandstop filters are present at different frequencies. As a result, both frequency components are present in the seeding signal, and will be amplified in the output undulator. This allows for the production of doublet spectral lines. The output signal from our setup is thus fully coherent, but shared between two separate longitudinal modes. The relative alignment tolerance of the crystal tilting angles should

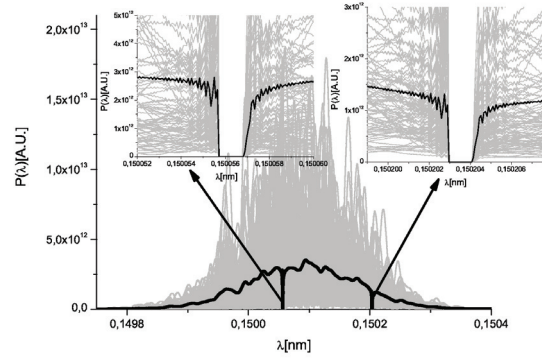


Figure 3: Spectrum after the diamond crystals, 100  $\mu\text{m}$ -thick, C(400) reflection. The bandstop effect is clearly visible. Grey lines refer to single shot realizations, the black line refers to the average over a hundred realizations.

Table 1: Parameters for the Low-charge Mode of Operation at LCLS used in this Paper

	Units	
Undulator period	mm	30
K parameter (rms)	-	2.466
Wavelength	nm	0.15
Energy	GeV	13.6
Charge	nC	0.02
Bunch length (rms)	$\mu\text{m}$	1
Normalized emittance	mm mrad	0.4
Energy spread	MeV	1.5

now be in the order of ten microrad, in order to allow for a stable frequency difference within the Darwin width.

While the radiation is sent through the crystals, the electron beam passes through a magnetic chicane, which accomplishes three tasks: it creates an offset for the crystals installation, it removes the electron microbunching produced in the first undulator, and it acts as a delay line for the implementation of a temporal windowing process. In this process, the magnetic chicane shifts the electron bunch on top of the monochromatic tail created by the bandstop filter thus temporally selecting a part of it. By this, the electron bunch is seeded with a radiation pulse characterized by a bandwidth much narrower than the natural FEL bandwidth. For the hard X-ray wavelength range, a small dispersive strength  $R_{56}$  in the order of a few microns is sufficient to remove the microbunching generated in the first undulator part. As a result, the choice of the strength of the magnetic chicane only depends on the delay that one wants to introduce between electron bunch and radiation. The optimal value amounts to  $R_{56} \simeq 12 \mu\text{m}$  for the low-charge mode of operation. Such dispersion strength is small enough to be generated by a short (4 m-long) magnetic chicane to be installed in place of a single undulator module. Such chicane is, at the same time, strong enough to create a sufficiently large transverse offset for installing the crystals.

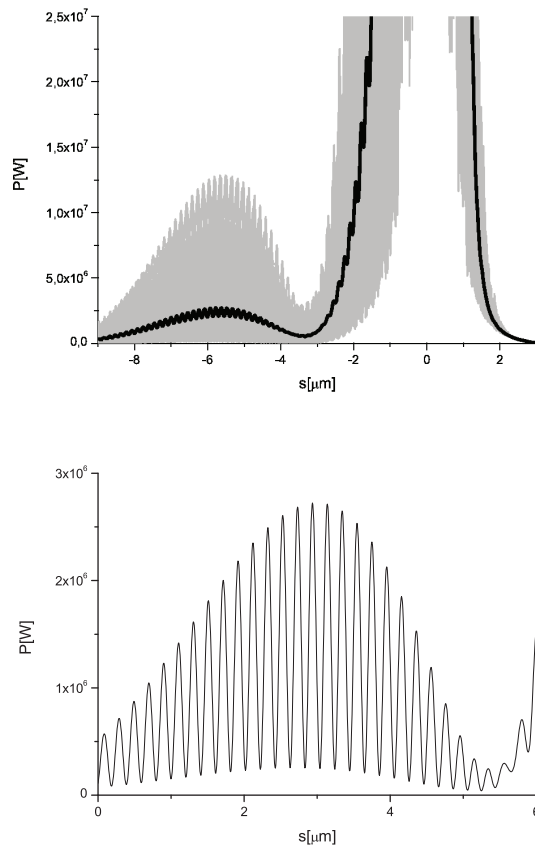


Figure 4: (upper) Power distribution after the diamond crystals. The monochromatic tail due to the transmission through the bandstop filters is now evident on the left of the figure. Grey lines refer to single shot realizations, the black line refers to the average over a hundred realizations. (lower) An enlargement of a single shot seed power distribution presented in the left part of the plot. The seed signal consists of two harmonic waves with slightly different wavenumbers. The form of this type of signal is interesting, and consists of a rapidly oscillating (at X-ray angular frequency) carrier wave multiplied by a simple sinusoidal envelope function at optical angular frequency. The beat of the sinusoidal envelope (see the maximum at 6  $\mu\text{m}$ ) is related to specific features of the transmittance profile of the band-stop filter.

The output power and spectrum of the setup is shown in Fig. 5. Since two bandstop filters are present at slightly different frequencies, the seed signal contains a “mode-beat” component whose frequency is related to the difference between central frequencies of the bandstop filters. In other words, the seeding power distribution is modulated at optical frequencies, as is evident from the lower part of Fig. 4, which is an enlargement of the average (black) line in the upper part of the same figure. As a result, the output from our setup exhibits a remarkable feature: namely we have a modulation of the output radiation power and of the energy

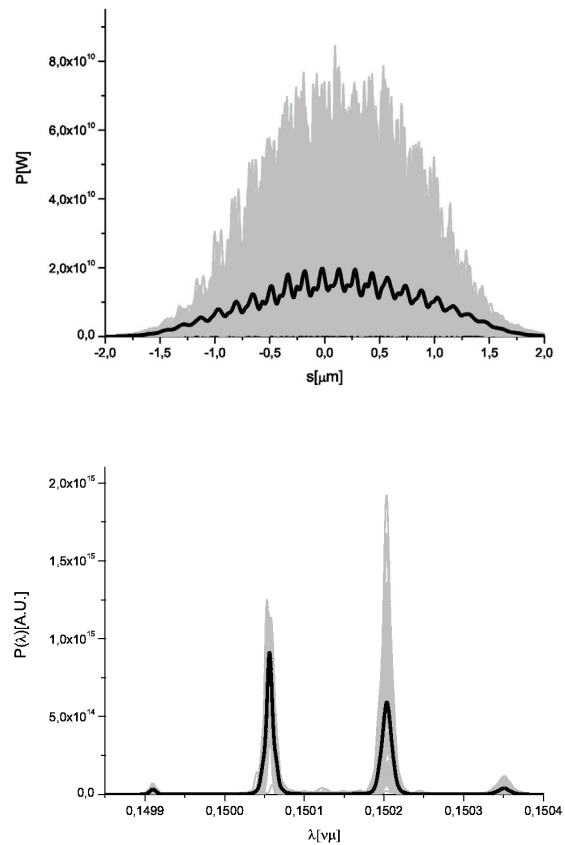


Figure 5: (upper) Power distribution of the X-ray radiation pulse at saturation. (lower) Spectrum of the X-ray radiation pulse. Grey lines refer to single shot realizations, the black line refers to the average over a hundred realizations.

loss and energy spread of the electron beam at a frequency related with the difference between the central frequencies of the bandstop filters.

One may take advantage of such energy modulation by transforming it into a density modulation, which can be used to produce powerful pulses of coherent radiation in the visible range. This can be done with the help of an extra magnetic chicane installed after the XFEL undulator at the LCLS baseline. A dispersive strength of 50 – 100 microns is enough to this end. The output particle file from Genesis is used as input to the code Elegant to study the electron beam dynamics through the magnetic chicane.

As a simple example of radiator one may consider an OTR station. It is technically possible to avoid interference between the OTR pulse production and the X-ray beam delivery. In fact, the vacuum chamber downstream of the main undulator has an effective aperture of 25 mm, which is the diameter of the BPM bore. Such aperture is sufficiently large to alter the electron beam trajectory (with the help of correctors) and to introduce an offset in the order of a centimeter, thus separating electron beam from X-rays.

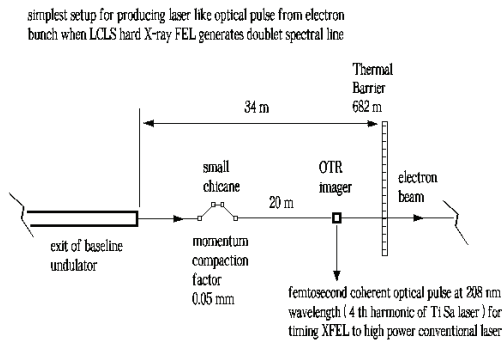


Figure 6: Installation of a small dispersive element (magnetic chicane) and of an OTR station after the LCLS baseline undulator will allow to produce laser-like optical pulses from electron bunches when the LCLS hard X-ray FEL generates doublet spectral lines.

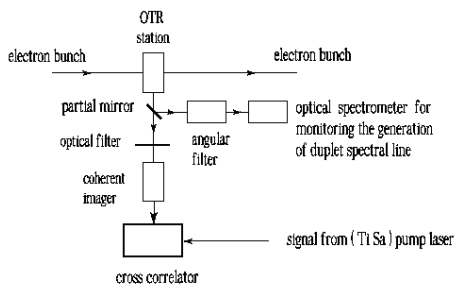


Figure 7: Block diagram view of possible coherent OTR pulse applications.

Since we deal with optical wavelengths, such electron orbit perturbation will not change the density modulation in the electron bunch.

Several applications can be considered. The presence of coherent pulses of OTR can be used, with the help of an optical spectrometer, to monitor the generation of the doublet spectral lines. Moreover, the OTR pulses are naturally synchronized with the electron bunches, and therefore with the main X-ray FEL pulses. After filtering, these pulses can be cross-correlated with a harmonic signal from a Ti:Sa pump laser in order to provide a timing of pump and probe pulses with an accuracy within a few femtoseconds.

## CONCLUSIONS

In this article we presented an extension to our previously proposed method for self-seeding, which was based on the use of a single Diamond crystal in Bragg geometry acting as a band-stop filter. Here we extend such treatment to a series of two or more crystals tuned at closely-spaced frequencies, and we demonstrate the possibility of generat-

ing doublet spectral lines through the self-seeding process. In other words, fully coherent radiation is shared between two longitudinal modes. Depending on the crystals settings one can have one mode dominating on the other, or a balance between the two<sup>1</sup>. Moreover, the spacing between the two modes can be tuned within the FEL gain band, i.e. within 10 eV. Once doublet spectral lines are generated, they can be used to study processes dealing with a large change in cross-section over a narrow wavelength range.

Furthermore, possibility of pump-probe experiments with sub-femtosecond resolution where an external optical laser is involved are enabled. In fact, a power beating between the two closely spaced wavelengths of the doublet yields a modulation of the SASE output power on the visible range. By energy conservation, such modulation is printed on the electron bunch as an energy modulation at the same frequencies, which can be transformed into a density modulation with the help of a weak dispersive element. The modulated electron bunch can then be made radiating coherently with the help of any radiator, e.g. an OTR screen. A powerful pulse of coherent radiation in the optical range is then produced, which is intrinsically synchronized to the X-ray photon pulse, and can be cross-correlated to an external pump-laser. Such correlation results in the possibility of measuring the jitter between SASE doublet and external optical pump with a few femtosecond accuracy. The coherent optical pulse may also be used to monitor the formation of the doublet, since it will appear only when the doublet is actually present, which enables beating.

From the technical viewpoint, the present method constitutes a minor upgrade of our previously proposed technique relying on a single crystal, of which it retains flexibility, simplicity of implementation, low cost and no risk for the recovering of the baseline mode of operation.

## REFERENCES

- [1] G. Geloni, V. Kocharyan and E. Saldin, "Generation of doublet spectral lines at self-seeded X-ray FELs", DESY 10-199 (2010) <http://arxiv.org/abs/1011.3910>, and Optics Communications, Volume 284, Issue 13, 3348-3356 (2011)

<sup>1</sup>It should be noted that the idea of radiation shared between longitudinal modes should be thought of from a statistical standpoint. In other words, here we are talking about an average over ensemble of shots, not about a single realization.