HARD X-RAY SELF-SEEDING FOR XFELS: TOWARDS COHERENT FEL PULSES

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Abstract

Start-up from shot noise limits the longitudinal coherence of typical SASE XFEL pulses. Self-seeding schemes provide an elegant solution to this problem. However, their applicability to the baseline of already working or designed XFELs is subject to constraints, including minimal changes to the baseline design and possibility to recover the baseline mode of operation. Here we discuss a recently proposed single-bunch self-seeding scheme for hard X-rays. The physical principles of this scheme can be extended to soft X-rays as well. The method is based on a particular kind of monochromator, which relies on the use of a single crystal in Bragg-transmission geometry. In its simplest configuration, the setup consists of an input undulator and an output undulator separated by such monochromator. Several, more advanced configurations can be considered. For example, for high repetition rates of the X-ray pulses, or when a high spectral purity of the output radiation is requested, the simplest two-undulator configuration is not optimal: three or more undulators separated by monochromators can then be used. Exemplifications, based on facilities working or under construction will be discussed. **These proceedings are based on [1]-[5], to which we address the interested reader for further information and references.**

INTRODUCTION

SASE X-ray beams are characterized by nearly complete transverse coherence, but due to the inherent nature of the SASE process, the pulses only possess partial longitudinal coherence. This is a consequence of the fact that in SASE FELs the amplification process starts up from noise. For conventional XFELs, the typical pulse bandwidth is much larger than the Fourier transform limited value for the radiation pulse duration. Self-seeding schemes have been studied to reduce the bandwidth of SASE X-ray FELs. A self-seeded XFEL consists of two undulators with an X-ray monochromator located between them. The implementation of such scheme for the hard X-ray range could exploit a crystal monochromator. Typically, self-seeding schemes make use of a four-crystal, fixed-exit monochromator in Bragg reflection geometry. The X-ray pulse thus acquires a cm-long path delay, which must be compensated. For a single-bunch self-seeding scheme this requires a long electron beam bypass, implying modifications of the baseline undulator configuration. To avoid this problem, a new method of monochromatization exploiting a single crystal in Bragg transmission geometry was proposed. A great advantage of this method is that the single crystal monochromator introduces no path delay of X-rays. This fact eliminates the need for long electron beam bypass, or for the creation of two precisely separated identical electron bunches, as required in the other self-seeding schemes (see references in [1]). An example setup is shown in Fig. 1. The first undulator operates in the linear high-gain regime starting from the shot-noise in the electron beam. In order not to spoil the electron beam quality, the power gain of the first undulator should be about three orders of magnitude smaller than the power gain of the X-ray SASE FEL at saturation. Here we consider a typical hard X-ray FEL, where the effective power of shot-noise in the electron beam is $P_{\mathrm{n}} \sim 3$ kW, and the power of the SASE radiation at saturation is $P_{\mathrm{sat}} \sim 30$ GW. Thus one requires that the power gain of the first undulator be no more than four orders of magnitude. After the first undulator, the output SASE radiation passes through the monochromator, which reduces the bandwidth to the desired value. According to the single-crystal monochromator principle, the SASE pulse coming from the first undulator impinges on a crystal set for Bragg diffraction. Then, the single crystal in Bragg geometry actually operates as a bandstop filter for the transmitted X-ray SASE radiation pulse, as shown in Fig. 2. When the incident angle and the spectral contents of the incoming beam satisfy the Bragg diffraction condition, the temporal waveform of the transmitted radiation pulse shows a long monochromatic tail. The duration of this tail is inversely proportional to the bandwidth of the absorption line in the transmittance spectrum. While the radiation is sent through the crystal, the electron beam passes through a magnetic chicane, which creates an offset for the crystal installation, removes the electron micro-bunching produced in the first undulator, and acts as a delay line for the implementation of a temporal windowing technique: the magnetic chicane shifts the electron bunch on top of the monochromatic tail created by the bandstop filter thus selecting (temporal windowing) a part of the tail. 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 ten microns (for the shortest bunch case corresponding to a 1 μm rms bunch length) is sufficient to remove the micro bunching in the electron bunch. As a result, the choice of the strength of the magnetic chicane only depends on the delay that we want to introduce between electron bunch and radiation. Moreover, the required dispersion strength is small enough

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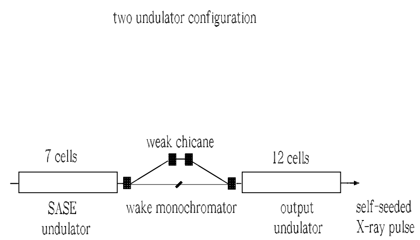

Figure 1: Self-seeding setup with single-crystal monochromator. Two undulator configuration.

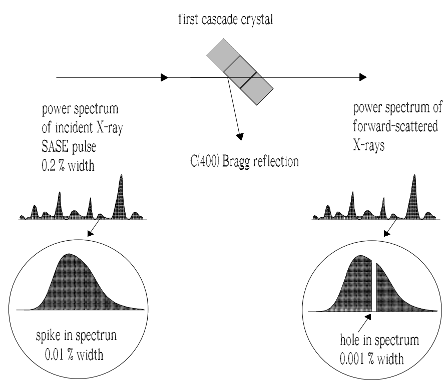

Figure 2: The crystal acts as a bandstop filter for the transmitted X-ray SASE radiation pulse.

to be generated by a short 5 m-long chicane to be installed in place of a single undulator module. The chicane is, however, strong enough to create a sufficiently large transverse offset of a few millimeters for installing the crystal.

In some experimental situations, like in the LCLS case, the simplest two-undulator configuration for self-seeding scheme is practically advantageous. In other cases it is not optimal, like for the European XFEL, where high heat-loading of the crystal due to the higher repetition rate. The obvious and technically possible extension is to use a setup with three or more undulators separated by monochromators. This cascade scheme is distinguished, in performance, by a small heat-loading of crystals at a very high repetition rate. There still remains room for improving the output characteristics of the XFEL. The most promising way to increase the output power is by tapering the magnetic field of the undulator. Significant further increase in power is achievable by starting the FEL process from a monochromatic seed rather than from noise. It is also possible to create a pair (or multiplet) of pulses with slightly different frequencies by setting two (or more) crystals in a series. In this contribution we summarize all these techniques. Also, start-to-end simulations for the electron beam can be included in the self-seeding simulations. We exemplify this possibility for the nominal (1 nC) mode of operation for the LCLS. Finally, we speculate how this self-seeding technique can be extended to the soft X-ray region as well.

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)	μm	1
Normalized emittance	mm mrad	0.4
Energy spread	MeV	1.5

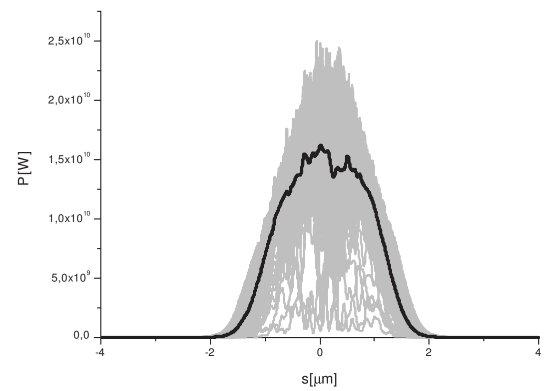

Figure 3: LCLS low charge mode of operation. Power distribution of the X-ray radiation pulse at saturation. Grey lines refer to single shot realizations, the black line refers to the average over a hundred realizations.

THE LCLS SHORT BUNCH MODE OF OPERATION

Following the introduction of the proposed method we summarize a feasibility study of the single-bunch self-seeding scheme with a wake monochromator for the LCLS. The LCLS enables both a low charge, short bunch mode of operation characterized by an electron beam charge of 0.02 nC and a 1 μm rms-long lasing part of the bunch, and a nominal charge, long bunch mode of operation, characterized by an electron beam charge of 0.25 nC and a 10 μm rms-long lasing part of the bunch. In this section we consider the low charge mode of operation for the LCLS. Parameters used are presented in Table 1. This study is discussed in more detail in [1], to which the reader is addressed for a comprehensive set of references. The output power and spectra are shown in Fig. 3 and Fig. 4 respectively. A peak power of about 15 GW is foreseen. Monochromatization is in the order of 10^{-4}.

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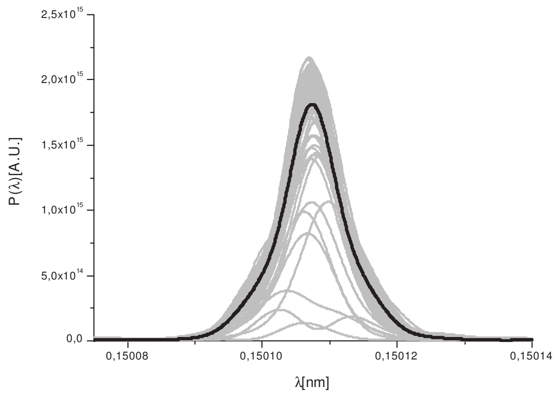

Figure 4: LCLS low charge mode of operation. Spectrum of the X-ray radiation pulse at saturation. Grey lines refer to single shot realizations, the black line refers to the average over a hundred realizations.

THE EUROPEAN XFEL SHORT BUNCH MODE OF OPERATION

To provide effective operation of the self-seeded XFEL, we must require that the power of the monochromatic seed signal P_{seed} at the entrance of the output undulator significantly exceeds the effective shot-noise power in the electron beam, i.e. $P_{\mathrm{seed}} \gg P_{\mathrm{n}}$. This in its turn requires a relatively long first undulator, which becomes problematic for the European XFEL due to the high repetition rate of X-ray pulses (about 10 trains of pulses per second, each train consisting of about 3000 pulses), which leads to a large heat-loading of the crystal. If the first undulator is shortened, the spectral purity of the output from the entire setup degrades, due to large SASE background contributions. A post-monochromator can be used to filter out the SASE signal. However, spectral purity can be of crucial importance for application of some other techniques like tapering and polarization manipulations, i.e. for the next steps of performance improvement. In this section we summarize a method to increase the value of P_{seed}. A high value of the signal-to-noise ratio at the entrance of the output undulator may be obtained by using more than one stage of amplification-monochromatization, which we will call "cascade". The scheme is discussed in more detail in [2], to which the reader is addressed for a comprehensive set of references. Two cascades can be arranged sequentially as shown in Fig. 5. To be specific, here we consider the case of two identical cascades. As discussed above, due to the shortness of the first undulator, the signal-to-noise ratio at the entrance of the second undulator cannot be much larger than unity. Nevertheless, the monochromatic field amplitude at the entrance of the third undulator will be much larger than that at the entrance of the second. The difference with respect to the previously discussed two-undulator configuration is that after amplification in the second undulator, the bandwidth of the X-ray pulse related with the monochromatic signal that impinges on the second crystal is near to the transform-limited bandwidth of the electron bunch i.e. c/σ_e. As a result, assuming the same amplification in the two cascades, the signal to noise ratio is enhanced by a factor $\sigma_e \Delta\omega_{SASE}/c$, where $\Delta\omega_{SASE}$ is the SASE bandwidth. A rough estimate for the signal to noise ratio at the entrance of the third (output) undulator is therefore $P_{\mathrm{seed2}}/P_{\mathrm{n}} \sim (P_{\mathrm{seed1}}/P_{\mathrm{n}})\sigma_e \Delta\omega_{SASE}/c \gg 1$. Since this value is much larger than unity, we conclude that a double cascade self-seeding scheme using a single-crystal monochromator is insensitive to noise and non-ideal effects. The two-cascade setup drastically relaxes the heat load on the crystals, and eliminates the presence of off-band SASE radiation, still retaining the advantage of a high signal to noise ratio. Referring to Table 2, here we consider an example when two cascades are present for the SASE2 line of the European XFEL. For simplicity we neglect the effects of wakefields on the electron bunch.

Following the second crystal, the radiation is used to seed once more the electron bunch. Radiation is collected at the exit of a third undulator. The upper and lower plots in Fig. 6 respectively show the output power and spectrum for the three-undulator configuration. By tapering the last (output) section of the FEL it is possible to increase the output power up to the TW level, Fig. 7.

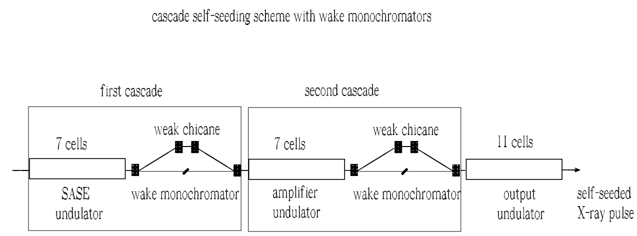

Figure 5: Design of an undulator system for narrow-bandwidth mode of operation. The scheme is based on the use of a cascade, single bunch self-seeding scheme with single-crystal monochromators.

Table 2: Parameters for the short pulse mode of operation of the European XFEL used in this paper.

	Units	
Undulator period	mm	48
K parameter (rms)	-	2.516
Wavelength	nm	0.15
Energy	GeV	17.5
Charge	nC	0.025
Bunch length (rms)	μm	1.0
Normalized emittance	mm mrad	0.4
Energy spread	MeV	1.5

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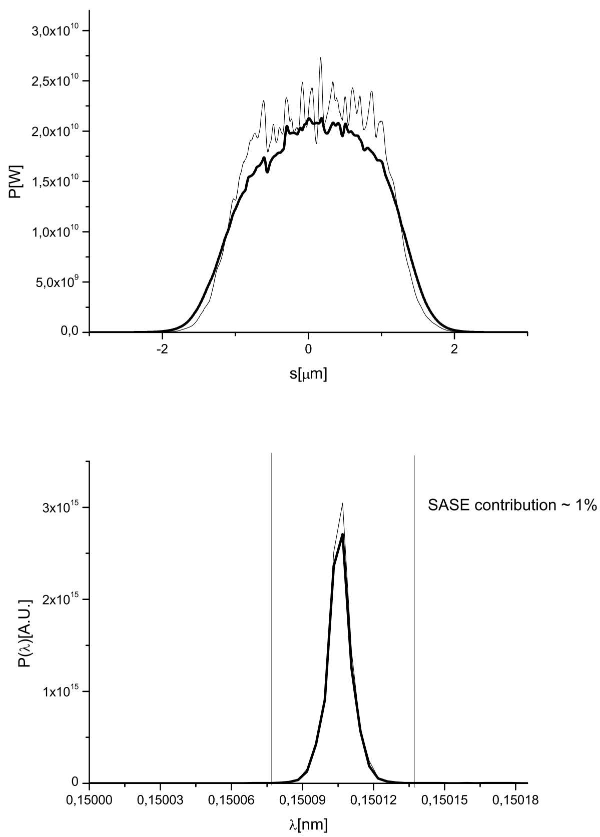

Figure 6: Three-undulator configuration. Short pulse mode of operation. Upper plot: average and typical single-shot output power (respectively, thick and thin solid lines). Lower plot: average and typical single-shot output spectrum (respectively, thick and thin solid lines). An estimation of the SASE contribution can be done by evaluating the total power outside the spectral window shown with black straight lines and dividing it to the spectral power integrated over all the spectrum.

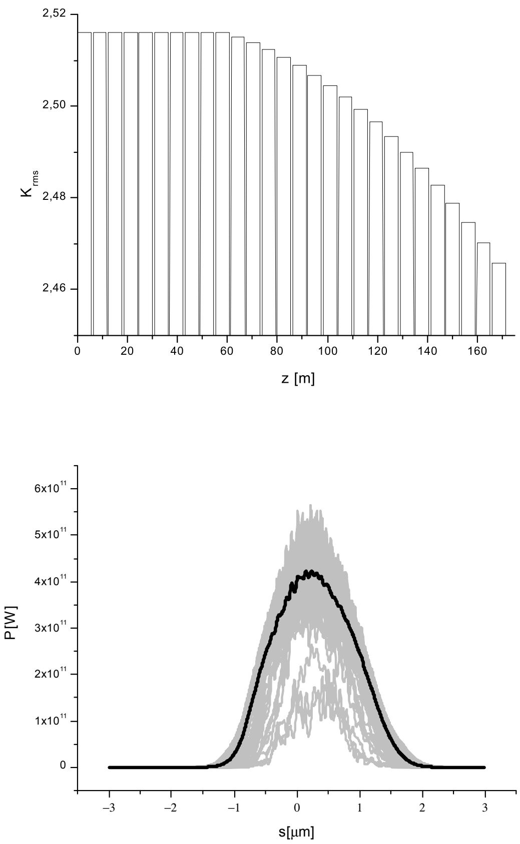

Figure 7: Short bunch mode of operation. Upper plot: tapering law. Lower plot: power distribution of the X-ray radiation pulse in the case of undulator tapering. Grey lines refer to single shot realizations, the black line refers to the average over a hundred realizations.

NOMINAL MODE OF OPERATION: THE LCLS CASE

Up to now we limited our consideration for the LCLS to the low charge mode of operation.

In this section we extend our considerations to the nominal charge mode of operation of the LCLS. The scheme is discussed in more detail in [3], to which the reader is addressed for a comprehensive set of references as well. We study the performance of our self-seeding scheme for the LCLS based on start-to-end electron beam simulations. Particle tracking through the LCLS linac for the nominal charge case was studied by the LCLS staff, and the resistive-wall wakefield in the LCLS undulator was also calculated including the frequency dependence of beam-pipe conductivity. This wakefield generates an energy change, different for each time-slice along the bunch, shifting slices out of resonance, and thus reducing the total FEL power. A feasibility study of the two-bunch self-seeding scheme for the LCLS nominal charge mode of operation was also presented (see Ref. 10 of [3]). We will consider that feasibility study as the reference point for our investigations. The setup which will be considered in this work is sketched in Fig. 8, and is composed of two undulator parts separated by a weak chicane. At variance with previously discussed schemes this time the chicane should provide a delay in the order of 50μm, meaning that $R_{56} \simeq 100\mu$m, and can be installed within the space of a single undulator segment (4 m long at the LCLS). Using a single crystal installed in the offset created by the chicane it is possible to decrease the bandwidth of the radiation well beyond the XFEL design down to $3 \cdot 10^{-5}$. Compared with the low charge case discussed before, where almost all the electrons radiate coherently, here we have a strong SASE signal due to the typical double-horn current profile and to the electron energy modulation generated by the undulator wakefield. Nevertheless, as proposed by the LCLS staff (see Ref. 10 of [3]), we can use a post-baseline monochro-

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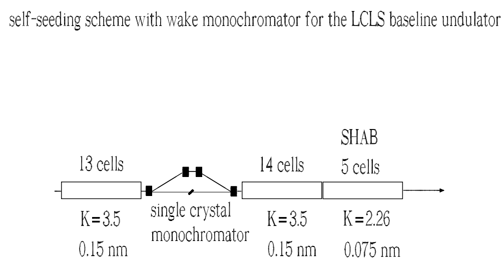

Figure 8: Design of the LCLS baseline undulator system for generating highly monochromatic hard X-ray pulses in the nominal charge (250 pC) mode of operation.

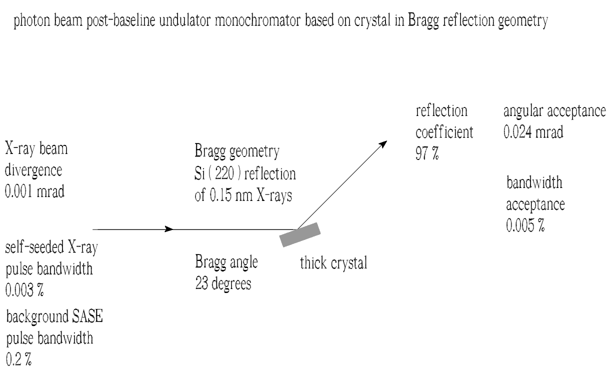

Figure 9: Concept of post-baseline undulator monochromator for SASE background suppression based on the use of a crystal in Bragg reflection geometry.

mator for SASE background suppression, based on the exploitation of a thick crystal in Bragg reflection geometry, Fig. 9. A feasibility study was performed with the help of the FEL code GENESIS 1.3 running on a parallel machine. The overall beam parameters used in the simulations are as in Ref. 10 of [3], and are presented in Table 3.

The electron beam distribution at the entrance of the undulator are shown in terms of energy and current in Fig. 4 and Fig. 5 of Ref. 10 in [3]. As mentioned above, the LCLS

Table 3: Parameters for the nominal charge mode of operation at LCLS used in this paper.

	Units	
Undulator period	mm	30
K parameter (rms)	-	2.466
Wavelength	nm	1.55
Energy	GeV	13.4
Charge	nC	0.25
Bunch length (fw)	μm	26.6
Normalized emittance	mm mrad	0.4
Energy spread	MeV	1.4

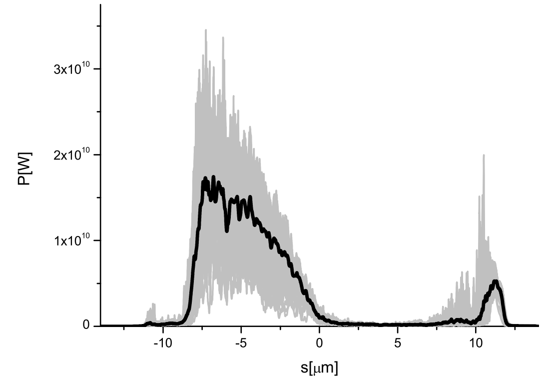

Figure 10: Output power of the setup. Grey lines refer to single shot realizations, the black line refers to the average over 70 realizations.

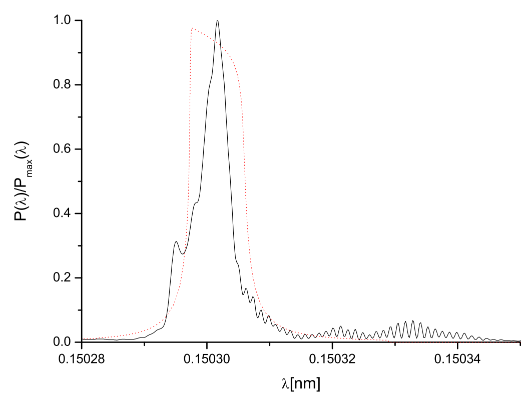

Figure 11: (Solid line) Average output spectrum of the setup, normalized. (Dotted line) Shape of the thick crystal filter Si(220).

beam operated at nominal charge mode is characterized by a ”double-horn” current distribution, which introduces additional energy modulation on the bunch due to wakefield effects in the undulator chamber. The resistive-wall energy loss in the LCLS undulator at nominal charge is shown in Fig. 6 of Ref. 10 in [3]. The output power of our setup is shown in Fig. 10. The corresponding average spectrum can be seen in Fig. 11. As one can see from the figures, our single-bunch self-seeding technique leads to the production of x-ray pulses with a relative bandwidth of about $3 \cdot 10^{-5}$, yielding about 12 GW power, and with 15 fs FWHM duration, very similar to the output results from Ref. 10 in [3], which is based on a two-bunch technique. Moreover not that, as said before, the output signal can be further filtered to obtain better spectral properties.

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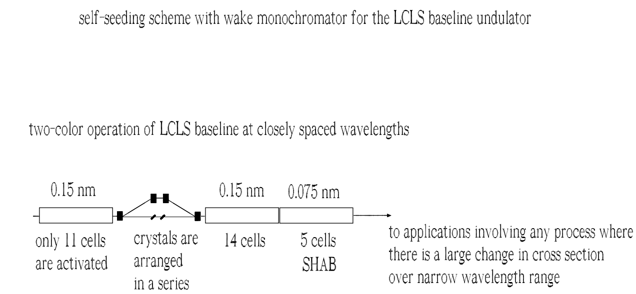

Figure 12: Design of the LCLS baseline undulator system for generation of doublet spectral lines.

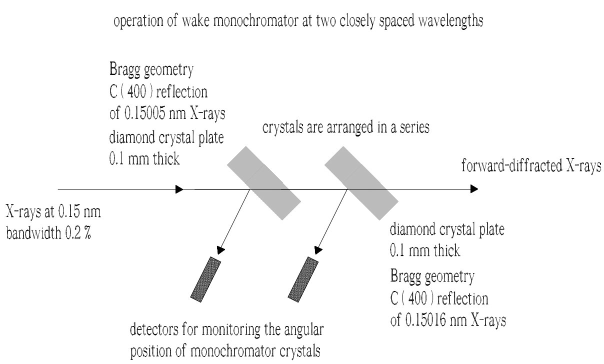

Figure 13: Forward diffraction in a series of crystals in Bragg geometry.

DOUBLET GENERATION

A possible extension of previously described techniques consists in using two -or more- crystals arranged in a series, instead of a single one, 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. Applications exist over a broad range of hard X-ray wavelengths involving any process where there is a large change in cross section over a narrow wavelength range. An overview of the proposed setup is sketched in Fig. 12. The scheme is discussed in more detail in [4], to which the reader is addressed for a comprehensive set of references. Two crystals, instead of one, are located in the transverse offset provided by the magnetic chicane. As before, the first undulator in Fig. 12 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. 13. 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

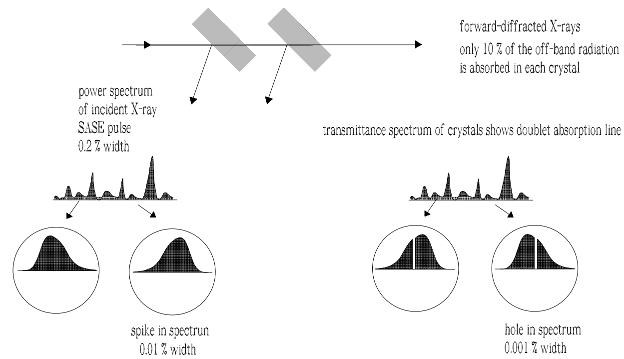

Figure 14: Two crystals bandstop filter as monochromator for the self-seeding scheme.

crystals operate as bandstop filters for the transmitted X-ray SASE radiation pulse, as shown in Fig. 14. 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. 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. At variance with previously considered schemes relying on a single crystal, here two bandstop filters are present at different frequencies. As a result, two frequency components are to be found 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 now be in the order of ten microradians, to allow for a stable frequency difference within the Darwin width. As usual, while the radiation is sent through the crystals, the electron beam passes through a magnetic chicane. A consequence of the presence of two bandstop filters at different frequency is that the seed signal contains a "mode-beat" component whose frequency is related to the difference between central frequencies of the bandstop filters. As a result, the output from our setup exhibits a remarkable feature: a modulation of the output radiation power and of the energy 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, as depicted in Fig. 15. 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, as sketched in Fig. 15 and Fig. 16. It is technically

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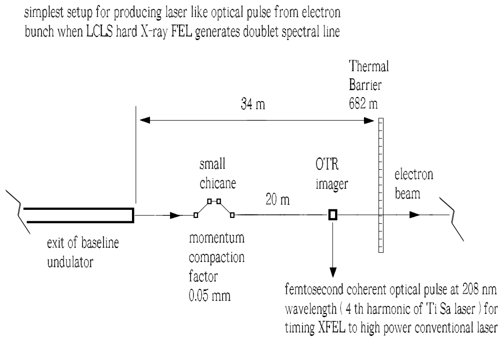

Figure 15: Installation of a small dispersive element (magnetic chicane) and of an OTR station after the LCLS baseline undulator.

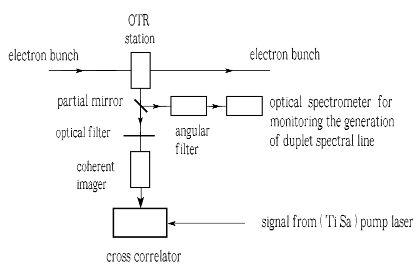

Figure 16: Block diagram view of possible coherent OTR pulse applications.

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 introduce an offset in the order of a centimeter, thus separating the electron beam and the X-ray. Since we deal with optical wavelengths, such electron orbit perturbation will not perturb the density modulation in the electron bunch. Several applications can be considered. With reference to Fig. 16 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.

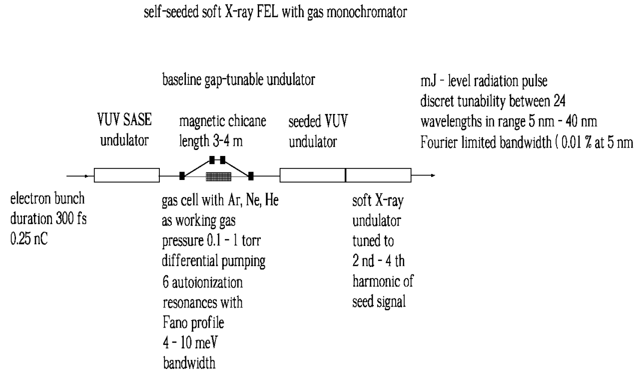

Figure 17: Design of the VUV - soft X-ray FEL undulator system for narrow bandwidth mode of operation.

EXTENSION TO SOFT X-RAYS

Self-seeding schemes have been proposed not only for hard X-rays, but also for the VUV and soft X-ray region. In this case, they make use of a grating monochromator. This introduces a path delay with respect to the straight path, which has to be compensated with the introduction of a bypass of the length of about 30 m for the case of the LCLS-II.

The previously discussed techniques for hard X-rays can be extended to the soft X-ray region exploiting a cell containing resonantly absorbing gas in the transmission direction. Such cell works, in analogy with the single-crystal monochromator method for the hard X-ray, as a bandstop filter. The scheme is discussed in more detail in [5], to which the reader is addressed for a comprehensive set of references. The proposed setup is extremely simple, and composed of two elements: a gas cell and a short magnetic chicane, Fig. 17. As for the hard X-ray case, the magnetic chicane accomplishes three tasks. It creates an offset for gas cell installation, it removes the electron micro bunching produced in the first undulator, and it acts as a delay line for the electron bunch. Thus, using a cell with rare gas installed within a short magnetic chicane in the baseline soft X-ray undulator as a bandstop filter, it is possible to decrease the bandwidth of the VUV radiation down to the Fourier limit. One can implement the proposed scheme in the soft X-ray region, exploiting the tunable-gap soft X-ray baseline undulator. One can first perform monochromatization at $20 - 40$ nm with the help of the gas-cell monochromator, and subsequently amplify the radiation in the first part the of output undulator. The amplification process can be stopped at some position well before the FEL reaches saturation, where the electron beam gets considerable bunching at the 2nd, 3rd and 4th harmonic of the coherent radiation. The undulator downstream that position can then be tuned to a given harmonic frequency to amplify the radiation further to saturation, Fig. 17. A feasibility study of the self-seeding scheme with gas monochromator for the LCLS-II has been described in detail in [5]. The main parameters are as in Table 4. The tentative de-

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Table 4: Parameters for the nominal pulse mode of operation of the soft X-ray setup.

	Units	
Undulator period	mm	60
K parameter	-	1.3-12
Wavelength (fundamental)	nm	19.2
Energy	GeV	3.5
Charge	nC	0.25

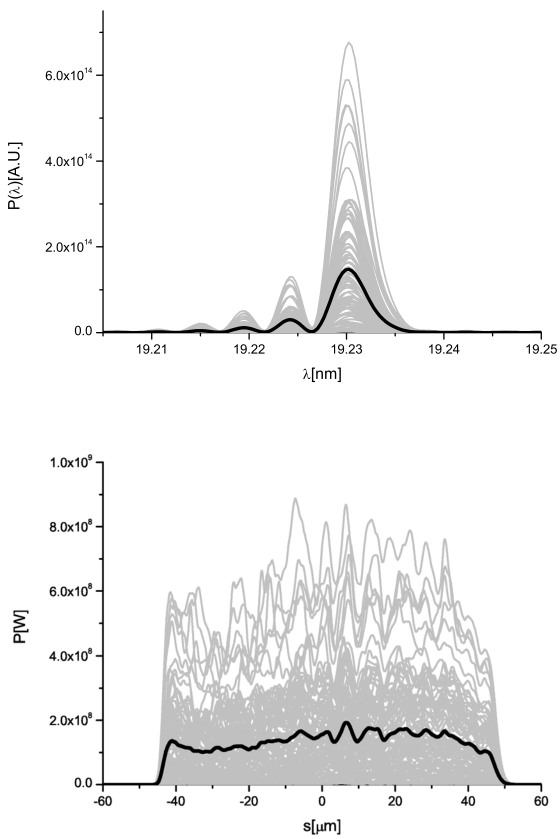

Figure 18: Spectrum (upper plot) and power (lower plot). Grey lines refer to single shot realizations, the black line refers to an average over 100 realizations. The second undulator is tuned at the fundamental.

sign for the proposed technique at LCLS-II allows to generate fully coherent radiation at a wavelength of about 5 nm. The output of the fundamental is shown in Fig. 18. The final output at the fourth harmonic is shown in Fig. 19, showing power and spectrum. A mJ, fully coherent pulse with a bandwidth in the order of the 0.01% is produced at a wavelength of 4.8 nm.

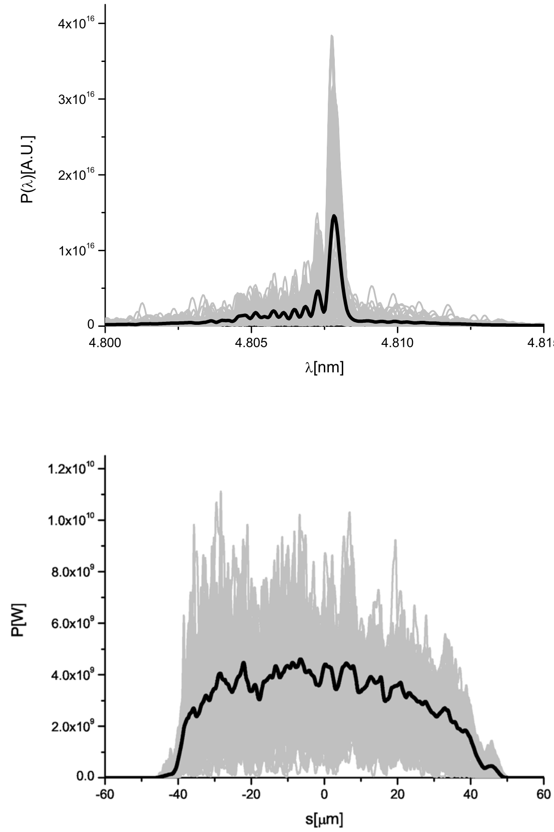

Figure 19: Spectrum (upper plot) and power (lower plot). Grey lines refer to single shot realizations, the black line refers to an average over 100 realizations. The second undulator is tuned at the fourth harmonic.

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