Extension of self-seeding to hard X-rays $> 10$ keV as a way to increase user access at the European XFEL

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Abstract

We propose to use the self-seeding scheme with single crystal monochromator at the European X-ray FEL to produce monochromatic, high-power radiation at 16 keV. Based on start to end simulations we show that the FEL power of the transform-limited pulses can reach about 100 GW by exploiting tapering in the tunable-gap baseline undulator. The combination of high photon energy, high peak power, and very narrow bandwidth opens a vast new range of applications, and includes the possibility to considerably increase the user capacity and fully exploit the high repetition rate of the European XFEL. In fact, dealing with monochromatic hard X-ray radiation one may use crystals as deflectors with minimum beam loss. To this end, a photon beam distribution system based on the use of crystals in the Bragg reflection geometry is proposed for future study and possible extension of the baseline facility. They can be repeated a number of times to form an almost complete (one meter scale) ring with an angle of 20 degrees between two neighboring lines. The reflectivity of crystal deflectors can be switched fast enough by flipping the crystals with piezo-electric devices similar to those for X-ray phase retarders at synchrotron radiation facilities. It is then possible to distribute monochromatic hard X-rays among 10 independent instruments, thereby enabling 10 users to work in parallel. The unmatched repetition rate of the European XFEL would be therefore fully exploited.

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Fig. 1. Sketch of an undulator system for high power mode of operation at a photon energy of 8 keV. The method exploits a combination of cascade self-seeding scheme with single crystal monochromator and undulator tapering technique. The amplification-monochromatization cascade scheme is distinguished, in performance, by spectral purity of the output radiation and smaller heat loading of crystals.

1 Introduction

Radiation from SASE XFEL consists of many independent spikes in both the temporal and spectral domains. Self-seeding is a promising approach to significantly narrow the SASE bandwidth to produce nearly transform-limited pulses [1]-[15]. We discussed the implementation of a single-crystal self-seeding scheme in the hard X-ray lines of European XFEL in [16, 17]. For this facility, transform-limited pulses are particularly valuable, since they naturally support the extraction of more FEL power than at saturation by exploiting tapering in the tunable-gap baseline undulators [18]-[25]. Tapering is implemented as a stepwise change of the undulator gap from segment to segment. Simulation results presented in [16, 17] show that the FEL power of the transform-limited X-ray pulses may be increased up to 0.4 TW by operating with the tapered baseline undulator SASE1 (or SASE2). In particular, it is possible to create a source capable of delivering fully-coherent, 7 fs (FWHM)-long X-ray pulses with $2 \cdot 10^{12}$ photons per pulse at a wavelength of 0.15 nm, Fig. 1.

We can apply the same scheme to harder X-rays, and obtain 100 GW fully-coherent X-ray pulses at a wavelength of 0.075 nm. In this paper we propose to perform monochromatization at 0.15 nm with the help of self-seeding, and amplify the seed in a first part of the 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 harmonic of the coherent radiation. A second part of the output undulator
tuned to the 2nd harmonic frequency, follows beginning at that position, and is used to obtain 2nd harmonic radiation at saturation. One can prolong the exchange of energy to the advantage of the photon beam by tapering the last part of the output undulator on a segment by segment basis. Fig. 2 shows the design principle of our self-seeding setup for harder photon energy mode of operation. Two self-seeding cascades, identical to those considered in [16, 17] (see Fig. 1), are followed by the same output undulator with changed gap configuration, compared to Fig. 1.

An advantage of the proposed scheme is the possibility to increase user capacity. In this paper we describe a photon beam distribution system, which may allow to switch the hard X-ray beam quickly among many experiments in order to make a more effective use of the facility. Monochromaticity is the key for implementing multi-user operation in the hard X-ray range, which can be granted by using crystal deflectors and small absorption of the radiation in crystals at photon energies larger than 15 keV. In contrast to the broadband SASE bandwidth, transform-limited hard X-ray bandwidths are of order of 0.007%, and match the Bragg width of crystals. Thus, using 0.05 mm thick diamond crystals one may obtain two beams, one transmitted and one Bragg reflected, with minimum intensity loss. We suggest to flip crystals for switching reflectivity similarly as for polarization switching techniques with X-ray phase retarders at synchrotron radiation facilities, that is based on the use of piezo-electric components. Crystal deflectors can be repeated a number of times to form an almost complete ring. It is then possible to distribute monochromatic hard X-rays among ten independent experiments.
Fig. 3. Concept for a hard photon beam deflector based on the use of a crystal in Bragg reflection geometry. High energy (16 keV) X-rays are associated with large penetration power, which makes it possible to use relatively thick diamond deflectors. The thickness of one crystal is 0.05 mm. The deflector can be simply switched off by tilting it, which results in a change of the angle of incidence of the radiation. The angular change necessary for switching on and off the reflected beam is less than 0.1 mrad. Only 4% of incoming 16 keV radiation is absorbed outside the reflection range.

2 Scheme for multiplying the hard X-ray beams to serve more users simultaneously

In this section we describe a concept for a photon beam distribution system, which may allow to switch the FEL beam quickly among many instruments in order to make a more effective use of the facility. The high photon energy, and monochromaticity of the output radiation are the key for reaching such result.

In fact, dealing with 16 keV monochromatic radiation one may use crystals as deflectors, Fig. 3. The deflector is constituted by a diamond plate with a thickness of 0.05 mm. The crystal is used in Bragg reflection geometry and exploits the C(111) reflection plane. For the C(111) reflection, the angular acceptance of the crystal deflector is of the order of 10 μrad, and the spectral bandwidth is about 0.006%. As a result, the angular acceptance of the deflector is much wider compared to the photon beam divergence, which is of the order of a microrad. The bandwidth of the hard X-ray pulse is of order of 0.007% and matches the Bragg width of the crystal. In this case, more than 99% of the peak reflectivity can be achieved and only 4% of the incoming 16 keV radiation is absorbed outside of the reflection range. Thus, by use of a 0.05 mm-thick diamond crystal one may obtain two beams, a transmitted as well as a Bragg reflected beam, with minimal intensity loss.
Fig. 4. The proposed hard X-ray SASE1 (or SASE2) undulator beamline, consisting of a series of three or more crystals in Bragg reflection geometry. A photon beam distribution system based on flipping crystals can provide an efficient way to obtain a many-user facility. The monochromaticity of the output at 16 keV constitutes the key for reaching such result.

One of the biggest advantages of using a crystal deflector in Bragg geometry is that the reflected beam can be switched on and off by changing the crystal angle only. The typical angular change necessary for the switching is less than 0.1 mrad. This opens a new possibility of fast switching of the reflectivity, which is necessary for many-user operation. In order to achieve a stable photon beam deflection, the rotation error must be less than 0.01 mrad. Existing technology enables rotating crystals to satisfy this requirement. For example, at synchrotron radiation facilities, X-ray phase retarder crystals are driven by piezo-electric devices operated at hundred Hz repetition rate, which flip the crystals with a rotation error of about a fraction of a micro-radian [22].

A photon beam distribution system based on flipping crystals can provide an efficient way to obtain a many-user facility. A possible layout is shown in Fig. 4. The output radiation passes through the distribution system, consisting of a series of crystals in Bragg geometry. Photon macro-pulses at 16 keV photon energy can then be fed into 10 separate beamlines. The switching crystals need to flip at frequency 1 Hz, so that each user receives one macro-pulse per second. It should be noted that the single crystal provides a sufficiently large deflection angle (of order of 20 degrees), so that the problem of separation of neighboring beamlines does not exist.

A second possible layout of a future hard X-ray laboratory based on a hard-photon ”ring” distribution system is shown in Fig. 5. One can use a number of crystal reflectors to form an almost complete ring. The photon beam transport line guiding photons from SASE1 (or SASE2) to the experimental
Fig. 5. Top view of a hard-photon "ring" distribution system. Separation between two neighboring lines is about 20 degrees. The layout of the user instruments follows a similar approach as for synchrotron radiation sources.

Hall is connected tangentially to one of the straight section of the photon ring, and the beam is injected by the reflecting crystal. Using flipping crystals in each photon ring cell it is possible to quickly switch the photon beam from one instrument to the other, thus providing many-user capability. This layout of the laboratory follows a similar approach as for synchrotron light sources.

Finally, it should be remarked that the proposed beam distribution system operates at fixed wavelength. However as reported in [26]: "for many scattering experiments it is not necessary to continuously vary the X-ray wavelength or fine-tune to a core shell resonance. Generally, however it is desirable to have a large photon energy exceeding 10 keV. This optimizes probing condensed matter systems on the atomic length scale by minimizing deleterious absorption, while preserving scattering cross sections". Obviously, our idea to increase the user access by means of a "photon ring" has advantages for such kind of experiments and can be applied to the European XFEL as well as to the LCLS-II design.

3 Feasibility study for a self-seeding setup at photon energy 16 keV

In this Section we report on a feasibility study performed with the help of the FEL code GENESIS 1.3 [27] running on a parallel machine. We will present a feasibility study for a short-pulse mode of operation of the SASE1 and SASE2 FEL lines of the European XFEL, based on a statistical analysis consisting of 100 runs. The overall beam parameters used in the simulations are presented in Table 1. We refer to the setup in Fig. 2. Up to the output
Table 1
Parameters for the low-charge mode of operation at the European XFEL used in this paper.

| Parameter                      | Units | Value |
|-------------------------------|-------|-------|
| Undulator period             | mm    | 40    |
| Periods per cell             | -     | 125   |
| K parameter (rms)            | -     | 2.15  |
| Total number of cells        | -     | 35    |
| Intersection length          | m     | 1.1   |
| Wavelength                   | nm    | 0.15  |
| Energy                       | GeV   | 14.0  |
| Charge                       | pC    | 28    |

undulator, simulations are identical to those already presented in [17]. The choice of the FODO lattice parameters is also kept identical. This is in agreement with the present concept to use the self-seeding setup at the European XFEL in [17] to produce monochromatic beams using harmonic generation simply by acting on the gap of the output undulator.

The expected beam parameters at the entrance of the SASE1 and SASE2 undulators are shown in Fig. 6, [28]. Wakes inside the undulators are also accounted for and expected to obey the dependence in Fig. 7, [28].

The output power and spectrum after the first part of the output undulator (5 cells) tuned at 0.15 nm is shown in Fig. 8.

The tapering law used in the last 19 cells is shown in Fig. 9.

The output power and spectrum of the entire setup, that is after the second part of the output undulator (19 cells) tuned at 0.075 nm, is shown in Fig. 10. The evolution of the output energy and of the variance of the energy fluctuations in the photon pulse are reported in Fig. 11. Finally, the expected transverse size and divergence of the electron beam can be seen in Fig. 12.

4 Conclusions

In this work we addressed the potential for enhancing the capabilities of the European XFEL. In the hard X-ray regime, a high longitudinal coherence, in addition to full transverse coherence, will be the key to a performance upgrade. High longitudinal coherence is achievable based on a single-crystal
In this paper we proposed a study of the performance of a self-seeding scheme with single-crystal monochromators for the European XFEL at X-rays energies higher than 8 keV. By combining the two techniques of self-seeding and undulator tapering, we found that 100 GW X-ray transform-limited pulses at the photon energy of 16 keV can be generated without modification to the TW mode of operation at photon energy of 8 keV.

This paper also describes an efficient way for obtaining a many-user facility, based on the high photon energy and high monochromaticity of the output radiation expected from our concept. We propose a photon beam distribution system based on the use of crystals in the Bragg reflection geometry as deflectors. About 99% reflectivity can be achieved for monochromatic
X-rays. Angular and bandwidth acceptances of crystal deflectors match bandwidth and divergence of the X-ray beam. Therefore, it should be possible to deflect the full radiation pulse of an angle of order of a radian without perturbations. The proposed photon beam distribution system would allow to switch the hard X-ray beam quickly between many instruments in order to make a more efficient use of the European XFEL source.
Fig. 9. Taper configuration for high-power mode of operation at 0.075 nm

Fig. 10. (Left plot) Output power and (right plot) output spectrum after the second part of the output undulator (19 cells) tuned at 0.075 nm. Grey lines refer to single shot realizations, the black line refers to the average over a hundred realizations.

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Fig. 11. (Left plot) Energy in the X-ray radiation and (right plot) variance of the energy fluctuations of the photon pulse versus the length of the second part of the output undulator tuned at 0.075 nm. Grey lines refer to single shot realizations, the black line refers to the average over a hundred realizations.

Fig. 12. (Left plot) Transverse plot of the X-ray radiation pulse energy distribution and (right plot) angular plot of the X-ray radiation pulse energy distribution after the second part of the output undulator tuned at 0.075 nm.

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