OPTIMIZATION OF A DEDICATED BIO-IMAGING BEAMLINE AT THE EUROPEAN X-RAY FEL

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Abstract

We recently proposed a basic concept for design and layout of a dedicated undulator source for bio-imaging experiments at the European XFEL. Here we present an optimization of that concept. The core of the scheme is composed by soft and hard X-ray self-seeding setups. Using an improved design for both monochromators it is possible to increase the design electron energy up to 17.5 GeV in photon energy range between 2 keV and 13 keV, which is the most preferable for life science experiments. Operating at such high electron energy one increases the X-ray output peak power. Moreover, 17.5 GeV is the preferred operation energy for SASE1 and SASE2 users. This choice will reduce the interference with other undulator lines. We include a study of the performance of the self-seeding scheme accounting for spatiotemporal coupling caused by the use of a single crystal monochromator. This distortion can be easily suppressed by the right choice of diamond crystal planes. The proposed undulator source yields about the same performance as in the case for a X-ray seed pulse with no coupling. Simulations show that the FEL power reaches 2 TW in the 3 keV - 5 keV photon energy range.

INTRODUCTION

The availability of free undulator tunnels at the European XFEL facility offers a unique opportunity to build a beamline optimized for coherent diffraction imaging of complex molecules, like proteins and other biologically interesting structures. Crucial parameters for such bio-imaging beamline are photon energy range, peak power, and pulse duration [1]-[4].

The highest diffraction signals are achieved at the longest wavelength that supports a given resolution, which should be better 0.3 nm. With photon energy of about 3 keV one can reach a resolution better than 0.3 nm with a detector designed to collect diffracted light in all forward directions, that is at angles $2\theta < \pi/2$. Higher photon energies up to about 13 keV give access to absorption edges of specific elements used for phasing by anomalous diffraction. The most useful edges to access are the K-edge of Fe (7.2 keV) and Se (12.6 keV), [5]. Access to the sulfur K-edge (2.5 keV) is required too. Finally, the users of the bio-imaging beamline also wish to investigate large biological structures in the soft X-ray photon energy range down to the water window (0.3 keV – 0.5 keV), [5].

Overall, one aims at the production of pulses containing enough photons to produce measurable diffraction patterns, and yet short enough to avoid radiation damage in a single pulse. This is, in essence, the principle of imaging by "diffraction before destruction" [2]. These capabilities can be obtained by reducing the pulse duration to 5 fs or less, and simultaneously increasing the peak power to the TW power level or higher, at photon energies between 3 keV and 5 keV, which are optimal for imaging of macromolecular structures [5].

The requirements for a dedicated bio-imaging beamline are the following. The X-ray beam should be delivered in ultrashort pulses with TW peak power and within a very wide photon energy range between 0.3 keV and 13 keV. The pulse duration should be adjustable from 10 fs in hard X-ray regime to 2 fs - 5 fs in photon energy range between 3 keV and 5 keV. At the European XFEL it will be necessary to run all undulator beamlines at the same electron energy and bunch charge. Therefore, bio-imaging experiments should be performed without interference with other main SASE1, SASE2 beamlines. This assumes the use of nominal electron energy and electron beam distribution.

A key component of the bio-imaging beamline is the undulator source. A basic concept for layout and design of the undulator system for a dedicated bio-imaging beamline at the European XFEL was proposed in [6]. All the requirements in terms of photon beam characteristics can be satisfied by the use a very efficient combination of self-seeding, fresh bunch, and undulator tapering techniques [7]-[26], [27]-[30]. A combination of self-seeding and undulator tapering techniques would allow to meet the design TW output power. The bio-imaging beamline would be equipped with two different self-seeding setups, one provide monochromatization in the soft X-ray range, and one to provide monochromatization in the hard X-ray range. The most preferable solution in the photon energy range for single biomolecule imaging consists in using a fresh bunch technique in combination with self-seeding and undulator tapering techniques. In [6] it was shown how the installation of an additional (fresh bunch) magnetic chicane behind the soft X-ray self-seeding setup enables an output power in the TW level for the photon energy range between 3 keV and 5 keV. Additionally, the pulse duration can be tuned between 2 fs and 10 fs with the help of this chicane, still operating with the nominal electron bunch distribution [31].

The overall setup proposed in [6] is composed of four undulators separated by three magnetic chicanes. The undulator parts consist of 4,3,4 and 29 cells. Each magnetic chicane compact enough to fit one 5 m-long undulator segment and the FODO lattice will not be perturbed. The undulator system will be realized in a similar fashion as other

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European XFEL undulators. In order to make use of standard components we favor the use of SASE3 type of undulator segments, which are optimized for the generation of soft X-rays. The present layout of the European XFEL enables to accommodate such new beamline. The previously proposed undulator source provides access to a photon energy range between 3 keV and 5 keV only at the reduced electron beam energy of 10.5 GeV. Although the 10.5 GeV is one of the nominal electron energy, it may not be the preferable mode of operation for SASE1, SASE2 beamline users. Note that the SASE3 undulator type would enable operation down to 0.7 keV at an electron energy of 17.5 GeV. However, the delay of photons induced in the grating monochromator (3 ps) and, consequently, the delay of the electrons required in the magnetic chicane of the soft X-ray self-seeding setup sets a limit to the electron energy.

This paper constitutes an update to the scheme proposed in [6]. The present design assumes the use of the same 40 cells undulator system, with an improved design of both self-seeding setups. To avoid any interference with other beamlines, we propose to extend the photon energy range of the self-seeding setup with a single crystal monochromator down to 3 keV [32]. As a result, the design electron energy can be increased up to 17.5 GeV in the photon energy range most preferable for bio-imaging. This is achieved exploiting 0.1 mm diamond crystals in symmetric Bragg geometry. Based on the use C(111), C(220), and C(400) reflections (σ-polarization) it will be possible to cover the photon energy range between 3 keV and 13 keV. In particular, we exploit C(111) reflection (σ-polarization) in photon energy range between 3 keV and 5 keV. Combination of self-seeding and fresh bunch techniques, as in the case of the original design, has the advantage that the pulse duration can be tuned between 2 fs and 10 fs.

The users of the bio-imaging beamline also wish to investigate their samples around sulfur K-edge, i.e. in the photon energy range between 2 keV and 3 keV. A solution suitable for this spectral range constitutes a major challenge for self-seeding designers. In fact, on the one hand crystals with right lattice parameters are difficult to be obtained. On the other hand, grating monochromator throughput is usually too low due to high absorption. As for the original design we propose a method around this obstacle, which is based in essence on a fresh bunch technique, and exploits a self-seeding setup based on grating monochromator in the photon energy range between 0.7 keV and 1 keV. It should be noted that due to extension of the single crystal monochromator setup down to 3 keV, the maximal photon energy of operation for the grating monochromator is reduced from 1.7 keV in the original design down to 1 keV in the current design.

Also, here we adopt an improved design of grating monochromator, which was recently proposed for the soft X-ray self-seeding setup at the LCLS [33], substituting a previously proposed one [34, 35]. In this novel design the optical delay is reduced down to below 1 ps. As a result, a self-seeding setup with such grating monochromator allows for reduced constraints on the magnetic chicane, and can operate at the European XFEL down to 0.7 keV at the highest nominal electron energy of 17.5 GeV. Such high electron energy enables to increase the X-ray output peak power in the most preferable photon energy range for bio-imaging experiments up to 2 TW.

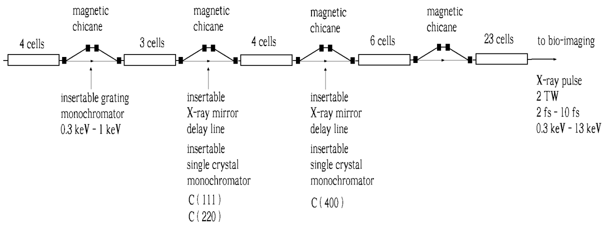

Figure 1: Design of the undulator system for the bio-imaging beamline. The method exploits a combination of self-seeding, fresh bunch, and undulator tapering technique. Each magnetic chicane accomplishes three tasks by itself. It creates an offset for monochromator or X-ray mirror delay line installation, it removes the electron microbunching produced in the upstream undulator, and it acts as a magnetic delay line.

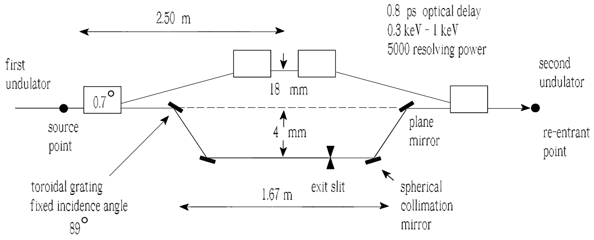

Figure 2: Compact grating monochromator originally proposed at SLAC [33] for soft X-ray self-seeding setup. The chicane fits in one European XFEL undulator undulator section (5 m).

SETUP DESCRIPTION

Self-seeding is a promising approach to significantly narrow the SASE bandwidth and to produce nearly transform-limited X-ray pulses [14]-[24]. In its simplest configuration, a self-seeding setup in the hard X-ray regime consists of two undulators separated by photon monochromator and electron bypass beamline, typically a 4-dipole chicane. The two undulators are resonant at the same radiation wavelength. The SASE radiation generated by the first undulator passes through the narrow-band monochromator, thus generating a transform-limited pulse, which is then used as a coherent seed in the second undulator. Chromatic dispersion effects in the bypass chicane smear out the microbunching in the electron bunch produced by the SASE

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lasing in the first undulator. Electrons and monochromatized photon beam are recombined at the entrance of the second undulator, and the radiation is amplified by the electron bunch in the second undulator, until saturation is reached. The required seed power at the beginning of the second undulator must dominate over the shot noise power within the gain bandpass, which is order of a few kW.

Despite the unprecedented increase in peak power of the X-ray pulses for SASE X-ray FELs (see e.g. [36]), some applications, including single biomolecule imaging, require still higher photon flux. The most promising way to extract more FEL power than that at saturation is by tapering the magnetic field of the undulator [7]-[25]. Also, a significant increase in power is achievable by starting the FEL process from a monochromatic seed rather than from noise [21]-[24]. Tapering consists in a slow reduction of the field strength of the undulator in order to preserve the resonance wavelength, while the kinetic energy of the electrons decreases due to the FEL process. The undulator taper could be simply implemented at discrete steps from one undulator segment to the next. The magnetic field tapering is provided by changing the undulator gap.

The setup suggested in this article constitutes an optimization of the original proposal in [6] and is composed of five undulator parts separated by four magnetic chicanes as shown in Fig. 1. These undulators consist of 4, 3, 4, 6 and 23 undulator cells, respectively. Each magnetic chicane is compact enough to fit one undulator segment. The installation of chicanes does not perturb the undulator focusing system. The implementation of the self-seeding scheme for soft X-ray would exploit the first magnetic chicane. The second and third magnetic chicanes create an offset for the installation of a single crystal monochromator or an X-ray mirror delay line, and act as a magnetic delay line. Both self-seeding setups should be compact enough to fit one undulator module.

For soft X-ray self-seeding, the monochromator usually consists of a grating [14]. Recently, a very compact soft X-ray self-seeding scheme has appeared, based on a grating monochromator [33]. The proposed monochromator is composed of a toroidal grating followed by three mirrors, and is equipped with an exit slit only. The delay of the photons is about 1 ps. The monochromator is continuously tunable in the photon energy range between 0.3 keV and 1 keV. The resolution is about 5000. The transmission of the monochromator beamline is up to 6%. The magnetic chicane delays the electron electron bunch accordingly, so that the photon beam passing through the monochromator system recombines with the same electron bunch. The chicane provides a dispersion strength of about 0.6 mm in order to match the optical delay and also smears out the SASE microbunching generated in the first 4 cells of the undulator. It should be noted that in [37] we studied the performance of a previous scheme of a grating monochromator for a soft X-ray self-seeding setup [34, 35]. For the present investigation we consider the new scheme in [33]. The layout of the bypass and of the monochromator optics is schematically shown in Fig. 2.

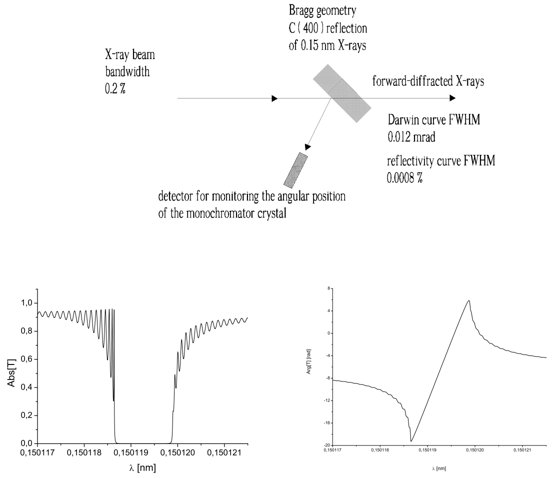

Figure 3: X-ray optics for compact crystal monochromator originally proposed in [20] for a hard X-ray self-seeding setup, based on the C(400) reflection (σ-polarization). Modulus and phase of the transmissivity are shown in the two lower plots.

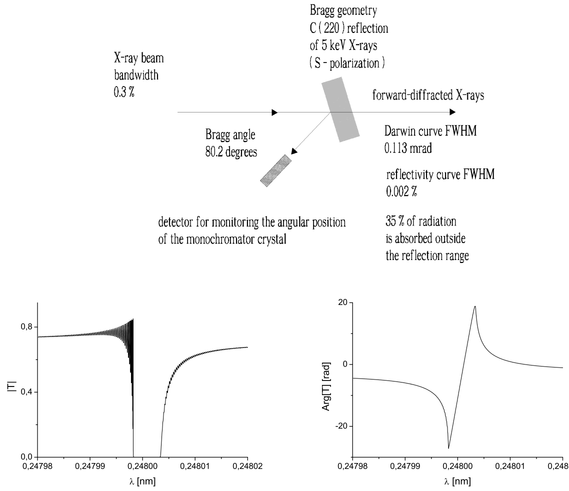

Figure 4: Schematic of single crystal monochromator for operation in photon energy range between 5 keV and 7 keV. In this range the C(220) reflection will be exploited. Modulus and phase of the transmissivity are shown in the two lower plots.

For hard X-ray self-seeding, a monochromator usually consists of crystals in the Bragg geometry. A conventional 4-crystal, fixed exit monochromator introduces optical delay of, at least, a few millimeters, which has to be compensated with the introduction of an electron bypass longer than one undulator module. To avoid this difficulty, a simpler self-seeding scheme was proposed in [20], which uses the transmitted X-ray beam from the single crystal to seed the same electron bunch. Here we propose to use a dia-

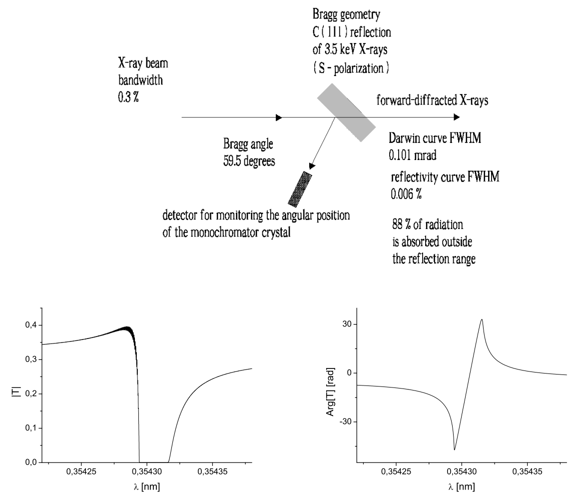

Figure 5: Schematic of single crystal monochromator for operation in photon energy range between 3 keV and 5 keV. In this range the C(111) reflection will be exploited. Modulus and phase of the transmissivity are shown in the two lower plots.

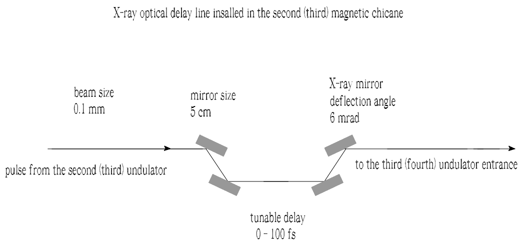

Figure 6: X-ray optical system for delaying the soft X-ray pulse with respect to the electron bunch. Two distinct X-ray optical systems can be installed within the second and the third magnetic chicane.

mond crystal with a thickness of 0.1 mm. Using the symmetric C(400) Bragg reflection, it will be possible to cover the photon energy range from 7 keV to 9 keV, Fig. 3. The range between 5 keV and 7 keV can be covered with the C(220) reflection, Fig. 4, while the range between 3 keV and 5 keV can be obtained using the C(111) reflection, Fig. 5.

One of the main technical problems for self-seeding designers is to provide bio-imaging capabilities in 2 keV - 3 keV photon energy range. Here we will use the same method already exploited in [6] to get around this obstacle. Our solution is based in essence on the fresh bunch technique [26] and exploits the above described conservative design of self-seeding setup based on a grating monochromator. The hardware requirement is minimal, and in order to implement a fresh bunch technique it is sufficient to install an additional magnetic chicane at a special position behind the soft X-ray self-seeding setup. The function of this second chicane is both to smear out the electron bunch microbunching, and to delay the electron bunch with respect to the monochromatic soft X-ray pulse produced in the second undulator. In this way, only half of the electron bunch is seeded, and saturates in the third undulator. Finally, the second half of the electron bunch, which remains unspoiled, is seeded by the third harmonic of the monochromatic radiation pulse generated in the third undulator, which is also monochromatic. The final delay of the electron bunch with respect to the seed radiation pulse can be obtained with a third, hard X-ray self-seeding magnetic chicane, which in this mode of operation is simply used to provide magnetic delay. The monochromatic third harmonic radiation pulse used as seed for the unperturbed part of the electron bunch is in the GW power level, and the combination of self-seeding and fresh bunch technique is extremely insensitive to non-ideal effects. The final undulator, composed by 29 cells, is tuned to the third harmonic frequency, and is simply used to amplify the X-ray pulse up to the TW power level.

In order to introduce a tunable delay of the photon beam with respect to the electron beam, a mirror chicane can be installed within the second magnetic chicane, as shown in Fig. 6. The function of the mirror chicane is to delay the radiation in the range between 0.7 keV and 1 keV relatively to the electron bunch. The glancing angle of the mirrors is as small as 3 mrad. At the undulator location, the transverse size of the photon beam is smaller than 0.1 mm, meaning that the mirror length would be just about 5 cm. The single-shot mode of operation will relax the heat-loading issues. The mirror chicane can be built in such a way to obtain a delay of the radiation pulse of about 23 μm. This is enough to compensate a bunch delay of about 20 μm from the magnetic chicane, and to provide any desired shift in the range between 0 μm and 3 μm. Note that for the European XFEL parameters, 1 nm microbunching is washed out with a weak dispersive strength corresponding to an R_{56} in the order of ten microns. The dispersive strength of the proposed magnetic chicane is more than sufficient to this purpose. Thus, the combination of magnetic chicane and mirror chicane removes the electron microbunching produced in the second undulator and acts as a tunable delay line within 0 μm and 3 μm with the required choice of delay sign.

Operation Into the Water Window

The five-undulator configuration in Fig. 1 can be naturally taken advantage of at different photon energies ranging from soft to hard X-rays. Fig. 7 shows the basic setup for the high-power mode of operation in the soft X-ray wavelength range. The second, the third and the fourth chicane are not used for such regime, and must be switched off. After the first undulator (4 cells-long) and the grating monochromator, the output undulator follows. The first section of the output undulator (consisting of second and third undulator) is composed by 3 untapered cells, while tapering is implemented starting from the second cell of the fourth undulator. The monochromatic seed is exponen-

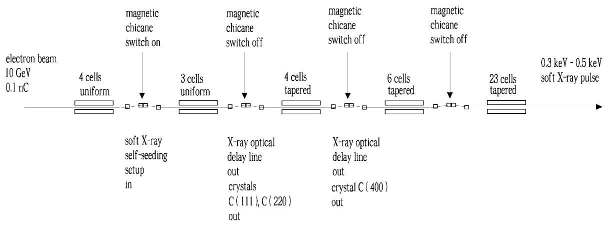

Figure 7: Design of the undulator system for high power mode of operation in the water window. The method exploits a combination of self-seeding scheme with grating monochromator and an undulator tapering technique.

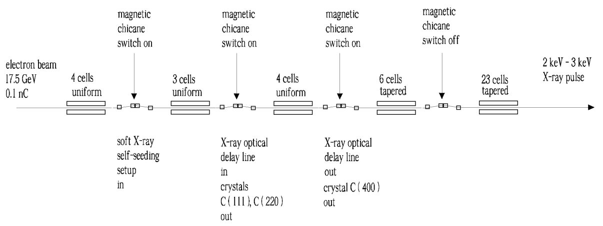

Figure 8: Design of the undulator system for high power mode of operation around the sulfur K-edge. The method exploits a combination of self-seeding scheme with grating monochromator, fresh bunch and undulator tapering techniques.

tially amplified by passing through the first untapered section of the output undulator. This section is long enough to allow for saturation, and yields an output power of about 100 GW. Such monochromatic FEL output is finally enhanced up to 1 TW in the second output-undulator section, by tapering the undulator parameter over the last cells after saturation. Under the constraints imposed by undulator and chicane parameters it is only possible to operate at the nominal electron beam energy of 10.5 GeV. The setup was optimized based on results of start-to-end simulations for a nominal electron beam with 0.1 nC charge. Results were presented in [37], where we studied the performance of this scheme for the SASE3 upgrade.

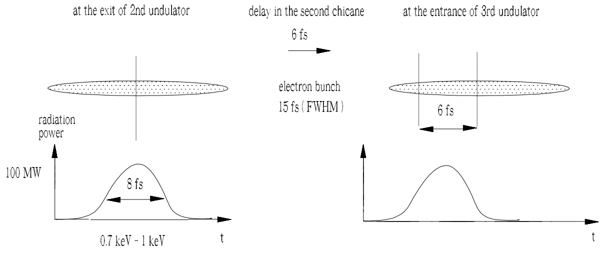

Figure 9: Principle of the fresh bunch technique for the high power mode of operation in the photon energy range between 2 keV and 3 keV. The second chicane smears out the electron microbunching and delays the monochromatic soft X-ray pulse with respect to the electron bunch of 6 fs. In this way, half of of the electron bunch is seeded and saturates in the third undulator.

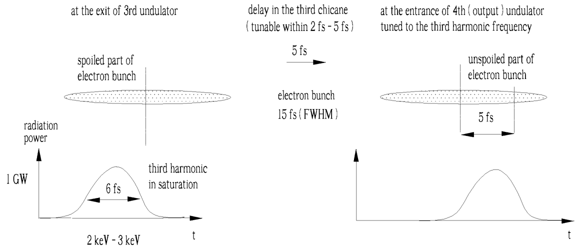

Figure 10: Principle of the fresh bunch technique for the high power mode of operation in the photon energy range between 2 keV and 3 keV. The third magnetic chicane smears out the electron microbunching and delays the electron bunch with respect to the radiation pulse. The unspoiled part of electron bunch is seeded by a GW level monochromatic pulse at third harmonic frequency. Tunability of the output pulse duration can be easily obtained by tuning the magnetic delay of the third chicane.

Operation Around the Sulfur K-edge

Figure 8 shows the basic setup for high power mode of operation in the photon energy range between 2 keV and 3 keV. The first three chicanes are used for such regime, and must be switched on, while the last fourth chicane is off. The third chicane is used as a magnetic delay only, and the crystal must be removed from the light path. We propose to perform monochromatization at photon energies ranging between 0.7 keV and 1 keV with the help of a grating monochromator, and to amplify the seed in the second undulator up to the power level of 0.2 GW. The second chicane smears out the electron microbunching and delays the monochromatic soft X-ray pulse of 2 μm with respect to the electron bunch. In this way, half of the electron bunch is seeded and saturates in the third undulator up to 40 GW. At saturation, the electron beam generates considerable monochromatic radiation at the third harmonic in the GW power level. The third magnetic chicane smears out the electron microbunching and delays the electron bunch with respect to the radiation of 2 μm. Thus, the unspoiled part of the electron bunch is seeded by the GW-level monochromatic pulse at the third harmonic frequency, Fig. 10. The fourth, 29 cells-long undulator is tuned to the third harmonic frequency (between 2 keV and 3 keV), and is used to amplify the radiation pulse up to 1 TW. The additional advantage of the proposed setup for bio-imaging is the tunability of the output pulse duration, which is obtained by tuning the magnetic delay of the third chicane. Simulations show that the X-ray pulse duration can be tuned from 2 fs to

5 fs. The production of such pulses is of great importance when it comes to single biomolecule imaging experiments.

The soft X-ray background can be easily eliminated by using a spatial window positioned downstream of the fourth undulator exit [6]. Since the soft X-ray radiation has an angular divergence of about 0.02 mrad FWHM, and the slits are positioned more than 100 m downstream of the third undulator, the background has much larger spot size compared with the 2 keV - 3 keV radiation spot size, which is about 0.1 mm at the exit of the fourth undulator. Therefore, the background radiation power can be diminished of more than two orders of magnitude without any perturbations of the main pulse.

With the monochromator design in [33], it will be possible to operate at an electron beam energy of 17.5 GeV. The setup was optimized based on results from start-to-end simulations for a nominal electron bunch with a charge of 0.1 nC. Results are presented in the following Sections of this article. The proposed undulator setup uses the electron beam coming from the SASE1 undulator. We assume that SASE1 operates at the photon energy of 12 keV, and that the FEL process is switched off for one single dedicated electron bunch within each macropulse train. A method to control the FEL amplification process is based on the betatron switcher technique described in [38, 39]. Due to quantum energy fluctuations in the SASE1 undulator, and to wakefields in the SASE1 undulator pipe, the energy spread and the energy chirp of the electron bunch at the entrance of the bio-imaging beamline significantly increase compared with the same parameters at the entrance of the SASE1 undulator. The dispersion strength of the first chicane has been taken into account from the viewpoint of the electron beam dynamics, because it disturbs the electron beam distribution. The other two chicanes have tenfold smaller dispersion strength compared with the first one. The electron beam was tracked through the first chicane using the code Elegant [40]. The electron beam distortions complicate the simulation procedure. However, simulations show that the proposed setup is not significantly affected by perturbations of the electron phase space distribution, and yields about the same performance as in the case for an electron beam without the tracking through the first chicane (see below).

Operation in the 3 *keV -* 7 *keV Photon Energy Range*

Starting with the energy range of 3 keV it is possible to use a single crystal monochromator instead of a grating monochromator at an electron energy of 17.5 GeV. Different crystal reflections and different positions of the monochromator down the undulator enable self-seeding for different spectral ranges.

For the range between 3 keV and 5 keV, Fig. 11, the first chicane is not used and is switched off. After the first 7 cells the electron and the photon beams are separated with the help of the second magnetic chicane, and the C(111) reflection is used to monochromatize the radiation. The seed is amplified in the next 4 cells. After that, the electron and the photon beam are separated again by the third chicane, and an X-ray optical delay line allows for the introduction of a tunable delay of the photon beam with respect to the electron beam. The following 6 cells use only a part of the electron beam as a lasing medium. A magnetic chicane follows, which shifts the unspoiled part of the electron bunch on top of the of the photon beam. In this way, a fresh bunch technique can be implemented. Since the delays are tunable, the photon pulse length can also be tuned. Finally, radiation is amplified into the last 23 tapered cells to provide pulses with about 2 TW power. The photon energy range between 5 keV and 7 keV can be achieved similarly, Fig. 12. The only difference is that now the C(220) reflection is used, instead of the C(111).

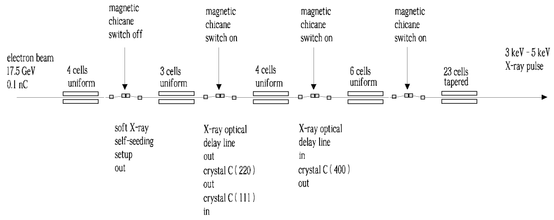

Figure 11: Design of the undulator system for high power mode of operation in the most preferable photon energy range for single molecule imaging, between 3 keV and 5 keV. The method exploits a combination of the self-seeding scheme with single crystal monochromator, fresh bunch and undulator tapering techniques.

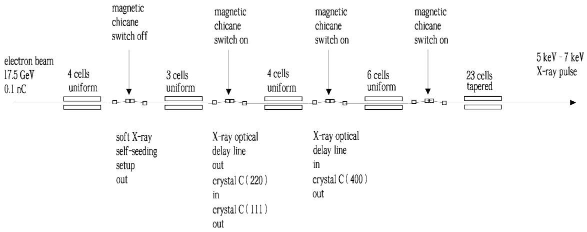

Figure 12: Design of the undulator system for high power mode of operation in the photon energy range between 5 keV and 7 keV. The method exploits a combination of self-seeding scheme with single crystal monochromator, fresh bunch and undulator tapering techniques.

It may be worth to point out the difference between the operation in the 3 keV - 7 keV range and the previously discussed range between 2 keV and 3 keV. In the 3 keV - 7 keV range we use seeding in combination of a fresh bunch technique, but we do not exploit harmonic generation. Moreover, the fresh bunch technique is only used for tuning the duration of the radiation pulse.

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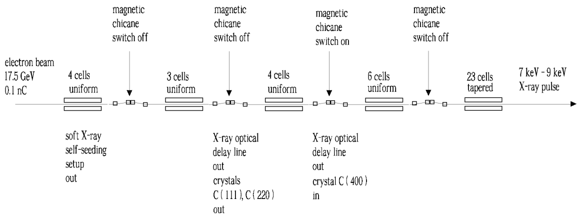

Figure 13: Design of the undulator system for high power mode of operation in the photon energy range in the photon energy range between 7 keV and 9 keV. The method exploits a combination of self-seeding scheme with single crystal monochromator and an undulator tapering technique.

Operation in the 7 keV - 9 keV Photon Energy Range

The energy range between 7 keV and 9 keV can be achieved by deactivating the first and the second magnetic chicane, thus letting the SASE process building up the radiation pulse to be monochromatized for 11 cells. After that, the third chicane is used for the monochromator setup, which makes use of the C(400) reflection. The last chicane is switched off, and the the output undulator is long enough to reach 1 TW power. The duration of the output pulses is of about 10 fs. If tunability of the pulse duration is requested in this energy range, this is most easily achieved by providing additional delay with the fourth magnetic chicane installed behind the hard X-ray self-seeding setup.

Operation Around the Selenium K-edge

Finally, for the energy range between 9 keV and 13 keV, a combination of self-seeding, fresh bunch tachnique and harmonic generation is used. The undulator line is configured as for the range between 3 keV and 5 keV, Fig. 11, the only difference being that the final undulator segments are tuned at the third harmonic of the fundamental thus enabling the 9 keV - 13 keV energy range. As before, the first chicane is not used and is switched off. After the first 7 cells the electron and the photon beams are separated with the help of the second magnetic chicane, and the C(111) reflection is used to monochromatize the radiation. The seed is amplified in the next 4 cells. After that, the electron and the photon beam are separated again by the third chicane, and an X-ray optical delay line allows for the introduction of a tunable delay of the photon beam with respect to the electron beam. The second chicane smears out the electron microbunching and delays the monochromatic soft X-ray pulse with respect to the electron bunch of 6 fs. In this way, half of of the electron bunch is seeded and saturates in the following 6 cells. A magnetic chicane follows, which shifts the unspoiled part of the electron bunch on top of the of the photon beam. In this way, a fresh bunch technique can be implemented. Since the delays are tunable, the photon pulse length can also be tuned. Since third harmonic bunching is considerable, the last 23 tapered cells are tuned at the third harmonic of the fundamental providing pulses with about 0.5 TW power.

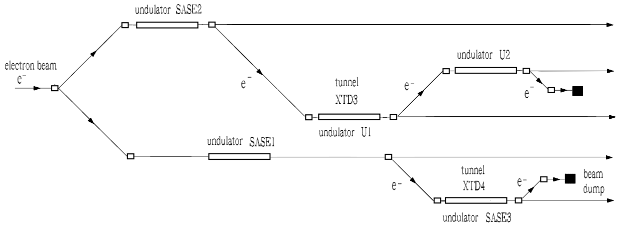

Figure 14: Original design of the European XFEL facility.

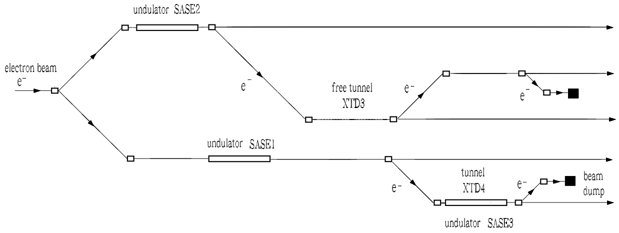

Figure 15: Current design of the European XFEL facility.

Possible Location of the Bio-imaging Line

The original design of the European XFEL [41] was optimized to produce XFEL radiation at 0.1 nm, simultaneously at two undulator lines, SASE1 and SASE2. Additionally, the design included one FEL line in the soft X-ray range, SASE3, and two undulator lines for spontaneous synchrotron radiation, U1 and U2, Fig. 14. The soft X-ray SASE3 beamline used the spent electron beam from SASE1, and the U1 and U2 beamlines used the spent beam from SASE2. In fact, although the electron beam performance is degraded by the FEL process, the beam can still be used in afterburner mode in the SASE3 undulator, which

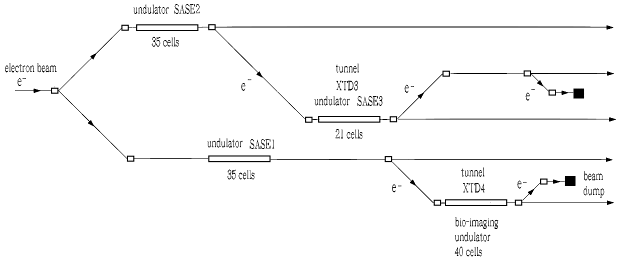

Figure 16: Schematic of the proposed extension of the European XFEL facility.

will be equipped with a 126 m-long undulator system, for a total of 21 cells.

After a first design report, the layout of the European XFEL changed. In the last years after the achievement of the LCLS, and the subsequent growth of interest in XFEL radiation by the scientific community, it became clear that the experiments with XFEL radiation, rather than with spontaneous synchrotron radiation, had to be prioritized. In the new design, the two beamlines behind SASE2 are now free for future XFEL undulators installations, Fig. 15.

Recently it was also realized that the amplification process in the XFEL undulators can be effectively controlled by betatron FEL switchers [38, 39]. The SASE3 undulator was then optimized for generating soft X-rays. However, due to the possibility of switching the FEL process in SASE1, it is possible to produce high power SASE3 radiation in a very wide photon energy range between 0.3 keV and 13 keV. The SASE3 beamline is now expected to provide excellent performance, and to take advantage of its location in the XTD4 tunnel, which is close to the experimental hall and has sufficient free space behind the undulator for future expansion (140 m). After this section, the electron beam will be separated from the photon beam and will be bent down to an electron beam dump, Fig. 14. In the photon energy range between 3 keV and 13 keV, the SASE3 beamline is now expected to provide even better conditions for users than SASE1 and SASE2.

In this article we propose to build the bio-imaging beamline in the XTD4 tunnel. The SASE3 undulator, which is composed by 21 cells, can be installed from the very beginning in the free XTD3 tunnel, which is shorter than the XTD4 tunnel but sufficiently long for such installation, Fig. 16. The undulator can be placed within the straight beam path that is defined by the last upstream and first downstream dipole of the electron deflection system. The limiting length given by these constraints is referred to as “available length”. For the XTD3 and the XTD4 tunnels this available length respectively amounts to 255 m and 460 m, see [42]. However, the electron beam optics requires sufficient space in front and the above-mentioned dipoles. The length that fits these electron optics restrictions is referred to as “potential length” and can be actually used for installations. For the XTD3 and the XTD4 tunnels, this potential length respectively amounts to 215 m and 400 m [42]. It should be mentioned that the potential length of the XTD4 tunnel is practically the same as the main SASE1 and SASE2 tunnels, and nicely fits with the undulator system for a dedicated bio-imaging beamline. It offers thus a great potential for future upgrades of this new beamline.

The bio-imaging beamline would support experiments carried out over a rather wide photon energy range. It is therefore proposed that the photon beam transport of the new beamline includes two lines. Line A uses 0.5m-long mirrors operating at a grazing angle of 2 mrad. This line is dedicated to the transport of X-ray radiation in the photon energy range from 3 keV up to 13 keV. This would be complementary to the Line B that is now optimized in the soft X-ray range between 0.3 keV and 3 keV. The distance from the 40-cells-long undulator exit to the first mirror system will be only of about 100m[1].

CONCLUSIONS

The highest priority for bioimaging experiments at any advanced XFEL facility is to establish a dedicated beamline for studying biological objects at the mesoscale, including large macromolecules, macromolecular complexes, and cell organelles. This requires 2 keV - 6 keV photon energy range and TW peak power pulses. However, higher photon energies are needed to reach anomalous edges of commonly used elements (such as Se) for anomalous experimental phasing. Studies at intermediate resolutions need access to the water window [5].

A conceptual design of a dedicated bio-imaging beamline based on the self-seeding scheme developed for European XFEL was suggested in [6]. The critical attribute of the proposed beamline, compared with the baseline SASE1 and SASE2 beamlines, is a wider photon energy range that spans from the water window up to the K-edge of Selenium (12.6 keV). With the current design of the European XFEL, the most preferable photon energy range between 3 keV and 5 keV cannot be used for biological scattering experiments, but the new proposed beamline could fill this gap operating at those energies with TW peak power.

The first goal in developing a design for a dedicated bio-imaging beamline is to make it satisfying all requirements. Once that is done, the next step is to optimize the design, making it as simple as possible. In order to improve the original design, here we propose to extend the photon energy range of the self-seeding setup with single crystal monochromator to lower photon energies down to 3 keV. An important aspect of this extension is that the self-seeding scheme with single crystal monochromator is now routinely used in generating of narrow bandwidth X-ray pulses at the LCLS [43]. It combines a potentially wide photon energy range with a much needed experimental simplicity. Only one X-ray optical element is needed, and no sensitive alignment is required. The range of applicability of this novel method is a slightly limited, at present, by the availability of a short pulse duration (of about 10 fs or less). However, this range nicely matches that for single biomolecule imaging.

Optimization of the bio-imaging beamline is performed with extensive start-to-end simulations, which also take into account effects such as the spatiotemporal coupling caused by the single crystal monochromator. One must keep this effect in mind when performing the design of any self-seeding setup. The spatial shift is proportional to $\cot(\theta_B)$, and is therefore maximal in the range for small

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[1] This is in contrast with SASE1 and SASE2 beamlines, where an opening angle of 0.003 mrad at 3 keV FEL radiation leads to unacceptable mirror length of 2 m due to long distance of about 500 m between the source and mirror system. For these beamlines there is no possibility to use identical configuration of mirrors within the photon energy range from 3 keV to 13 keV.

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Bragg angles θ_B. A Bragg geometry close to backscattering (i.e. θ_B close to $\pi/2$) would be a more advantageous option from this viewpoint, albeit with a decrease in the spectral tunability [44]-[46]. It is worth mentioning that this distortion is easily suppressed by the right choice of crystals within the photon energy range between 3 keV and 9 keV. Here we propose to use a set of three diamond crystals. For the C(111), the C(220) and the C(400) Bragg reflections (σ-polarization), it will be possible to respectively cover the photon energy ranges 3 keV - 5 keV, 5 keV - 7 keV, and 7 keV - 9 keV. Finding a solution suitable for the spectral range between 9 keV and 13 keV is major challenge due to the large value of $\cot(\theta_B)$ for the C(400) reflection case. Fortunately, even in this case, this obstacle can be overcome by using a fresh bunch technique, and exploiting the self-seeding setup with a C(111) single crystal monochromator, which is tunable in the photon energy range around 4 keV, in combination with harmonic generation techniques.

The goal of the present optimized proposal for a dedicated bio-imaging beamline presented here is to aim for experimental simplification and performance improvement. The design electron energy in the most preferable spectral range 3 keV - 5 keV is increased up to 17.5 GeV. The peak power is shown to reach a maximum value of 2 TW. The new design takes additional advantage of the fact that 17.5 GeV is the most preferable operation energy for the SASE1 and the SASE2 beamlines. Because of this, the optimized beamline is not sensitive to the parallel operation with other European XFEL beamlines.

Detailed FEL studies and a treatment of the spatiotemporal transformation caused by the use of a single crystal monochromator are not included here for reasons of space and can be found in [47].

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