CONCEPTUAL DESIGN OF AN UNDULATOR SYSTEM FOR A DEDICATED BIO-IMAGING BEAMLINE AT THE EUROPEAN X-RAY FEL

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Abstract

We describe a future possible upgrade of the European XFEL consisting of a new undulator beamline dedicated to coherent diffraction imaging of complex molecules. Crucial parameters are photon energy range, peak power, and pulse duration. The peak power is maximized in the photon energy range between 3 keV and 12 keV by the use of a very efficient combination of self-seeding, fresh bunch and tapered undulator techniques. The unique combination of ultra-high peak power of 1 TW in the entire energy range, and ultrashort pulse duration tunable from 2 fs to 10 fs, would allow for single shot coherent imaging of protein molecules with size larger than 10 nm. Also, the new beamline would enable ima ing of large biological structures in the water window, between 0.3 and 0.4 keV. In order to make use of standardized components, at present we favor the use of SASE3-type undulator segments. The number segments, 40, is determined by the tapered length for the design output power of 1 TW. The present plan assumes the use of a nominal electron bunch with charge of 0.1 nC. Experiments would be performed without interference with the other three undulator beamlines.

INTRODUCTION

Structural biology aims at understanding biological functions of proteins by studying their three-dimensional structures. The main technique for elucidating three-dimensional structures of macromolecules is X-ray crystallography (see references in [1]). One of the requirements of X-ray crystallography of biological molecules is that they form crystalline samples large enough for crystallographic study. This requirement severely limits the number of biological molecules that can be studied as many fail to form crystals. The development of XFELs promises to open up new areas in life science by allowing structure determination without the need for crystallization. In fact, as suggested in (see references in[1]), sufficiently short and intense pulses from X-ray lasers may allow for the imaging of single protein molecules.

This article describes a possible future upgrade of the European XFEL. We present a study for a dedicated beamline for single-biomolecular imaging. The main idea is to use one of the free undulator tunnels of the European XFEL for providing the user community with the three SASE1, SASE2 and SASE3 lines, with the addition of a fourth beamline where the combination of 1 TW peak power in the energy range between 3 keV and 13 keV, and tunability of the pulse duration from 2 fs to 10 fs will provide significantly better conditions for single shot coherent imaging of protein molecules than at other XFEL facilities.

The European XFEL equipped with a dedicated bio-imaging beamline represents a development half way in between a proof-of-principle and a fully dedicated bio-imaging XFEL facility with high-rate of protein structure determination. The main advantage of the new beamline is the operation point at 1 TW with 2 fs-5 fs long pulses in the particular energy range between 3 keV and 5 keV, where the diffraction signal is strong. Operation at 1 TW in this peculiar energy range will not be accessible to other XFEL facilities at least until the end of the next decade. These characteristics would enable new exciting possibilities for coherent imaging of protein molecules with size larger than 10 nm.

BASIC CONCEPT OF THE BIO-IMAGING BEAMLINE

For the realization of the bio-imaging beamline we propose to use the same undulator technology optimized for the generation of soft X-rays at the European XFEL. The installation and commissioning of the new beamline can take place gradually. In the beginning, the new beamline would just extend the soft X-ray (SASE3) beamline and take advantage of the long XTD4 tunnel. An additional undulator composed by 19 cells would be added into the 300 m-long XTD4 tunnel. This undulator would extend the existing SASE3 line, composed by 21 cells, and have the same period of SASE3, in order to obtain a total cell number of 40. With this, SASE3 would be de facto converted into a bio-imaging beamline. Then, a new soft X-ray beamline, identical to the SASE3 baseline, could be installed in the free 150 m-long XTD3 tunnel.

Setup Description

The proposed setup is composed of four undulators separated by three magnetic chicanes as shown in Fig. 1. These undulators consist of 4, 3, 4 and 29 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 and hard X-ray would exploit the first and the third magnetic chicane, respectively. Both self-seeding setups should be compact enough to fit one undulator module.

A retractable grating monochromator based on a recent SLAC design (see references in [1]) will be introduced in the space created by the first chicane to enable soft X-ray

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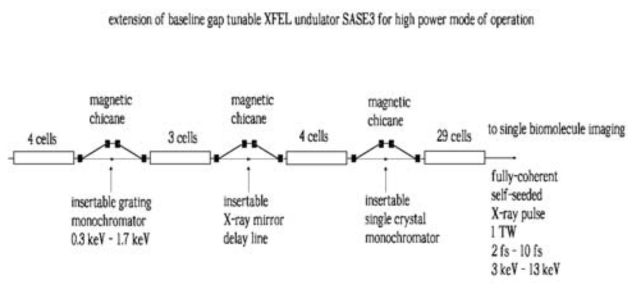

Figure 1: Design of the undulator system for the bio-imaging beamline. The method exploits a combination of self-seeding, fresh bunch, and undulator tapering technique. Each magnetic chicane accomplishes three tasks by itself. It creates an offset for monochromator or X-ray mirror delay line installation,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

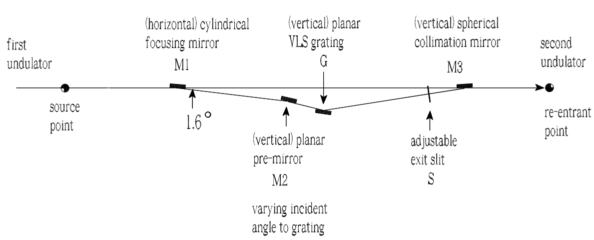

Figure 2: Optics for the compact grating monochromator originally proposed at SLAC (see references in[1]) for the soft X-ray self-seeding setup.

self-seeding, Fig. 2. The final design is currently under active investigations by the SLAC staff. A retractable mirror chicane will be introduced in the second chicane, and will introduce a tunable delay between electrons and photons, Fig. 3. Finally, a single-crystal monochromator (also retractable) will be inserted in the third chicane, to enable

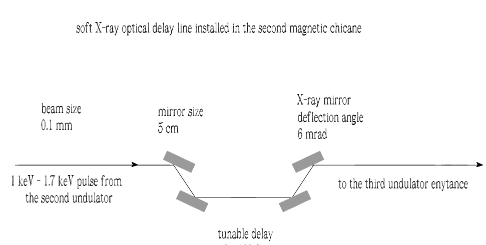

Figure 3: X-ray optical system for delaying the soft X-ray pulse with respect to the electron bunch. The X-ray optical system can be installed within the second magnetic chicane of the fresh bunch setup.

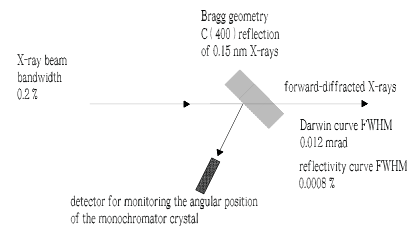

Figure 4: X-ray optics for compact crystal monochromator (see references in [1]) for a hard X-ray self-seeding setup.

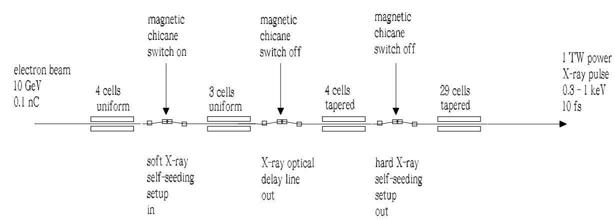

Figure 5: Design of the undulator system for 1 TW power mode of operation in the soft X-ray photon energy range. The method exploits a combination of self-seeding scheme with grating monochromator and an undulator tapering technique.

hard X-ray self-seeding, Fig. 4.

Generation of TW Pulses in the 0 3 keV - 1 7 keV Photon Energy Range

The four-undulator configuration in Fig. 1 can be naturally taken advantage of at different photon energies ranging from soft to hard X-rays. Fig. 5 shows the basic setup for the high-power mode of operation in the soft X-ray wavelength range. The second and the third chicanes 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 7 untapered cells , while tapering is implemented in the fourth undulator. The monochromatic seed is exponentially 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 an electron beam energy of 10 GeV. The setup was optimized based on results of start-to-end simulations for a nominal electron beam with 0.1 nC charge (see [1] for

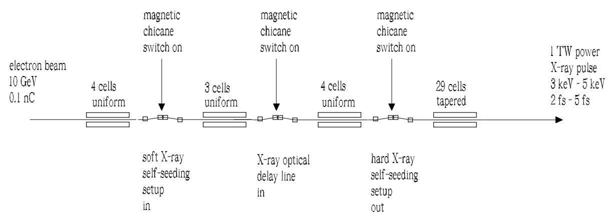

Figure 6: Design of the undulator system for 1 TW power mode of operation in the 3 keV - 5 keV photon energy range. The method exploits a combination of self-seeding scheme with grating monochromator, fresh bunch and undulator tapering techniques.

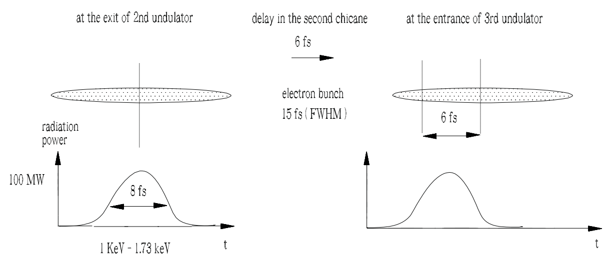

Figure 7: Principle of the fresh bunch technique for the high power mode of operation in the photon energy range between 3 keV and 5 keV. The second chicane smears out the electron microbunching and delays the monochromatic soft X-ray pulse with respect to the electron bunch of 6 fs. In this way, half of of the electron bunch is seeded and saturates in the third undulator.

references). Results in [1] show the feasibility of nearly Fourier-limited, TW-level pulses in this energy range.

Generation of TW Pulses in the 3 keV - 5 keV Photon Energy Range

Fig. 6 shows the basic setup for high power mode of operation in the most preferable photon energy range for single biomolecule imaging. All three chicanes are used for such regime, and must be switched on. 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 1 keV and 1.7 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, Fig. 9. 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

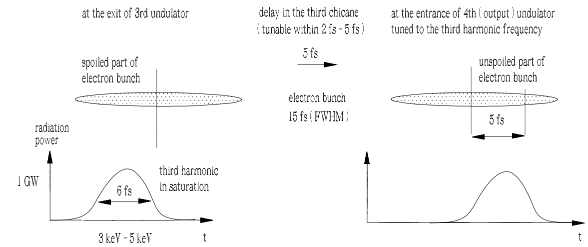

Figure 8: Principle of the fresh bunch technique for the high power mode of operation in the photon energy range between 3 keV and 5 keV. The third magnetic chicane smears out the electron microbunching and delays the electron bunch with respect to the radiation pulse. The unspoiled part of electron 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.

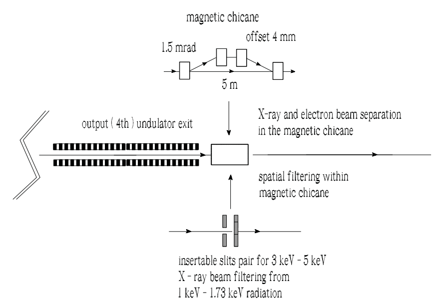

Figure 9: Schematics of a background filtering setup downstream of the extended SASE3 undulator. The scheme for spatial filtering will make use of a short magnetic chicane immediately behind the exit of the output undulator, so that the electron beam bypasses the slits. Vertical and horizontal slits will positioned at 70 m (Phase one) or 200 m (Phase two) downstream of the third undulator, where the background radiation (between 1 keV and 1.73 keV) is characterized by a spot size ten times larger than that of the main X-ray beam (between 3 keV and 5 keV).

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 3 keV and 5 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

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undulator exit, Fig. 9. 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 3 keV - 5 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.

Under the constraints imposed by the soft X-ray self-seeding setup, it is only possible to operate at an electron beam energy of 10 GeV. The setup was optimized based on results of start-to-end simulations for a nominal electron bunch with a charge of 0.1 nC. Results are presented in Section 4. 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 betatron switcher (see references in [1]). 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 increases compared with the same parameters at the entrance of the SASE1 undulator. The dispersion strength of the first chicane has been taken 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 first one. The electron beam was tracked through the first chicane using the code Elegant (see references in [1]). The electron beam distortions complicate the simulation procedure. However, simulations show (see Section 4) 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 chicane transformation (see below).

Finally, the design of the grating monochromator for the soft X-ray self-seeding scheme is under active investigation. For example, a more compact grating monochromator design has appeared very recently (see references in [1]). This novel design is based on the use of a toroidal grating, and adopts a constant entrance-angle mode of operation. The resolution and the photon energy range are the same, but the delay of the photons is about three times smaller. Therefore, the perturbations of the electron beam distributions generated in this way would be negligible. Results in [1] show the feasibility of nearly Fourier-limited, TW-level pulses in this energy range.

Generation of TW Pulses in 8 keV- 13 keV Energy Range

Fig. 10 shows the basic setup for the high-power mode of operation in the hard X-ray photon energy range. The first and the second chicane are not used in this regime, and

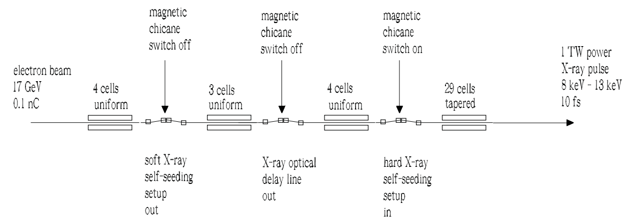

Figure 10: Design of the undulator system for 1 TW power mode of operation in the 8 keV - 13 keV photon energy range. The method exploits a self-seeding scheme with crystal monochromator.

are switched off. After the first three undulators and the single-crystal monochromator, a fourth output-undulator follows. Under the constraints imposed by the undulator parameters it is possible to operate at two nominal electron beam energies of 14 GeV and 17.5 GeV. The setup was optimized based on results of the start-to-end simulations for an electron beam energy of 17.5 GeV and a nominal electron beam with 0.1 nC charge. Results are presented in section 4. The output undulator is long enough to reach 1 TW power. The duration of the output pulses is of about 10 fs. In this mode of operation there is no possibility to tune the pulse duration without changing the electron beam distribution. If tunability of the pulse duration is requested in this energy range, this is most easily achieved by providing additional delay with a magnetic chicane installed behind the hard X-ray self-seeding setup. Results in [1] show the feasibility of nearly Fourier-limited, TW-level pulses in this energy range.

REFERENCES

[1] G. Geloni, V. Kocharyan and E. Saldin, ”Conceptual design of an undulator system for a dedicated bio-imaging beamline at the European X-ray FEL”, DESY 12-082, http://arxiv.org/abs/1205.6345 (2012).

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