OPTICAL DESIGN AND TIME-DEPENDENT WAVEFRONT PROPAGATION SIMULATION FOR A HARD X-RAY SPLIT-AND-DELAY UNIT FOR THE EUROPEAN XFEL

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Abstract

For the European XFEL [1] an x-ray split-and-delay unit (SDU) is built covering photon energies from 5 keV up to 20 keV [2]. This SDU will enable time-resolved x-ray pump / x-ray probe experiments as well as sequential diffractive imaging [3] on a femtosecond to picosecond time scale. The set-up is based on wavefront splitting, which has successfully been implemented at an autocorrelator at FLASH [4]. The x-ray FEL pulses will be split by a sharp edge of a silicon mirror coated with Mo/B4C and W/B_4C multilayers. Both partial beams will then pass variable delay lines. For different wavelengths the angle of incidence onto the multilayer mirrors will be adjusted in order to match the Bragg condition. Hence, maximum delays between +/- 2.5 ps at hν = 20 keV and up to +/- 23 ps at hν = 5 keV will be possible. The time-dependent wave-optics simulations have been done with SRW software, for the fundamental at hν = 5 keV. The XFEL radiation was simulated using an output of time-dependent SASE code FAST. Main features of the optical layout, including diffraction on the splitter edge, and optics imperfections were taken into account. Impact of these effects on the possibility to characterize spatial-temporal properties of FEL pulses are analyzed.

INTRODUCTION

The advent of new hard x-ray sources providing ultrashort and ultrabright light pulses allows for new classes of x-ray experiments. This is a great challenge for optical instrumentation. In addition to the already operating LCLS at the Stanford Linear Accelerator Center (USA) [5] and SACLA in Japan [6] the European XFEL is now under construction in Hamburg (Germany). Operating at electron bunch energies of 17.5 GeV the machine will provide photon energies between hν = 3 keV and hν = 24 keV at the undulator sources SASE1 and 2. Pulse energies of up to E_{pulse} = 2 mJ and an ultrashort pulse duration from a few fs up to 100 fs [1] are expected. In the burst mode very high pulse rates of 2700 pulses at 4.5 MHz per burst at a pulse rate of 10 Hz are possible, due to superconducting accelerators. In order to gain information about the temporal properties of the x-ray pulses, like temporal coherence and pulse-duration, two jitter-free pulse replicas are needed. Also for x-ray pump / x-ray probe experiments and for time-resolved diffractive imaging a split- und delay unit is required. In this paper we describe the design of a new x-ray split-and-delay unit based on a multilayer mirror coating, that covers photon energies between hν = 5 keV and hν = 20 keV. With this energy range the SDU can be integrated into the SASE 1 or SASE 2 undulator beamlines. Due to the high absorbance and the small reflectivity at large incident angles a grazing incident geometry is utilized. For the xuv- and soft x-ray spectral regime such a set-up has successfully been integrated into the FLASH SASE FEL. With this device the spatio-temporal coherence properties [4,7] as well as the pulse duration [8] of a soft x-ray FEL have successfully been measured for the first time. Further, ionization dynamics in expanding clusters have been investigated by XUV pump / XUV probe spectroscopy [9] and femtosecond sequential imaging has been realized for the first time [3]. The new SDU at the European XFEL will enable similar experiments in the x-ray spectral regime. While for the energy range of FLASH carbon (DLC) coated silicon mirrors still yield a sufficient reflectivity at photon energies up about to hν = 200 eV, this will not be the case for the hard x-ray pulses of the European XFEL. Therefore, Si-substrates coated with multilayers will be utilized.

OPTICAL CONCEPT

The high absorbance and the small reflectivity at large incident angles are severe limitations for optical instrumentation in the x-ray range and therefore demand for a grazing incident geometry.
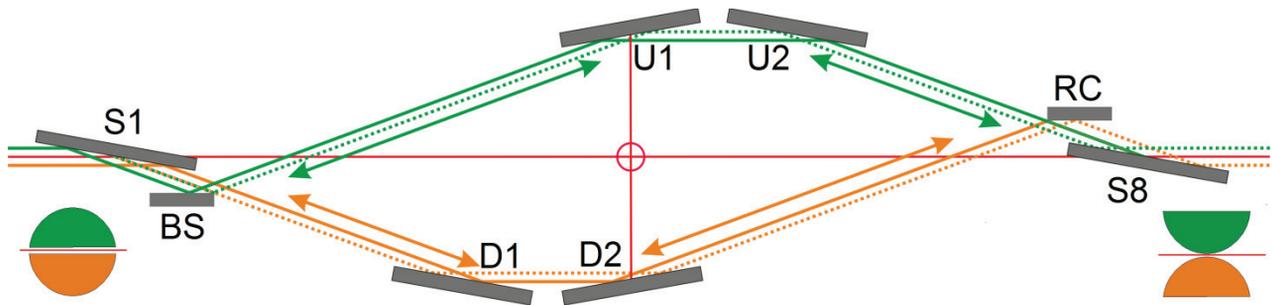
Figure 1: The optical concept of the SDU.

The optical concept will have to meet various requirements, like: A high reflectivity, transmission of the whole spatial beam-profile, delay with sub-fs resolution, a large delay range, and the wide photon energy range of the XFEL (5 –20 keV). These properties have to be achieved with a minimal disturbance of the beam position and direction, a high mechanical stability making a temporal resolution in the sub 100 attosecond regime feasible. The design and construction should of course incorporate elements, which allow a realization of the SDU in a practicable size. In order to meet these requirements a point symmetric optical concept based on a geometrical wavefront beam splitter and multilayer Bragg coatings which permit larger grazing angles has been developed. The whole set-up of the optical pathway is schematically shown in Fig. 1. The XFEL beam enters the SDU from the left side and is reflected by the first mirror (S1) downwards in the direction of the beam splitter (BS). The lower green part of the beam is reflected into the upper delay arm while the upper orange part passes the sharp edge in the direction of the lower delay arm. The mirrors of both delay arms can be moved along the split beam direction in order to introduce a temporal delay between both partial beams. After the orange beam has passed the lower delay line it is reflected by the recombination mirror (RC) in the direction of the last mirror (S8). The green beam passes the sharp edge of the recombination mirror unaffected. Thus, in this point symmetric concept the recombination mirror acts as the counterpart of the beam splitter. The last mirror (S8) reflects both beams into their original direction. It should be noted that the beam shape of both arms is rotated by 180° due to the odd number of reflections. In order to perform experiments the beams will have to be overlapped. This can be achieved by slightly rotating the recombination mirror, RC.

As already mentioned the mirrors are intended to work at grazing incidence angles. For photon energies from $h\nu = 5$ keV to $h\nu = 20$ keV multilayers will be used on the mirrors which possess high reflectivity. Since for multilayers the grazing angle depends on the wavelength, the mirrors have to be aligned for different wavelengths.

MECHANICAL LAYOUT

The projected sub-fs resolution as well as the essential pointing stability of the partial beams demand an extensive mechanical stability of the 6 m long construction. For the SDU at FLASH an intrinsic mechanical stabilization of the entire system is achieved by increasing the stiffness of the whole system. Thereby vibrations are significantly reduced. To ensure the mechanical sturdiness all components are mounted inside an optical bench which consists of an octagonal structure of stainless steel. For the SDU for the European XFEL a similar octagonal structure will be utilized, see Fig. 2. The mechanical stability of the optical bench is further improved by supporting frames. As discussed before the FEL beam is divided geometrically and both partial beams travel along two paths whose lengths can be adjusted. The path-length difference of one beam with respect to the other and in consequence the temporal delay is changed by moving the mirrors of both arms along the 2.4 m long guide rails. In order to adjust the correct angles for different photon energies all mirrors are turnable and the angle of the guide rails is variable. By moving the mirror the path length which the beam travels along the hypotenuse instead of the (shorter) adjacent of a triangle is varied, compare Figures 1 and 2.
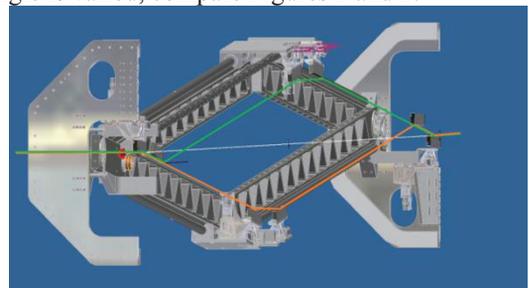
Figure 2: The mechanical layout of the SDU.

To obtain the designed sub-100 as resolution of the delay this longitudinal motion of the mirrors has to be of excellent precision. Under a grazing angle of $\theta = 0.56°$ (for $h\nu = 20$ keV) a movement of the mirror of $\Delta l = 10$ µm results in a path length difference of the light of 1.9 nm which corresponds to a temporal delay of $\Delta t = 6$ as. If

the grazing angle is $\theta = 2.28°$ (for $h\nu = 5$ keV) the corresponding delay for a movement of $\Delta l = 10$ µm is $\Delta t = 100$ as. Since the grazing angles of multilayer mirrors depend on the photon energy, an adjustability of the angles of incidence is required. The mirror mountings will therefore possess an angular precision of better than $\Delta\alpha = 1$ µrad. For the last mirrors, that reflect the beam to the experiment an additional piezo driven fine tuning is foreseen. In order to provide the experiments with an unaffected XFEL beam the whole optical bench can be moved horizontally so that the beam does not hit any mirror of the SDU.

MULTILAYER COATINGS

The silicon mirror substrates will be coated with different multilayers. Therefore, the grazing angle θ depends on the photon energy of the incident FEL beam. As it is obvious from Fig. 1 the grazing angle θ under which the beam splitter and the recombination mirror are to be positioned will be twice as large as the grazing angle of the other mirrors. Hence, different multilayer periods will have to be utilized for these two mirrors. In this regard, it has to be ensured that a maximum total transmission over the whole photon energy range is achieved. Since the absorption and correspondingly the reflectivity of different layer materials vary within the projected operating spectral regime of the SDU different materials will be used for the multilayers in order to provide the best reflectivity for each photon energy. These coatings will be applied beside each other. It possible to change between the multilayers by moving the whole optical bench in the horizontal direction (transverse to the beams direction). For photon energies above 10 keV Mo/B$_4$C multilayers with a periodicity of $d = 3.2$ nm for the delay mirrors and one of $d = 1.57$ nm for the beam splitter and recombination mirrors will be used. The reflectivity of a first test mirror has been measured at the ESRF.
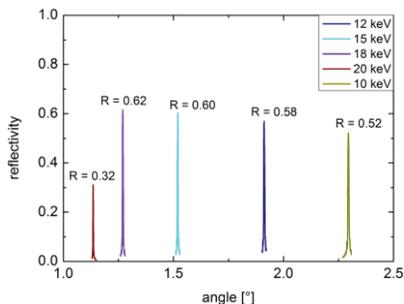
Figure 3: Reflectivity measurement of a Mo/B4C coating for the beamsplitter.

Figure 3 exemplarily shows the reflectivity of the multilayers for the beam splitter and recombination mirror with a periodicity of $d = 1.57$ nm. Due to the influence of the substrate's roughness and interdiffusion between these very thin layers the reflectivity reaches a maximum of $R = 0.62$ at $h\nu = 18$ keV.
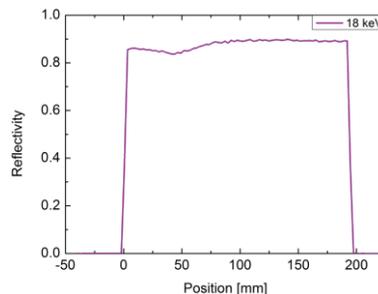
Figure 4: Measurement of the homogeneity of the Mo/B$_4$C multilayer.

In comparison a reflectivity of $R = 0.89$ is measured for the corresponding S1, S8 and the delay mirrors with a periodicity of $d = 3.2$ nm. With these values a total transmission of $T = 0.39$ is calculated. One major issue for a proper transmission of the beam through the SDU is the homogeneity of the reflectivity of the multilayer coatings along the whole footprint of the beam. Figure 4 shows a scan along the Mo/B$_4$C multilayer with a period of $d = 3.2$ nm with 18 keV radiation.

The measurement shows a perfectly homogenous coating between $l = 75$ mm and $l = 190$ mm. For $l = 50$ mm the reflectivity drops by 6% which is still tolerable. For photon energies below 10 keV Ni/B$_4$C multilayers with a period of $d = 4$ nm will be used for S1, S8 and the delay mirrors. For the beamsplitter and the recombination mirror the period will be $d = 1.96$ nm because such a thin periodicity Ni/B$_4$C layers do not grow properly. Thus W/B$_4$C will be utilized instead.

WAVEFRONT PROPAGATION SIMULATIONS

In order to evaluate the influence of diffraction effects from the non-ideal mirror surfaces and especially from the sharp edge, where the beam is split into two partial beams, time dependent wavefront propagation simulations were performed [10,11]. With these simulations of the two interfering half beams the capability of the SDU to measure the temporal coherence properties of the XFEL can be prognosticated. The simulations have been performed for SASE pulses using data generated by means of the FEL-simulation code FAST [12]. Figure 5 shows the spiky SASE pulse after the SDU for zero delay, $\tau = 0.24$ fs and for $\tau = 10$ fs.
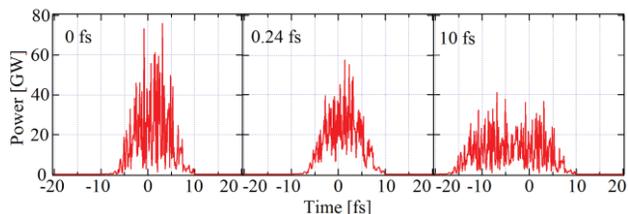
Figure 5: SASE power versus time for zero delay, $\tau = 0.24$ fs and $\tau = 10$ fs.

For a photon energy of $h\nu = 5$ keV Fig. 6 shows the interference pattern of both half beams overlapping each other under an angle of $\theta = 1.54$ µrad in a distance of

d = 130 m from the SDU and zero time delay. The interference pattern yields a maximum visibility of $v = (I_{max}-I_{min})/(I_{max}+I_{min}) = 0.92$. In comparison Fig. 7(a) shows the interferences for a time delay of $\tau = 240$ as, which is the theoretically estimated coherences time of the pulses. Here the visibility is $v = 0.42$. From figure 7(b) it is obvious that for a large delay of $\tau = 10$ fs the interference fringes vanish. Here only fringes resulting from diffraction at the edge of the beamsplitter are apparent.

The mirrors inside the SDU will show a peak-to-valley height error of ~8 nm, which will cause wavefront perturbations that are not negligible. On the detector which will be placed in a distance of ~130 m behind the SDU these perturbations will raise additional fringes.
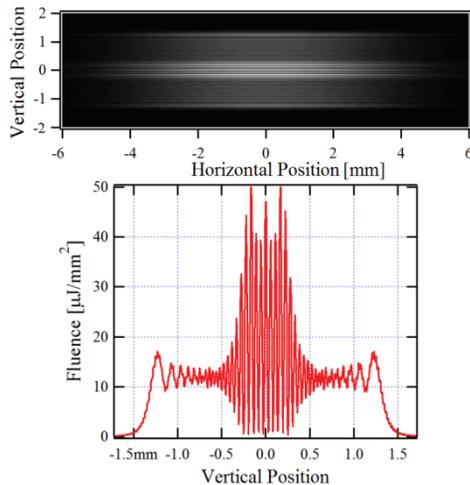
Figure 6: Two-beam interferences at zero delay (5 keV).
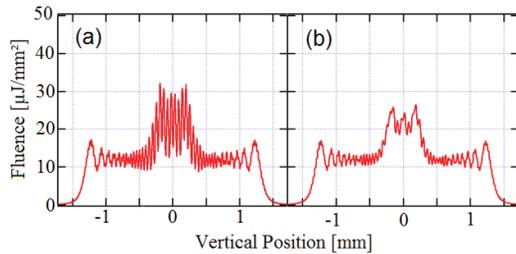
Figure 7: Two-beam interference for $\tau = 240$ as (a) and $\tau = 10$ fs (b).

In order to evaluate the influence of this effect simulations for non-perfect mirror surfaces [2] have been performed. Figure 8 shows the interference pattern of both half beams for the same parameters as in Fig. 6 ($\theta = 1.54$ µrad, d = 130 m and zero time delay). Compared to Fig. 5 the fringes caused by wavefront perturbations from the non-perfect surfaces of the mirrors are obvious. Nevertheless, the fringes from two-beam interference are still clearly visible. For a time-delay in the order of the coherence time ($\tau = 240$ as) between the two interfering beams the two-beam interference fringes are still visible, however, their amplitude is already in the order of the fringes caused by the imperfect surfaces, see Fig. 9(a). In Figure 9(b) only the fringes caused by the splitting edge

and by the wavefront perturbations from the mirrors are visible for a delay of $\tau = 10$ fs.
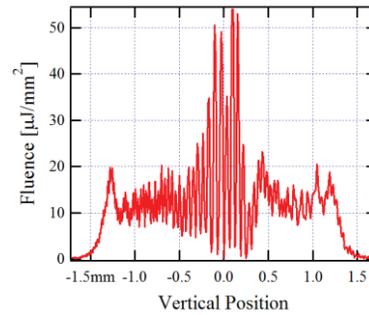
Figure 8: Two-beam interference with non-perfect mirror surfaces.
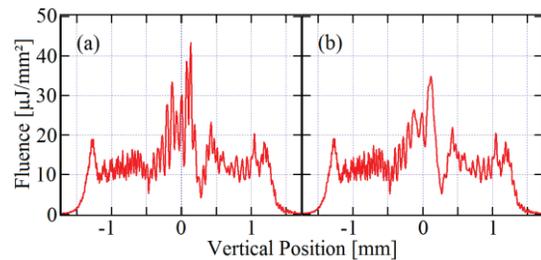
Figure 9: Two-beam interference for $\tau = 240$ as (a) and $\tau = 10$ fs (b) for a mirror with a height error of 8 nm (pv).

Thus there is an influence of the wavefront perturbations on the measurement of the temporal coherence properties of the XFEL pulses. Consequently, a simple evaluation of the temporal coherence by just calculating the visibility of the interference fringes will not be feasible in this case.

However, together with thoroughly conducted wavefront propagation simulations the SDU will be a beneficial device to investigate the temporal coherence properties of the European XFEL beam.

CONCLUSION

A new split- and delay-unit for the European XFEL is designed and constructed for photon energies between hν = 5 keV and hν = 20 keV. This SDU will serve the users with two time delayed x-ray pulses for x-ray pump / x-ray probe experiments and it will enable a characterization of the temporal properties of the XFEL. Wavefront propagation simulations have been performed taking into account real SASE pulse data generated with the FEL-simulation code FAST. In this regard the capability of the SDU to evaluate the temporal coherence properties of the XFEL pulses has been proven for ideal and also for real mirror surfaces with a peak-to-valley height error of ~8 nm. Detailed time-dependent wavefront propagation calculations, with the use of final mirror metrology data, may greatly help in the advanced diagnostics and analysis of properties of real X-ray FEL pulses.

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