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Design and Throughput Simulations of a Hard X-Ray Split and Delay Line for the MID Station at the European XFEL

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Abstract. A hard X-ray Split and Delay Line (SDL) under development for the Materials Imaging and Dynamics (MID) station at the European X-Ray Free-Electron Laser (XFEL.EU) is presented. This device will provide pairs of X-ray pulses with a variable time delay ranging from -10 ps to 800 ps in a photon energy range from 5 to 10 keV. Throughput simulations in the SASE case indicate a total transmission of 1.1% or 3.5% depending on the operation mode. In the self-seeded case of XFEL.EU operation simulations indicate that the transmission can be improved to more than 11%.

INTRODUCTION

The intense, ultra-short, and coherent X-ray pulses provided by X-ray free-electron lasers (XFELs) open up areas of research with X-rays that were previously inaccessible. Taking advantage of these outstanding beam properties, the forthcoming Materials Imaging and Dynamics (MID) instrument at European XFEL facility [1, 2] aims at the investigation of nanoscale structure and dynamics by X-ray scattering and imaging. Applications to a wide range of materials from hard to soft condensed matter and biological samples are envisaged.

The European XFEL facility (XFEL.EU) will provide X-ray pulses separated by 220 ns in 0.6 ms long bunch trains arriving with a repetition rate of 10 Hz [1]. Probably, special operation modes will permit the pulse spacing within the trains to be reduced to ~800 ps (defined by the accelerator RF frequency) for a few pulses per train. Shorter time separation between individual pulses cannot be provided by the accelerator. Hence, in order to access ultrafast dynamics below 800 ps in the time domain an X-ray split and delay line (SDL) is required at the MID station.

In this proceeding article, we report about the concept and the mechanical design of hard X-ray SDL for the MID station at XFEL.EU. The SDL is optimized to operate in a photon energy range from 5 to 10 keV and provides pairs of jitter-free X-ray pulses with a variable time delay ranging from -10 ps to 800 ps. Simulations are presented to address the total throughput of the SDL in the optical splitting scheme, both with SASE and self-seeded beams.

CONCEPTUAL LAYOUT

Figure 1 shows a sketch of the SDL concept based on symmetric Bragg diffraction from perfect Si (220) crystals. The incoming FEL pulse is separated in two parts by a beam splitter and the split pulses take two different trajectories (upper and lower branch). By changing the path length of the upper branch, the difference in arrival times (Δt) between the two pulses can be varied from 0 to the desired 800 ps with a few fs precision. In order to

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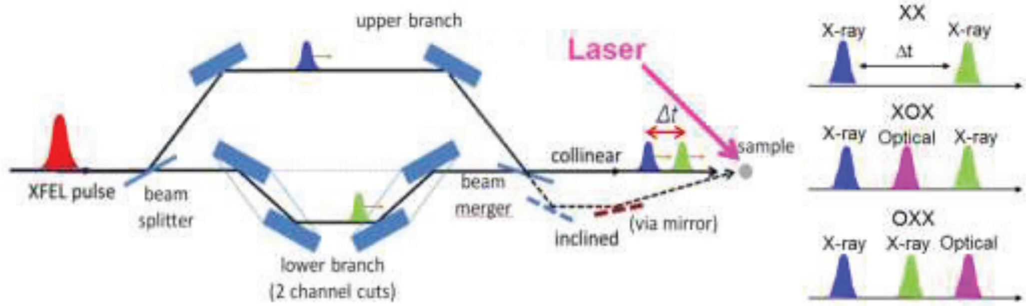
achieve a negative delay time between the two pulses (required to scan Δt and experimentally determine Δt=0), two channel-cut crystals are employed in the lower branch to extend the beam path slightly. The beam merger can be adjusted such that either a collinear or a parallel, non-collinear mode is provided. In the latter case, the two beams are overlapped at the sample by use of an additional mirror. In such an inclined mode the two diffraction patterns resulting from interaction with a sample will be spatially separated on the detector. This device will allow the study of ultrafast dynamics using experimental techniques, e.g. time-resolved X-ray Photon Correlation Spectroscopy (XPCS) [3], Speckle Visibility Spectroscopy (SVS) [4], ultrafast X-ray tomography [5] and temporally and spatially resolved X-ray holography [6]. In addition, with the powerful tunable and synchronized optical laser system at the MID station, not only X-ray Pump-probe experiments, but also X-ray probe - optical pump - X-ray probe (XOX) and optical pump - X-ray probe - X-ray probe (OXX) experiments are enabled by the SDL.

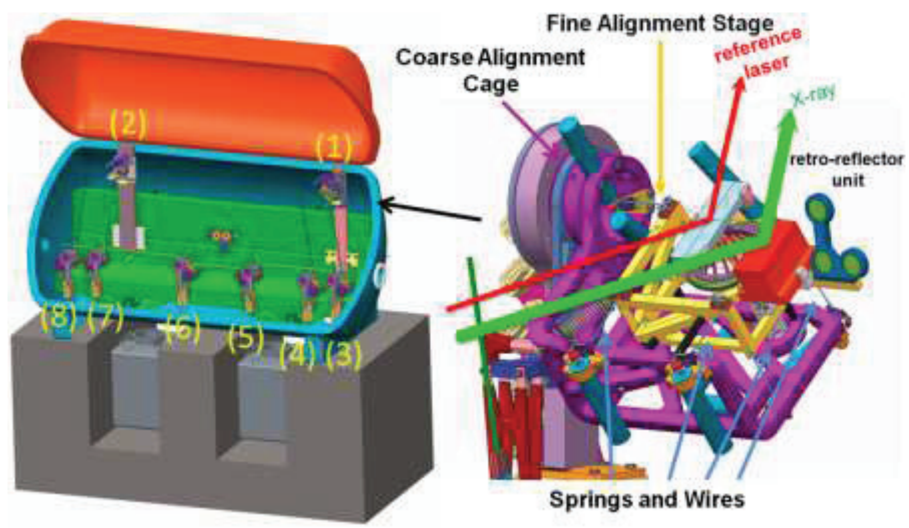


(a) (b)

FIGURE 1. (a) Schematic layout of the split and delay line (SDL) and (b) the possible pump-probe schemes at MID.

CURRENT MECHANICAL DESIGN

The SDL is situated towards the end of the MID optics hutch ~8 m upstream of the sample position. This location is downstream of a pre-monochromator, hence reducing the heat load on the first beam splitter crystal. The SDL is at this position as close as possible to the sample enabling optimum beam stability.



(a) (b)

FIGURE 2. (a) Mechanical design of the SDL and (b) Double cage configuration to host the Bragg crystals.

Figure 2 presents mechanical design of the SDL. The vacuum vessel in Fig. 2(a) is about 2 meters long and supported by a massive granite block to ensure mechanical stability of the setup. Inside the vessel, the rails for the translations of the two upper branch crystal cages (1), (2) are mounted on the vertical extend of an L-shaped optical bench. Linear encoders will be installed on all translations of the upper branch to monitor the positions. The splitter cages (3), (4), channel cut cages (5), (6) and merger cages (7), (8) in the lower branch are mounted on the other vertical side of the bench. Two different concepts will be employed to split the beam, ideally in 1:1 splitting. One concept is denoted optical splitting ensured by a thin perfect crystal of a few µm thickness [7] inserted into the beam. It diffracts a portion of the beam intensity and transmits the remainder. The other concept is geometrical splitting where a thick crystal intersects half of the beam and diffracts that portion while the other half passes over the crystal [8]. The beam merger will be realized using the same concepts. These two versions of splitters (3), (4) and mergers (7), (8) will be installed at different position alone beam direction, as close as possible. The thin crystal splitter (merger) precedes the geometric splitter (merger). In this way, one can split the beam with the thin crystal and continue in the inclined mode by using a thick crystal merger without compromising on the maximum delay time. All these lower branch elements can be shifted downwards to move out of the X-ray beam path if desired.

Due to the 8 m distance between the SDL and the sample, we demand alignment accuracies of 0.1 µrad in pitch angle (vertical beam shift) and 0.2 µrad in the roll angle (horizontal beam shift) for all the Bragg crystals. However, the parasitic tilt motions of the upper branch translations are expected to be much more than these requirements because of the long travel range of about 1 meter for each arm. In order to measure parasitic crystal displacements during movement, a 3-axes laser interferometer system has been designed. To compensate these undesired tilt motions the crystals are mounted in double cages as show in Fig. 2(b). The outer cage's coarse pitch alignment can be adjusted in a range from 18.8º to 40.2º corresponding to the Si (220) Bragg angle from 10 to 5 keV. Inside the outer cage (purple), a fine alignment stage (yellow) is pulled by six motor driven wires against the restoring spring force from the left and the bottom side. By changing the length of the individual wires, this inner stage can be orientated to compensate small parasitic tilt motion of the outer cage introduced by the translations. The fine alignment stage has nrad resolution. An optical mirror for alignment purposes by a "reference laser" and the X-ray Si (220) crystal are mounted on this stage. A retro-reflector unit necessary for operating the laser interferometer system is also located on this stage, as close as possible to the Si crystal. The parasitic tilt displacements of the crystals will be measured by the laser interference signal and corrected for by the fine alignment stage.

Further developments concerning control system, X-ray diagnostics and temperature stabilization are still under discussion and in progress.

THROUGHPUT SIMULATIONS

To address the total throughput of the SDL we have performed simulations for the optical splitting scheme both with SASE and self-seeded pulses. The simulation is based on the sketch in Fig. 1 (a) with all crystals as Si(220). Additionally, the pre-monochromator upstream of the SDL is also taken into account. The transmission and reflection of the thin crystals are calculated using dynamical diffraction theory in the two-beam approximation which is implemented in the x-ray optics module of the OCELOT framework [9].

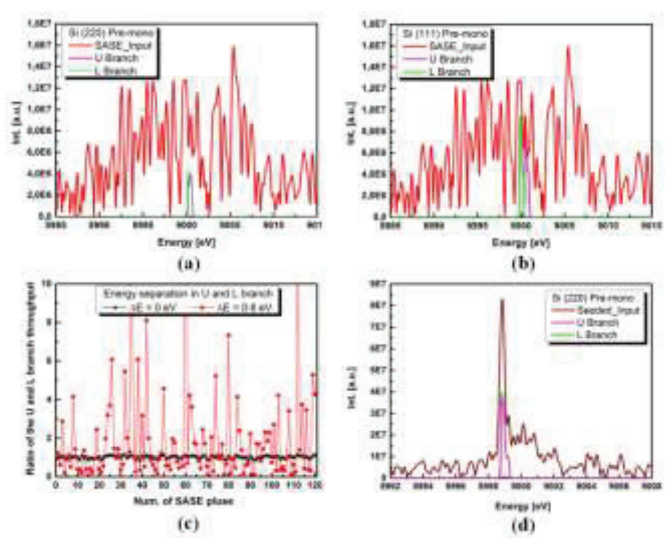


FIGURE 3. Throughput simulations for the intensity splitting scheme with 9 keV, 20 fs SASE and self-seeded pulses. (a) and (b) show the spectra of SASE input pulse and output pulses with Si(220) and Si(111) pre-monos, respectively. (c) shows the intensity ratio of the two output pulses in the two cases (a, black) and (b, red). (d) illustrates the spectra of self-seeded input pulse and output pulses using a Si(220) pre-mono.

In the SASE case, 120 individual pulses were simulated in Genesis 1.3 [10] assuming a 17.5 GeV electron beam radiating at 9 keV using undulator tapering and electron beam parameters from start-to-end linac simulations for a 20 fs radiation pulse [11]. As an example, the spectrum of a simulated SASE pulses is presented in Fig. 3(a) in red. Due to the large bandwidth of the SASE pulse, the pre-monochromator can be either Si(220) or Si(111). With a Si(220) pre-monochromator (0.6 eV bandwidth), the upper and lower branch crystals need to share the same spectral component of the input pulse coming from the pre-monochromator. The spectra of the two output pulses are illustrated in the Fig. 3(a) in green and magenta. A constant intensity ratio between the upper and lower pulse is expected (star points in Fig. 3 (c)) as they share the same spectral component and an average throughput of ~1.1% is obtained. By using a Si(111) pre-monochromator (1.3 eV bandwidth), the upper and lower branch energies can be slightly separated (0.6 eV in this simulation) by adjusting the crystal angles. Hence, the upper and lower branches transmit different spectral components of the incident beam. The spectra are shown in Fig.3(b). In this configuration, the total throughput of the SDL can be increased to 3.5%. However, due to the spectral randomness of SASE, large pulse-to-pulse fluctuations of the intensity ratio between the two branches are observed, as shown by circles in Fig.3(c).

In the self-seeded case, the 120 pulses are simulated with OCELOT using the same electron beam parameters as above and assuming a two-chicane self-seeding setup with tapered undulators currently under design for the SASE-2 beamline [12]. A self-seeded spectrum and output pulse spectra from the SDL are shown together in Fig.3(d). Since the bandwidth is already narrow only the Si(220) pre-monochromator is considered in this scenario. The two output pulses have the exact same photon energy and a constant intensity ratio (not shown), similar to the SASE case with Si(220) pre-mono, but here with 10 times higher throughput (11.2% instead of 1.1% is obtained).

SUMMARY

A hard X-ray split and delay line is under development for the MID station at European XFEL facility. The device is designed to operate in an energy range from 5 to 10 keV and provides pairs of X-ray pulses with variable delay between -10 to 800 ps. In the self-seeded case the device operates both with a high transmission (> 11%) and an optimum stability of the intensity ratio between the two pulses.

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