The Laser Infrastructure at the SXP instrument of the European XFEL

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P. Grychtol, V. Vardanyan, D. Doblas-Jimenez, and M. Izquierdo
European XFEL, Holzkoppel 4, 22869 Schenefeld, Germany
E-mail: sxp@xfel.eu

Abstract. This contribution presents the laser infrastructure concept of the Soft X-ray Port (SXP) instrument at the European X-ray Free Electron Laser (XFEL) for day one operation. This scientific platform is conceived as an open port complementing the scientific scope of the other two, already operating baseline instruments at the SASE 3 soft x-ray undulator focusing on atomic, molecular and non-linear optical (SQS) as well as condensed matter physics (SCS). The main driving force behind SXP originates from the time-resolved X-ray photo-electron spectroscopy community contemplating key questions in the dynamics of materials science at interfaces. Nonetheless, proposals to investigate high-valent metal intermediates in biological and inorganic catalysts for chemical bond activation by means of fluorescence spectroscopy as well as research on highly charged ions in the light of astrophysics are also pursued. The outstanding capabilities of the European XFEL pave the way for ultrafast pump-probe investigations at the SXP instrument combining intense and tunable soft X-rays with versatile optical laser capabilities, which are provided by two synchronized femtosecond laser systems, whose wavelength ranges can be extended into the infrared as well as extreme ultraviolet region.

1. Motivation

Highly brilliant X-ray free electron laser (XFEL) facilities producing photons with energies of several thousands of electron volts (eV) have opened up intriguing possibilities to explore the realm of atoms, molecules and condensed matter [1]. Their energy-tunable, ultrafast and highly coherent photon pulses enable site-specificity investigations of light-matter interactions on the natural time scales of the fundamental nuclear as well as electronic motion in great detail [2, 3]. For this purpose, time-resolved experiments have generally employed a pump-probe technique, in which the system under investigation is excited by a *pump* pulse and its subsequent response is followed by a temporally shifted *probe* pulse. In case these pulses originate from different and autonomous light sources, such as an accelerator-based XFEL and an optical laser (OL), the temporal resolution of any measurement is limited by the duration of the respective pulses as well as the timing jitter in between them. Therefore, in order to successfully conduct pump-probe experiments with the highest possible time resolution, it is not only important to generate extremely short laser pulses, but also to properly synchronize the different light sources. Moreover, to benefit from site-specificity and address all kinds of electronic, magnetic and phononic degrees of freedom in a time-resolved experiment, it is crucial to be able to tune the investigative photon sources over a large range of wavelengths, with full control over the polarization and ideally over the entire electro-magnetic field of the ultrafast photon pulses.

2. Overview

In the following, this contribution presents the concept of the laser infrastructure at the Soft X-Ray Port (SXP) instrument of the European XFEL [4, 5]. This scientific platform is primarily designed for time- and spin-resolved X-ray photo-electron spectroscopy, but investigations of complex chemical and bio-inorganic molecular systems with fluorescence spectroscopy as well as research on highly charged ions are also envisioned. It is located behind the SASE 3 soft X-ray undulator providing photons with variable polarization in an energy range between 260 eV and 3000 eV exceeding 10^{12} photons per pulse with up to 27000 pulses per second. Two high-quality elliptical mirrors in Kirkpatrick-Baez (KB) configuration can focus the femtosecond XFEL pulses to a spot size of approximately 1 µm in diameter, resulting in an intensity of more than $10^{18}\,W/cm^2$ in the interaction region. Together with various synchronized femtosecond laser systems, whose wavelength ranges can be extended into the infrared as well as extreme ultraviolet region, it will pave the way for ultrafast pump-probe investigations at the SXP instrument combining intense and tunable soft X-rays with versatile optical laser capabilities.

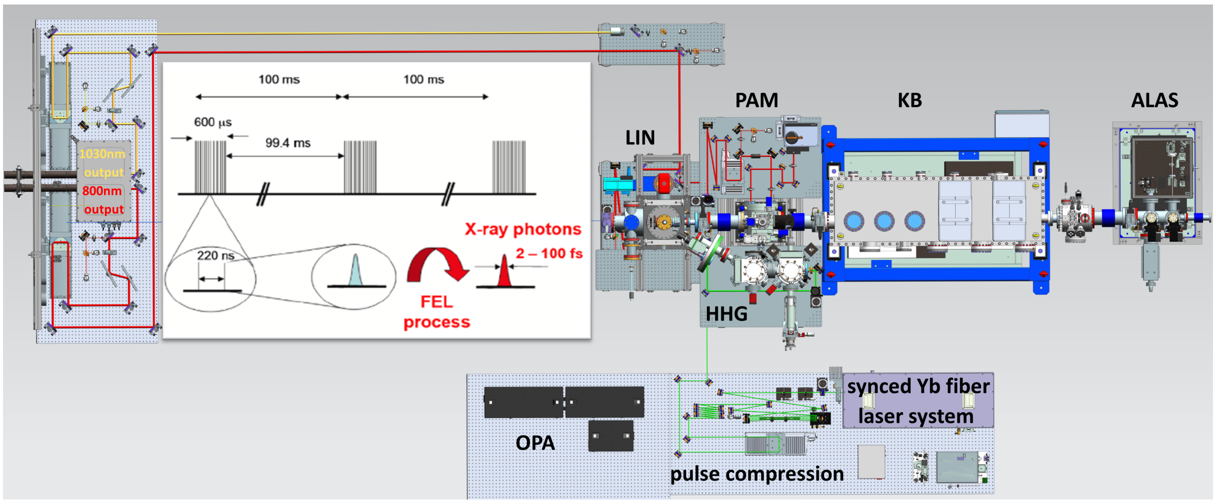

Figure 1. Top view of the SXP instrument model and tentative laser beam paths.

A top view of the SXP instrument model without an experimental end-station but including the permanent beamline components and an exemplified outline of the laser beam paths for day one operation is presented in Fig 1. The FEL beam enters the SXP instrument on the right side of this figure and passes first through the alignment laser system (ALAS) entering the KB optics tank thereafter. Before the soft X-ray beam is focused into the interaction region, it is lead into the photon arrival time monitor (PAM) and the laser in-coupling unit (LIN). While the PAM is used to measure the relative arrival times between the XFEL and the OL pulses, the LIN allows for coupling the OL beam into the path of the XFEL in a co-linear manner, such that both beams can be properly focused onto the sample under investigation.

3. Alignment laser system - ALAS

The ALAS is an optical laser and imaging system whose purpose is to (pre-)align the beamline components farther downstream. It is supposed to simplify the alignment procedure of the SXP instrument, thereby also saving valuable user beam time, and reducing the risk of beam damage as well as wear on all components that can potentially be exposed to the focused XFEL radiation. A mechanical model of the ALAS placed right in front of the KB optics tank is displayed in Fig 2. In this figure, the XFEL beam enters the ALAS chamber from the bottom through a CF 40 flange and it passes through two combined 4-way-crosses, each of which hosting a manipulator.

The first manipulator is equipped with a drop-in mirror to inject an optical laser beam along the beam path of the XFEL, while the second manipulator holds a set of fluorescent screens to be used for monitoring the positions of both laser beams. In combination with additional pop-in screens located farther downstream in the PAM or the LIN sections, it is possible to align the SXP instrument without having to resort to valuable XFEL operation.

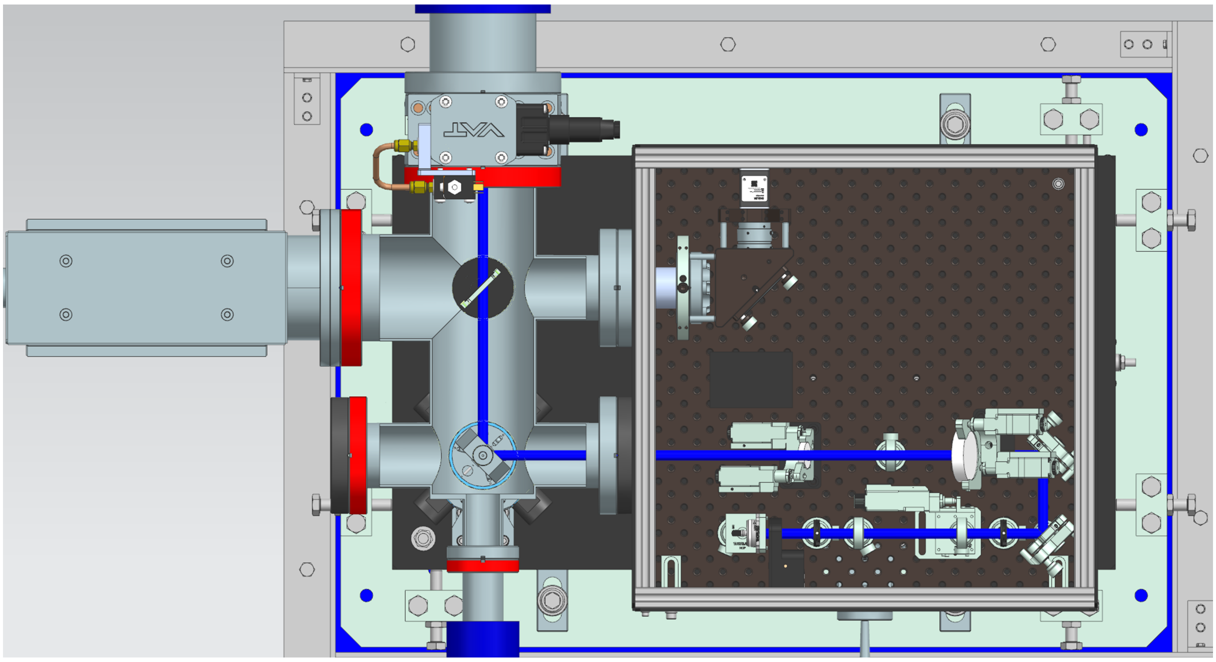

Figure 2. Top view of the ALAS mechanical model.

Mounted in the black box perpendicular to both manipulators the corresponding laser diode module including a set of alignment optics and a CCD camera assembly can be found. To maximize the utility of the ALAS, it should not only propagate coaxially with the XFEL beam, but also mimic its profile and divergence. That is how it is also possible to adjust the KB mirrors to focus on the sample using an optical beam only. To this end, a telescope has been placed after the laser diode allowing for the expansion of the optical beam to the size of the X-ray beam.

4. Optical pump-probe laser systems - LAS

Ultrafast optical pulses at the SXP instrument are mainly provided by the central pump-probe laser developed by the European XFEL Laser (LAS) group [6]. This laser operates in a 20 Hz burst mode with an intra-burst pulse structure matching that of the European XFEL, as illustrated in the inset of Fig 1. The 20 Hz operation allows for sending the beam simultaneously to the two baseline experiments at SASE 3. Thus, both instruments (SQS and SCS) are able to work at 10 Hz with the same pattern as the X-ray pulses. While it is foreseen to offer laser pulses in a wide range of wavelengths around the visible spectrum via various frequency conversion schemes, two beams will be delivered to the SXP experiment hutch in the first place: one centered at 800 nm with pulse durations in the femtosecond range (mainly 15 fs and 50 fs) and the other centered at 1030 nm with pulse durations in the picosecond regime (mainly 0.9 ps and 400 ps). Both beams are passed through the dedicated SCS instrument laser hutch entering the SXP experiment hutch by means of an elaborate delivery system, as seen on the left side of Fig 1. The SASE 3 central pump-probe laser has primarily four set points with the intra-burst pulse pattern matching the one of the XFEL and they are summarized in the following table:

Table 1. Operating points of the central pump-probe laser at the SASE 3 undulator.

set point	intra-burst rep. rate [MHz]	pulse energy: 800 nm [mJ]	1030 nm [mJ]
1	4.5	0.05	1
2	1	0.2	4
3	0.2	1	20
4	0.1	2	40

Both laser beams allow for optical excitations at discrete wavelengths in the ultraviolet region by frequency up-conversion through second-, third- and fourth-harmonic generation reaching as high as 257 nm. In case of the 800 nm beam, however, fourth-harmonic generation is not feasible at these high pulse energies, because absorption of the generated light by the conversion crystals leads to its rapid degradation. To fill the spectral gaps until about 250 nm, an optical parametric amplifier (OPA) system can be used, which at the same time allows for tuning the wavelength into the mid-infrared region until approximately 15 µm to enable resonant excitations of collective low-energy modes, such as phonons, magnons, spin density waves, etc. [6].

Furthermore, the SXP instrument is equipped with an additional Yb fiber laser system centered at 1030 nm, delivering 250 fs short and 200 µJ strong laser pulses at a repetition rate of about 300 kHz. An internal acoustic-optical modulator allows for mimicking the characteristic 10 Hz bunch pattern and its pulse train can be fully synchronized to the European XFEL [7]. As indicated at the bottom of Fig 1, it is planned to compress the pulse duration below 40 fs using a Herriott-type multi-pass cell [8] and extend the wavelength range into the extreme ultraviolet (XUV) region employing high harmonic generation (HHG) techniques [9].

5. Photon Arrival Monitor - PAM

To perform pump-probe experiments with the highest possible time resolution combining an OL with a XFEL, it is not only important to generate ultrafast laser pulses, but also to properly synchronize these light sources and to compensate any residual jitter between them. By utilizing a dedicated balanced optical cross-correlation technique based on the actively stabilized distribution of an optical reference signal, a relative in-loop timing jitter on the sub-10 fs level has been achieved at European XFEL [7]. A feasible approach to mitigate any residual jitter is to measure the relative arrival time of the pump and probe pulses on a single shot basis and sort the data accordingly in the subsequent analysis process, potentially reaching sub-femtosecond accuracy [10]. For this purpose, the SXP instrument is equipped with a PAM placed downstream of the KB optics tank. As indicated in Fig 3, it receives a weak portion of the OL pulses that are split off the main beam pumping the sample under investigation. After passing over a delay stage, these pulses are stretched in time propagating through a thick piece of glass and they are focused onto a thin semi-transparent membrane, which at the same time is illuminated by the soft X-ray beam coming from the KB optics chamber. The XFEL pulses change the refractive index and thus transmission of the membrane material, whose transient response is measured by the chirped optical pulses such that their relative delays to the soft X-ray pulses are mapped onto the optical laser spectrum. This established technique is known as spectral encoding [11].

The PAM was designed and set up by the X-ray photon diagnostics group of the European XFEL [12]. It has already been successfully employed to monitor the relative arrival times between XFEL and synchronized OL pulses resulting in a timing jitter of about 58 fs (FWHM). Moreover, it was demonstrated that applying corresponding time-of-arrival corrections in pump-probe experiments can significantly improve their temporal resolution [13, 14].

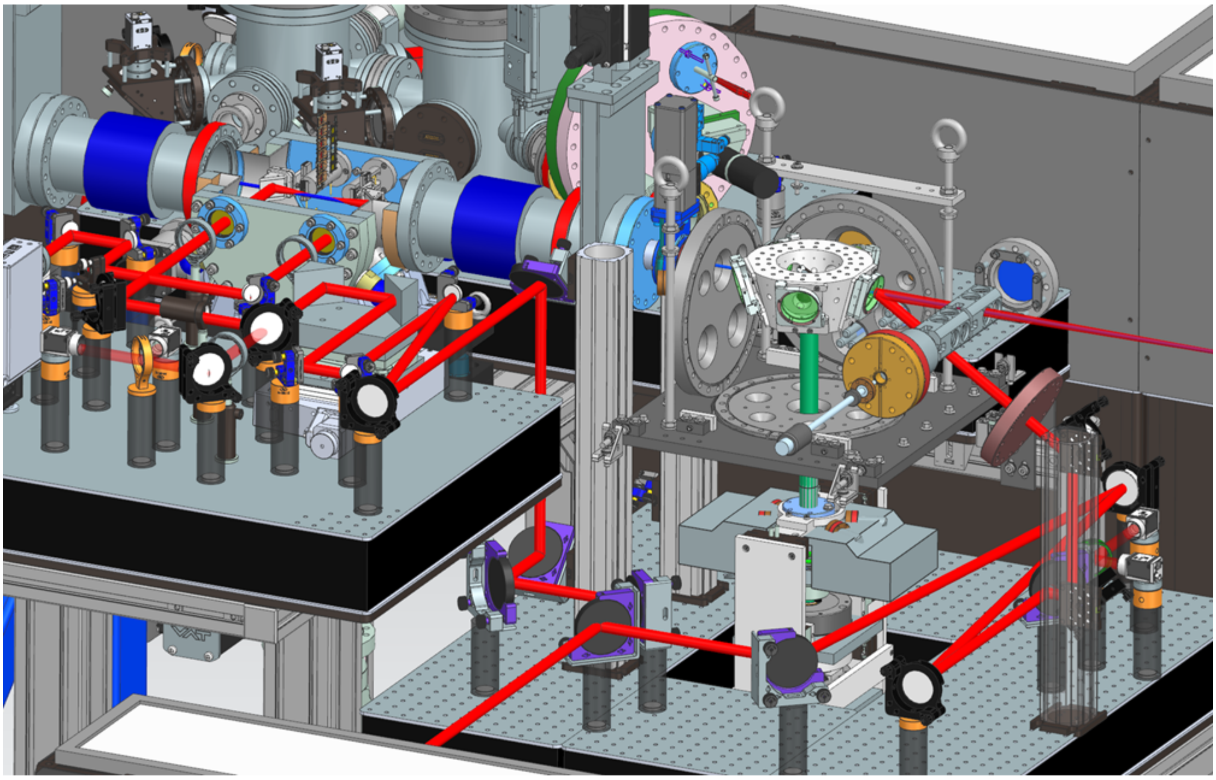

Figure 3. Close-up view of the PAM and LIN showing the tentative 800 nm laser beam path. Some mechanical components in this figure have been omitted for the sake of illustration.

6. Laser Incoupling - LIN

The LIN chamber is the most downstream beamline component of the SXP instrument placed right in front of any experimental end-station. As indicated in Fig 3, it serves for collinearly coupling the OL beam, which is focused onto the sample under investigation by a curved mirror system outside the chamber, into the XFEL beam path. In order to admit a large bandwidth of laser wavelengths without having to break the vacuum, this chamber can host several in-vacuum mirrors mounted on a two story rotatable carousel, the properties of which can be chosen according to the requirements of a particular experiment. The mirrors can have a diameter of either 2" or 3" and they are mounted at an angle of 15° with respect to the XFEL beam, which can pass collinearly with the OL via holes milled through the centre of each mirror. Vacuum compatible piezo motor driven mirror mounts can be used to align the OL beam with nm precision. Downstream of the in-coupling mirrors, a scintillator on a manipulator can be moved into the beam paths to image the OL as well as the XFEL beams for spatial overlap, at the same time allowing for the alignment of the entire beamline when combined with the ALAS. Moreover, the manipulator is equipped with an ultrafast photodiode that can be used to narrow down the temporal overlap of both beams to less than 100 ps. A conservative assessment utilizing ray-tracing simulations reveal that by using a pair of curved mirrors placed onto the optical breadboard below the LIN chamber, a focus with a diameter of about 100 µm at the sample interaction region can be obtained. This translates to an intensity of more than $10^{15}\,W/cm^2$ per mJ pulse energy on target using the 800 nm beam with a pulse duration of 15 fs.

7. Summary

This contribution presents an overview of the laser infrastructure concept for day one operation of the SXP instrument at the European XFEL. Here, the permanent beamline components are introduced and their purpose as well as functionality are briefly described. The first and most upstream component is the alignment laser system (ALAS), which is used to align the SXP instrument without having to resort to the precious XFEL beam. It is followed by the soft X-ray Kirkpatrick-Baez (KB) optics that are used to focus the XFEL beam into the sample region. Before reaching a diameter of about 1 µm, the X-rays are lead into the photon arrival time monitor (PAM) and the laser in-coupling unit (LIN). The former is used to measure the relative arrival times between the XFEL and the OL laser pulses, while the latter allows for coupling the OL into the path of the XFEL in a co-linear manner. Thus, both beams can be properly focused onto the sample under investigation eventually reaching intensities at the order of $10^{15}\,W/cm^2$ and $10^{18}\,W/cm^2$, respectively. This sophisticated infrastructure paves the way for ultrafast pump-probe investigations at the SXP instrument combining intense and tunable soft X-rays with versatile optical laser capabilities, which are provided by two synchronized femtosecond laser systems, whose wavelength ranges can be extended into the infrared as well as extreme ultraviolet region of the electromagnetic spectrum.

Acknowledgments

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