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P. Grychtol[1], N. Kohlstrunk[1], J. Buck[2,3], S. Thiess[3], V. Vardanyan[1], D. Doblas-Jimenez[1], J. Ohnesorge[1], S. Babenkov[4], M. Dommach[1], D. La Civita[1], M. Vannoni[1], K. Rossnagel[2,3], G. Schönhense[5], S. Molodtsov[1] and M. Izquierdo[1]

[1]European XFEL, Holzkoppel 4, 22869 Schenefeld, Germany
[2]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany
[3]Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany
[4]Université Paris-Saclay, CEA, CNRS, LIDYL, 91191 Gif-sur-Yvette, France
[5]Institut für Physik, Johannes Gutenberg Universität Mainz, 55099 Mainz, Germany

E-mail: `sxp@xfel.eu`

Abstract. The successful implementation of the baseline instruments at the European XFEL has triggered a second phase of instrument developments aiming to extend the portfolio of available techniques. At the soft X-ray undulator (SASE 3), the Soft X-ray Port (SXP) instrument is currently under construction. Conceived as an open port, it focuses primarily on femtosecond time-resolved X-ray photoelectron spectroscopy (TR-XPES), which has proven to be a powerful tool to understand the properties of materials and the interaction between their internal degrees of freedom. The extension of this technique to the soft X-ray energy range is only possible at MHz free electron lasers (FELs) due to space-charge effects which limit the maximum photon flux per pulse on the sample. In this contribution, the SXP instrument at the European XFEL and the implementation of TR-XPES using a momentum microscope are presented. The photon energy range available at SASE 3, 0.25 keV to 3.5 keV, and the variable polarization will allow for the simultaneous characterization of the electronic, magnetic, chemical and structural properties of materials with femtosecond time resolution. To this end, a wide range of laser excitation wavelengths, ranging from the XUV to the THz region, will be available.

1. Introduction

The European X-Ray Free Electron Laser (XFEL) produces coherent and ultrafast electromagnetic radiation in the soft and hard X-ray regimes by accelerating electrons up to 17.5 GeV in a superconducting (SC) linear accelerator. This technology allows to increase the typical 10 Hz to 120 Hz repetition rate achievable with warm linear accelerators (linacs) into the MHz regime. At the end of the European XFEL, a fan of 5 tunnels has been built ending up in an experiment hall that allows to host up to three experiments per undulator tunnel. In the first implementation phase, three of the tunnels have been equipped with planar undulator systems to generate Self-Amplified Spontaneous Emission (SASE) type FEL radiation. The SASE 1 and SASE 2 undulator systems produce horizontally polarized hard X-ray photons photons in a range from 5 keV to 30 keV [1, 2]. On the other hand, SASE 3 has been optimized to produce soft X-rays starting below the carbon edge around 0.25 keV and reaching up to 3.5 keV [3]. This initial configuration has been recently upgraded with the installation of an afterburner to generate FEL light with variable polarization, which is currently under commissioning [4].

The FEL radiation produced at the SASE 3 undulator is used since 2018 by the two soft X-ray baseline instruments: Spectroscopy and Coherent Scattering (SCS) and Small Quantum Systems (SQS) [1]. The Soft X-ray Port (SXP) presented in this contribution is part of a development program at SASE 3 launched after the successful start of the operation of these baseline instruments. It aims to provide a FEL beamline where one can easily integrate user provided setups exploiting techniques not available at SCS or SQS. The user community has proposed three new classes of experiments so far: femtosecond time-resolved X-ray photoelectron spectroscopy to investigate quantum materials, charge transfer materials for light harvesting, new catalysts, etc.; fluorescence spectroscopy and inelastic scattering of very diluted high-valent metal intermediates in biological and inorganic catalysts for chemical bond activation and highly charged ions experiments to test new atomic and molecular theories, understand astrophysical phenomena occurring in hot plasmas, unsolved questions in quantum electrodynamics and also to gain insight into atmospheric processes and climate change. From the facility side, the SXP instrument could be used to test new diagnostics, detectors and experimental techniques. A more detailed description of these first implementations can be found in [3].

The first expression of interest represents the largest community thanks to the creation of the time-resolved X-ray photoemission spectroscopy (TR-XPES) consortium. The community aims to use the extended photon energy range of SASE 3 to perform *complete* time-resolved X-ray photoelectron spectroscopy. *Complete* refers to the idea of performing simultaneous characterization of the electronic, spin, chemical and structural properties of materials with femtosecond time resolution. This will allow to deepen the understanding of their properties in great detail, to advance theoretical frameworks and also to develop new materials and methods to improve current technology. While femtosecond TR-XPES experiments of the electronic and spin properties are available since decades using pulsed laser and high harmonic generation (HHG) sources, the chemical and structural investigations require soft X-rays with pulse energies only available at FELs. Since space-charge effects [5] limit the photon flux dramatically, the generalization of TR-XPES requires the high repetition rate of SC FELs. FLASH and the European XFEL are currently the only SC FELs available for this purpose. LCLS-II and SHINE will soon be available. TR-XPES has been already successfully implemented at FLASH [6] allowing to extend femtosecond TR-XPES to chemical and structural studies [7, 8]. However, the fundamental photon energy is limited to about 0.3 keV, while higher energies can be accessed using third harmonic limiting the photon energy to less than 1 keV.

TR-XPES at the SXP instrument of the European XFEL is a perfect extension of the FLASH capabilities. The photon energy range, 0.25 keV to 3.5 keV in first harmonic, would allow time-resolved structural studies using X-ray photoelectron diffraction in forward scattering, which has a straightforward interpretation. Moreover, the bunch pattern of the European XFEL, bursts of 2700 pulses at 4.5 MHz and 10 Hz base frequency, is expected to increase the data throughput. Pump-probe experiments will be performed using the central laser producing pulses with the same pattern as the XFEL. The fundamental wavelengths centered around 800 nm and 1030 nm can be frequency converted from the extreme ultraviolet (XUV) to the THz range [9, 10].

2. X-ray transport system

The SXP instrument shares the SASE 3 undulator and the first part of the X-ray transport system [11, 12] with the baseline instruments SCS and SQS. The X-ray transport system, depicted in Fig. 1, can be divided into four parts: (i) The offset mirrors, (ii) the monochromator, (iii) the distribution mirrors and (iv) the focusing system. The offset mirrors and the monochromator parts are common to all the instruments.

The offset mirror system is a combination of a flat mirror, M_1, and an adaptive optics, M_2, deflecting the beam horizontally. They are arranged in a chicane configuration to suppress the spontaneous radiation produced by the source. The incident angle of both mirrors can be

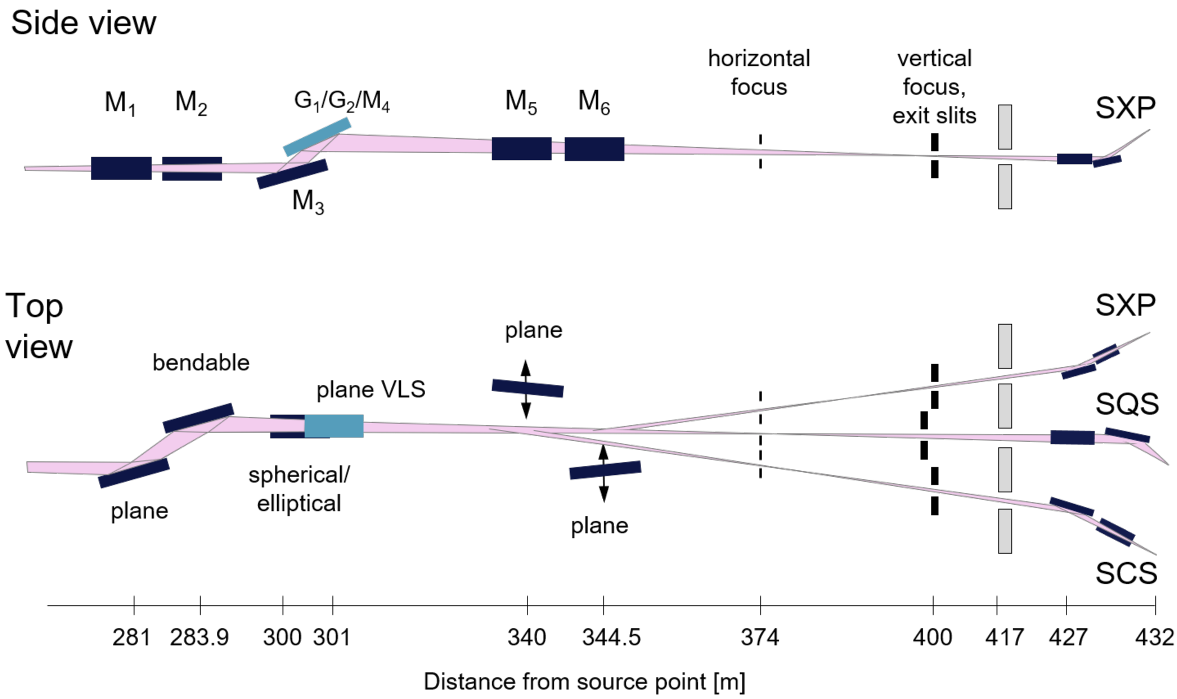

Figure 1. Side and top view sketch of the SASE 3 X-ray transport system.

adjusted between 6 mrad and 20 mrad in order to suppress the higher order harmonics. The M_2 bending system is used to optimize the mirror aperture with respect to the source divergence and to produce an intermediate horizontal focus. The optics have extremely tight tolerances in slope errors to work in the diffraction limit: $20 - 50$ nrad (RMS) slope profile errors and 2 nm peak-to-valley (PV) [11]. All X-ray optical elements in the system are coated with a B_4C layer, chosen to minimize damage effects at high pulse energies. Up to 17 mJ have been demonstrated.

The monochromator section is made of two pre-mirrors followed by two gratings, G_1 and G_2 and a plane mirror M_4. The fix radius pre-mirrors are installed at fixed incidence angles: 20 mrad and 9 mrad for the low energy (LE) and high energy (HE) pre-mirrors, respectively. The LE mirror covers the energy range from 0.25 keV to 1.5 keV and the HE mirror that between 1.5 keV and 3 keV. M_4 is flat and allows to use the pink beam. The grating G_1 has 50 lines/mm and G_2 150 lines/mm providing a resolving power of $\sim$3000 and $\sim$10000, respectively.

The specific X-ray optics of SXP are the M_6 distribution mirror and the Kirkpatrick-Baez focusing system (KBS). M_6, positioned at 344.5 m from the source, steers the beam to the SXP branch. It is flat and has a nominal length of 0.95 m. The mirror quality is similar to that of the offset mirrors and it is also coated with B_4C.

The KB focusing system will be installed in the SXP experiment hutch. It has been conceived with two bendable mirrors that allow to set different interaction points after the last permanent beamline component, the laser in-coupling (LIN) unit [9]. The X-ray beam will impinge on the horizontal focusing mirror first and on the vertical focusing mirror thereafter at a grazing angle of 9 mrad. This will focus the intermediate horizontal focused beam realized with M_2 and the intermediate vertical focused beam produced by the monochromator system. Two interaction points F1 and F2, separated by 1.5 m, have been defined. They can be reached using the configurations BTL#1 and BTL#2 shown in Fig. 2. An additional work through focus point F3 has been defined to allow for changing the spot size between approximately 1-2 µm at F1, and

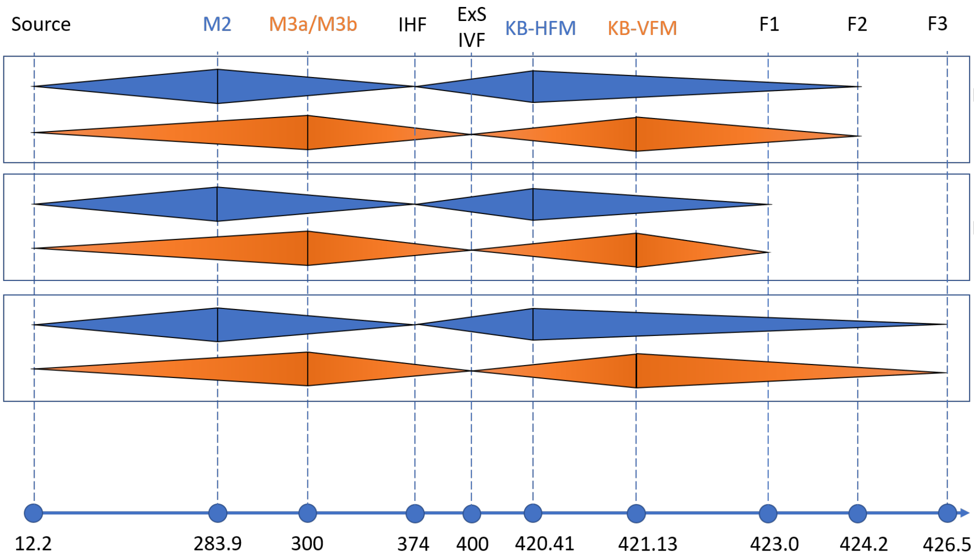

Figure 2. Focusing schemes considered in the design of the bendable KB system. Three optical configurations are proposed: F1 and F2 and a walk-through focus F3. The blue drawings represent the horizontal focusing plane, and the orange drawing corresponds to the vertical one.

100 µm (FWHM). The first KB implementation will be realized by means of fixed radii mirrors, which are supposed to provide a spot size of approximately 30 µm.

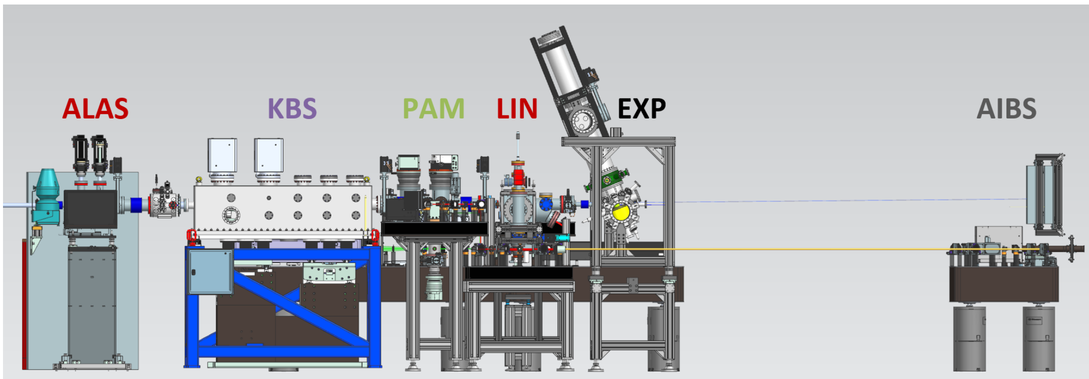

Figure 3. Side view of the SXP instrument in day one configuration.

3. Day one configuration

The day one configuration of the SXP instrument is depicted in Fig. 3. Besides the KBS described in the previous section, the SXP instrument hutch hosts the permanent beamline components, the optical laser infrastructure and the TR-XPES experimental station. The permanent beamline components (PBC) represent the minimum set required to ensure an efficient operation of the SXP instrument. The PBC are: the alignment laser (ALAS), developed to pre-align all SXP components without using the FEL beam; the pulse arrival monitor (PAM), designed to measure the relative arrival time of the pump and probe pulses on a single shot basis using the spectral encoding technique [13]. The arrival time is afterwards used to sort the data during the analysis process in order to reach potentially sub-femtosecond time resolution. The

LIN, located after the PAM, has been designed to couple the optical laser pulses with the FEL or HHG ones at the interaction point. The laser related components and the optical laser system are described in [9]. At the end of the wall an active instrument beam stop (AIBS) will be installed. This radiation safety device measures the fluorescence of air in case the FEL beam escapes from the experimental station sending a signal to disable the beam at the instrument.

4. TR-XPES experimental station

The TR-XPES experimental station is composed of a main chamber equipped with the photoelectron spectrometer and the sample manipulator with a cryostat cooling down to 20 K, a sample preparation chamber, a LEED chamber and a load-lock for fast sample exchange.

The main feature of the system is the time-of-flight (ToF) momentum microscope photoelectron spectrometer. It represents a novel approach to angle-resolved photoelectron spectroscopy (ARPES) allowing for measuring two dimensional maps over large momentum areas (k_x, k_y), thus providing the highest degree of parallelization possible in ARPES experiments. k–microscopy uses a basic optical concept: in imaging systems, the reciprocal image represents the distribution of the transversal momentum components. Since $k_{\|}$ is conserved in the photoemission process, the reciprocal image formed in the back-focal plane of a cathode lens maps the transversal momentum distribution of the electrons inside the crystal. Valence and core electrons can be directly accessed providing images of either the electronic structure in energy-momentum space or the chemical and atomic structure in real space.

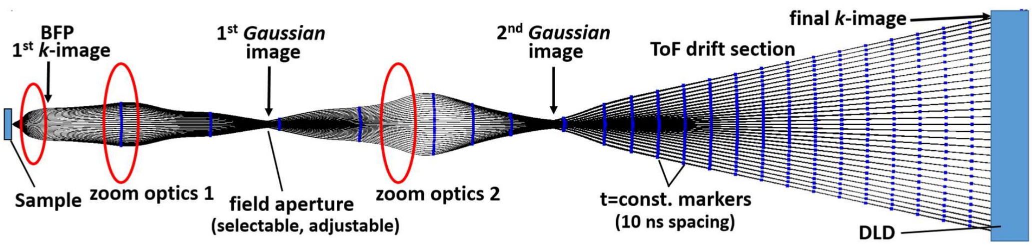

Figure 4. Simulated trajectories for the electron optics of the high energy k-microscope.

The soft X-ray range of the SXP instrument has required the development of new electron optics. The resultant lens accepts the full half-space above the surface with initial kinetic energies of up to several keVs [14]. This value represents an increase of the maximum k field radius by a factor of 3 as compared to standard low-energy designs. The larger acceptance angle results in the enhancement of the total intensity by one order of magnitude. The scheme of the lens system is depicted in Fig. 4. Three lens groups are indicated by ellipses; Gaussian and reciprocal planes are denoted. The first k image in the back-focal plane is formed by a special objective lens designed for minimum spherical aberration. The electron beam is transformed to the desired drift energy in the imaging ToF column by zoom lens 2. Energy-dependent k momentum maps are taken simultaneously in an energy interval defined by the drift energy. For high resolution, band-mapping intervals of up to 10 eV are imaged in best focus. Much larger intervals can be recorded with a reduced resolution determined by the chromatic aberration. To achieve a good energy resolution and minimize the "crosstalk" between the longitudinal and transversal momentum components, time markers with 10 ns spacing are defined as planar isochrones.

Besides the lens system, the other key components of the spectrometer are the 900 mm long drift tube and the detector. The applied voltage selects the energy interval of the electrons reaching the detector. The detector is an 80 mm diameter delay-line (DLD) with a spatial resolution of 80 µm and a temporal resolution of 150 ps. This allows for resolving about 1 Megapixel image points, which higher than the resolution of the electron optics. The time resolution allows a maximum count rate of $8 \cdot 10^6$ counts per second. The DLD records all counting events in the energy window selected by the voltage of the drift tube [15].

The energy resolution of the ToF microscope is defined by the length and potential of the drift tube and the temporal resolution of the detector. The SXP k-microscope can achieve an energy resolution ΔE between 70 meV and 9 meV [16] when working with drift energies between 60 eV and 10 eV, exceeding the energy resolution provided by the SASE 3 monochromator. Given the 150 ps time resolution of the DLD, the time gap of 222 ns (4.5 MHz mode) allows for resolving 1,500 time slices, thus enabling high-resolution work. The effect of temporal aliasing may restrict the usable working range, as described in [15].

Spin detection capabilities will be added in a second stage by inserting a spin-filter crystal (SFC) after the zoom optics 1 shown in Fig. 4. This lens will focus a parallel electron beam on the spin-filter. The reflected spin filtered electrons will enter into another ToF column with zoom optics 2, a drift tube and a DLD detector similar to those of the spin-integrated detector. Azimuthal rotation of the SFC will allow for switching from the transversal to the in-plane spin component thus enabling vectorial spin detection.

5. Summary

This contribution presents an overview of the day one implementation of the SXP instrument at the European XFEL. The X-ray optics system, the day one configuration and the first experimental station, TR-XPES, are outlined. The TR-XPES station, equipped with a time-of-flight momentum microscope and the soft X-ray energy range of the SASE 3 undulator system, 0.25 keV to 3.5 keV, will allow for the simultaneous characterization of electronic, spin, chemical and structural properties of materials. All together, the TR-XPES at SXP will represent one of the few worldwide instruments where to realize complete time-resolved photoelectron spectroscopy studies with femtosecond time resolution.

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