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CONCEPTUAL DESIGN REPORT

Scientific Instrument FXE

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Summary

The Femtosecond X-ray Experiments (FXE) scientific instrument will permit ultrafast pump-probe studies of solid and liquid samples, using different structural tools: X-ray absorption spectroscopies (XANES, EXAFS), requiring tunability of the incident monochromatic ($\Delta E/E$ down to a few 10^{-5}) radiation, X-ray emission spectroscopies (XES, RIXS, etc.), and X-ray diffraction (XRD) capabilities (WAXS, SAXS, Bragg) requiring both large (1 Mpx) and small (< 128 kpx) area detectors. All detectors need to be compatible with the burst-mode operation of the European XFEL.

The FXE instrument is a side branch of the SASE1 beamline, and thus three mirrors are needed to suppress the Bremsstrahlung and to deflect the beam. The experimental setup will focus on ambient condition experiments with adjustable spot sizes (line, spot) in the 5–1000 µm range via one Kirkpatrick-Baez (KB) pair, and provide a vacuum chamber for studies with sensitive samples or surfaces, and with samples requiring cryogenic cooling. This setup strategy will thus permit the installation of a highly versatile secondary spectrometer including large rotational movements around the sample position. A large area detector with a central hole (adjustable in size up to ca. 10 mm) will permit SAXS/WAXS studies from a distance of a few cm (*q* range up to 10 A^{-1} at 18–20 keV) up to 4.5 m, and the transmitted pink X-ray beam can be further analysed with a dispersive transmission spectrometer for transmission XANES/EXAFS. The additional smaller detector (< 128 kpx) will be available for special solid-state experiments and mounted to permit collecting specific large-angle reflections.

Table 1: *Summary of the FXE instrument parameters*

Parameter	**Amount**
Energy range / keV	3–20
Pulse energy / mJ	1.5–0.25 (250 pC); 5.4–0.5 (1 nC)
Pulse intensity / 10^{11} photons	31–0.5 (250 pC); 109–2.1 (1 nC)
Harmonic suppression	< 10^{-4} (ca. 10^{-6} for E > 7.5 keV)
Polarization	Linear
Beamline optics	2 offset mirrors,1 deflection mirror 2 KB focusing mirrors
Natural bandwidth	(3–1) x 10^{-3} (3–20 keV)
Primary monochromator	Si(111) (bandwidth 2 x 10^{-4}) Si(311) (bandwidth 5 x 10^{-5}) or Si(333) (2 x 10^{-5})
Beamline throughput (3–10 keV)	0.5–0.8
Beamline throughput (10–20 keV)	~ 0.8
Pulse duration	< 2–25 fs (15 fs laser) up to 1 nC
Spot size on sample	5–1 000 µm, freely adjustable (line, spot)
Synchronization	< 15 fs
Equipment*	< 15 fs burst mode laser (0.2 mJ / 800 nm) + SHG/THG + NOPA + laser diagnostics Sample positioner (xyz, angular) < 128 kpx detector positioner (angular, distance) X-ray emission spectrometer (rotatable) 4.5 MHz detectors (1 Mpx, 128 kpx, < 128 kpx, time monitor) Dispersive spectrometer (I_0, I_1)

* Mpx = megapixel, kpx = kilopixel

Introduction

The European XFEL facility will deliver a remarkably different pulse pattern than any other femtosecond hard X-ray source. This conceptual design report (CDR) seeks to exploit this capability to the fullest extent possible, as it offers the advantage of unprecedented average X-ray flux and extremely fascinating opportunities for the investigation of time-dependent phenomena, even down to the most dilute samples imaginable. This CDR thus naturally embraces the unique pulse structure available to perform hitherto unimaginable experiments in the fields of chemical and biological dynamics with few-femtosecond time resolution, over difficult catalytic studies on surfaces, sometimes even triggered with femtosecond-pulsed far-IR sources (THz radiation), to material science studies on crystalline and non-crystalline samples. In short, the overarching theme of the scientific instrument for femtosecond X-ray experiments (FXE instrument) is to take snapshots and film the very first instants of microscopic materials in action. This naturally includes the "molecular movies" capabilities advocated elsewhere, but in addition seeks to dig into the very origin of atomic motion, which is found in the extremely fast-changing electronic and spin structures, most often driven by light. The FXE instrument seeks to unravel the elementary steps of motion itself, which reign over all processes occurring in nature. Already, this fascinating goal warrants the construction of the most powerful hard X-ray source, and some fascinating goals envisioned appear uniquely solvable at the European XFEL facility

The scientific scope and the realization of the FXE instrument, as described in this CDR, should be evaluated in comparison to the related end station(s) at the first femtosecond free-electron laser source for hard X-radiation, LCLS, especially in view of what really new science can be done after its inauguration in 2015. This CDR describes, in particular, the unique characteristics of the European XFEL facility operation (including heat load issues). The FXE instrument is designed to exploit the X-ray burst mode at the highest pulse intensities possible. Processing up to 2 700 pulses at 4.5 MHz per burst at 10 Hz (Figure 1) is foreseen, which differentiates this

facility from all the others, be they operational, under construction, or in the planning stage.

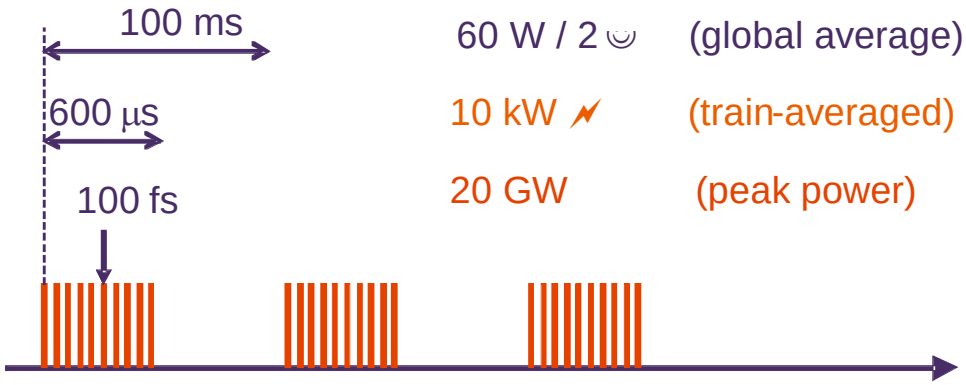

Figure 1: *Pulse operation mode of the European XFEL and corresponding average and peak power values*

Eventually, the present concept emphasizes the use of an extremely versatile secondary spectrometer in the hard X-ray domain, while maintaining the simultaneous capability for revealing X-ray diffraction studies down to the few-femtosecond time scale. This versatility can be preserved for a rather simple sample environment, thus the startup design will focus on dynamic studies in liquid or physiological environments, but also permit the study of solid samples, which require vacuum and cryogenic conditions. This concept is different from the other five scientific instruments planned for startup at the European XFEL, and thus provides specific capabilities that cannot be (easily) followed at any other scientific instrument at the European XFEL facility.

Science case

The European XFEL facility will provide transversely coherent X-radiation with up to 2 700 pulses at 4.5 MHz at an overall 10 Hz burst repetition rate. Within one such burst, the individual pulse-filling pattern can be selected, as requested by the experiment. For example, to monitor the temporal behaviour of a photoexcited protein over the entire 100 fs – 600 µs time scale, one could request a “logarithmic” filling pattern with few (e.g. around 30) individual X-ray pulses entering the sample at different time delays on the fs, ps, ns, and µs time scale. In such experiments, the fs laser pulse would strike the sample at 10 Hz, and each sequence of time-delayed X-ray pulses within one burst would monitor a different time domain of the ensuing dynamics and subsequent kinetics. This capability is unique to the European XFEL, and will be implemented at the FXE instrument.

For flux-demanding experiments, one can seek to use every single X-ray pulse at 4.5 MHz to collect the required statistics, and this strategy appears very promising for dynamic studies of dilute (e.g. biological) samples in physiological media. Some examples of the envisioned scientific program are given below. These represent a selection of research proposals for the FXE instrument, as discussed during the FXE workshop in December 2009.

Ultrafast studies of nuclear, charge, and spin dynamics: The interplay between nuclear, electronic, and spin degrees of freedom is commonplace in transition metal compounds. Such compounds are key ingredients in certain proteins, and often are at the very beginning of light-driven biological functions [1]. Such compounds are also being studied in chemistry due to their rich magnetic switching behaviour [2], but also for their charge-transfer properties in light-harvesting applications [3]. Many of these systems are believed to exhibit correlated electron dynamics in an extremely non-Born–Oppenheimer regime, but observation of the elementary steps towards e.g. spin transition dynamics has remained so far in the dark [4]. The FXE instrument will permit structural studies on the 25 fs time scale, and ultrafast XANES, EXAFS, and RIXS are key tools to unravel the very first steps in these systems.

Dynamics of solids and phase transitions, surface studies via X-ray reflectivity: Particularly interesting is the structural dynamics associated with photoexcited carrier relaxation, as well as carrier-lattice interactions and the subsequent phase transitions [5] as observed via XRD [6]. In addition, dynamic studies of diffuse scattering away from the Bragg peaks are envisioned. Non-crystalline samples are foreseen as well as crystals. Special interest will be given to single-shot irreversible and reversible phase transitions, i.e. amorphous-to-crystalline (and vice versa) phase switching in photoexcited chalcogenides [7]. In addition, both the diffraction and spectroscopy communities have emphasized the importance of dynamic magnetic structure studies using resonant diffraction techniques. Surface studies attempt to exploit the specular reflectivity from plane interfaces and the diffuse scattering from rough surfaces to investigate changes in the electronic density in solids near a vacuum–solid interface after impulsive excitation (light or pulsed magnetic field).

Dynamics of photoactive proteins: Static X-ray crystallography has been the most powerful tool for determining the atomic structure of proteins. However, to understand the details (and beginning) of biological functions, it is important to catch the protein in action, and this requires down-to-a-few-femtosecond time resolution. Picosecond studies on such protein crystals at synchrotrons has shown that significant changes already have taken place on time scales much shorter than the temporal resolution of the experiment [1, 8]. Extending such time-resolved studies to the 25 fs regime will allow capturing the very first steps in protein structural dynamics. Finally, X-ray spectroscopic tools will permit unraveling the very initial steps involving changing electronic and spin state structures, in concert with the early dynamic structural changes.

Chemical dynamics in the solution phase including solvation dynamics: The vast majority of chemical and biological phenomena in nature (but also in industrial processes) occur in the liquid phase, very often in water itself. It is also recognized that the specific nature of hydrogen-bonded water influences the outcome of chemical reactions in aqueous solutes. These guest–host interactions have been investigated over several decades with femtosecond optical tools [9], but many details still remain unclear. To tackle guest–host interactions, often combined with intramolecular dynamic processes on the

same femtosecond time scales, is extremely difficult in the experiment. For this purpose, one would at least like to observe the whereabouts of the caging solvent molecules together with the actual intramolecular structural changes inside the solute. These are often generated and accompanied by electronic and spin state changes [10]. This type of chemical dynamics research aims directly at the femtosecond capabilities of the FXE instrument: Local structural dynamics can be captured via EXAFS and XANES, and electronic structural changes via XES and RIXS. Diffuse X-ray scattering tools can bridge the knowledge gap between solute-only interactions and solute-solvent dynamics, and combining these tools into one single setup is highly beneficial for these types of studies.

The conceptual idea of the FXE instrument is thus to embrace the different spectroscopic and imaging techniques into one single setup, to permit simultaneous (or quasi-simultaneous) studies of the same sample with these different tools, down to the shortest time scales available. This has never been achieved in a single time-resolved setup, and even less for repetition rates that match those of the burst mode at the European XFEL facility (4.5 MHz). For the present design, it is thus vital to know that (a) such a combining strategy is indeed feasible (user-friendly) and (b) desirable to enhance our understanding of the science. This type of combined setup has been carried out just recently (March 2011) at MHz repetition rates at Beamline ID26 (ESRF) and at Sector 7 (APS) on liquid phase samples. There we performed picosecond time-resolved feasibility studies at MHz repetition rates, which exploit for the first time every single synchrotron radiation pulse in a time-resolved experiment, thus producing unprecedented S/N in TR-XANES, TR-XES, and TR-XRD in one single setup. These results also serve as vital input for utilizing the burst-mode frequency (4.5 MHz) at the European XFEL facility with current MHz laser sources (here: pulse energies in the 5–10 µJ range), as we can now estimate S/N for a large variety of future femtosecond X-ray experiments.

Instrument and beam transport requirements

The FXE instrument is dedicated to ultrafast studies of chemical and biological dynamics and of solid-state phenomena. After the scientific scope was presented in the European XFEL CDR (2006), a workshop was held in December 2009 to identify the key areas of research at the FXE instrument. The tools to be implemented are summarized in Table 2.

Table 2: *Techniques used by the FXE instrument*

Tool	**Tuning range**	**ΔE/E**
XANES	0.5–1%	Monochromatic (10^{-4}) (Option: pink beam and dispersive analyser)
EXAFS	≤ 14%	Monochromatic (10^{-3}–10^{-4})
Non-resonant XES	Single energy	0.1 %
Resonant XES	≤ 2 x 10^{-3}	10^{-5}
X-ray diffuse scattering (liquids)	Single energy (18–20 keV)	0.1 %
X-ray diffraction on solids (crystals, noncrystalline, grazing incidence)	Single energy (6–20 keV)	10^{-2}–10^{-4}

The tools dedicated to this instrument include XANES, EXAFS, XES, RIXS, and XRD variants, thus covering many aspects of imaging and advanced X-ray spectroscopies, and, for this reason, the sample environment will be kept very simple to enhance the flexibility of ultrafast investigations. Few-femtosecond time resolution will be achieved by using the shortest pulses available at the European XFEL and by exciting the sample with equally short laser pulses. The X-ray pulse width as a function of electron bunch charge in Figure 5 decreases to below 25 fs for electron bunch charges < 250 pC, and these operational conditions are consequently selected for the majority of femtosecond experiments performed here, while experiments at the highest pulse intensities (1 nC) will remain equally possible.

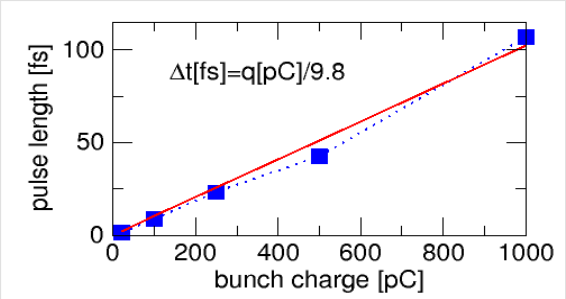

Figure 5: *Calculated X-ray pulse length as a function of electron bunch charge*

A femtosecond laser system operating in burst mode with pulse widths < 25 fs will deliver the pump beam, and optical parametric amplifiers will ensure wavelength tunability throughout the UV-NIR range. An additional THz laser beam will be guided and focused onto the sample with reflective optics (e.g. for ultrafast catalytic studies).

The SASE1 beamline has been designed by the X-Ray Optics and Beam Transport group (WP73) and its basic layout is reproduced in Figure 6.

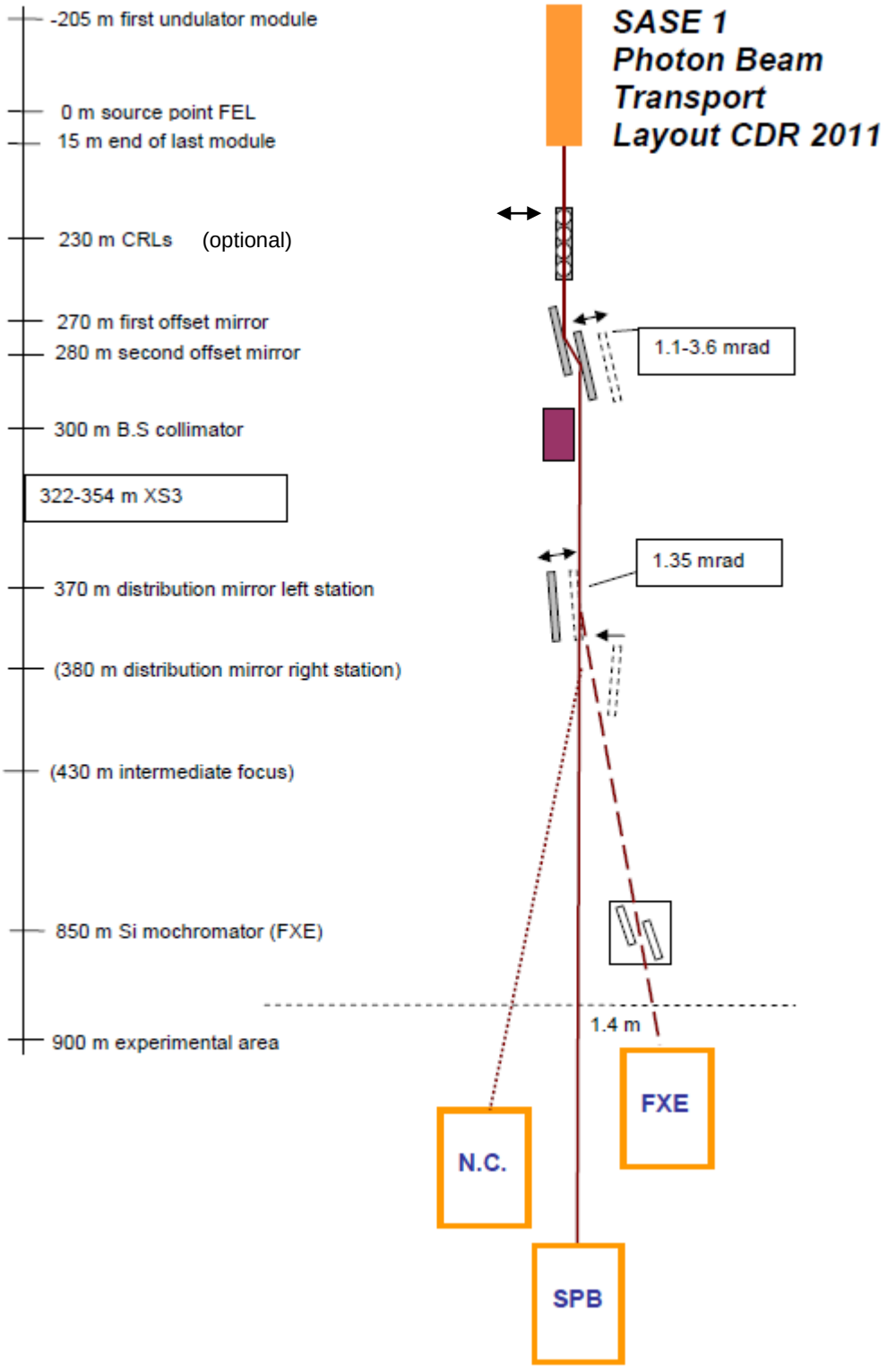

Figure 6: *Conceptual beam transport for the FXE (and SPB) instrument.*
(Source: CDR: X-Ray Optics and Beam Transport*, April 2011.)*

The X-ray beam exiting the SASE1 undulator has a natural divergence (2.5–0.6 µrad in the 3–20 keV range), leading to spot sizes in the experiment hall shown in Figure 7 (left) as a function of photon energy and electron bunch charge. The first crystal of a DCM monochromator will experience heating by the SASE beam during the burst, which gradually shifts the diffracted wavelength outside of the rocking curve acceptance of the second crystal, and in consequence will decrease the overall throughput during the burst. This leads to a maximum number of successive SASE pulses that can enter the experiment area, as shown in Figure 7 (right) for a channel-cut Si(111). For the standard operation mode (charge < 250 pC), one can expect to use > 1 000 pulses in monochromatic mode (green down-triangles in the figure).

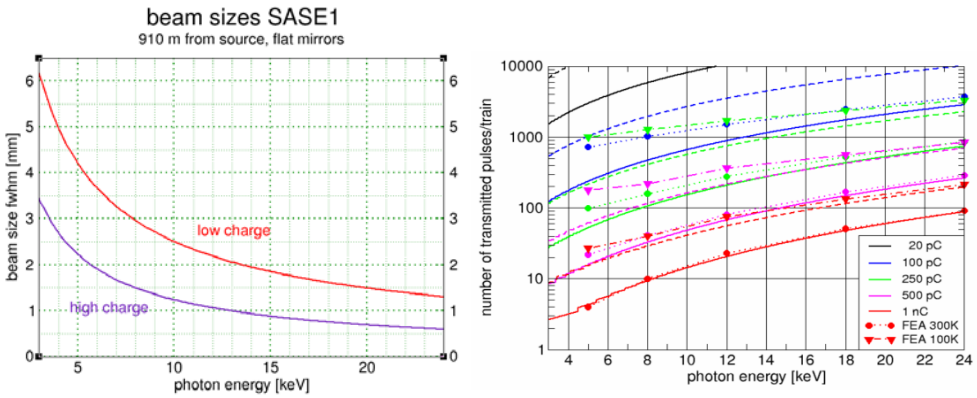

Figure 7: Left: *Beam size in the experiment hall of the unfocused beam.* Right: *Cryo-cooled channel-cut Si(111) monochromator will transmit > 1000 pulses/burst in the 3–24 keV range.*
(Source: CDR: X-Ray Optics and Beam Transport*, April 2011.)*

For the FXE instrument, we seek to be able to use most or all of the SASE1 radiation, in both pink and monochromatic modes, and this requires suitable focusing optics that do not suffer damage to the incident beam. We have studied the effect of Be lenses (CRLs) in the SASE beam, using the maximum acceptance for such curved lenses (for r ≈ 1.5 mm about 0.6 mm aperture), and this leads to permanent damage in burst mode for X-ray energies < 7 keV (250 pC) and < 11 keV (1 nC), as shown in Figure 8. Therefore, we will use KB mirrors to refocus the SASE beam.

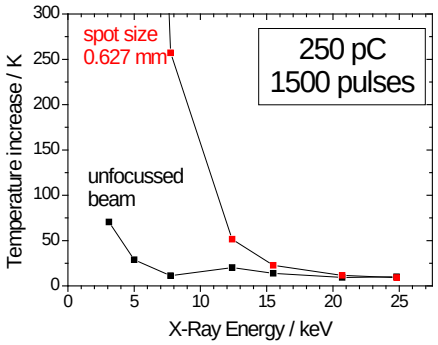

Figure 8: *Temperature increase for 0.1 mm Be after 1 500 pulses (at 250 pC) in the unfocused beam, compared to the case of a constant beam size of 0.627 mm (current CRL acceptance). Collecting entire bursts with 1 nC charges would destroy any CRL for energies < 11 keV (5 keV: 1 300 K).*

Placing the sample ca. 5 m downstream from the KB mirror exit will permit adjusting the beam size anywhere in the 5–1 000 µm range. There is no need to work in the focal spot region for the femtosecond X-ray experiments performed at the FXE instrument. In addition, one can select different spot shapes quite freely, e.g. line foci. These offer the possibility to perform studies on destructive samples (e.g. absorbing liquid jet) even in burst mode, since fast jets can remove the sample sufficiently quick (conventional jets today: 35 m/s, but improvements up to 80 m/s are foreseeable).

A KB system is also much more flexible towards the varying beam sizes demanded by users, and also permits an extension of the energy range beyond 5 keV to the lower limit of 3 keV. This design would require two 1 m mirrors. There are different solutions possible, depending on the actual choice of beam preconditioning with the offset and distribution mirrors. Figure 9 shows the example for a versatile KB system, which can accept the unfocused beam.

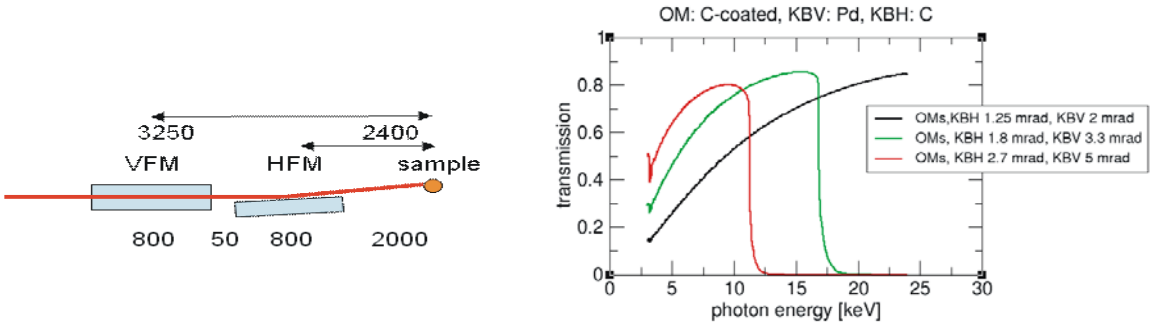

Figure 9: *Schematic of a KB arrangement for focusing the SASE beam in the FXE hutch, yielding a minimum spot size (focus) of 1 um, ca. 2.4 m behind the horizontal focusing mirror (HFM). The FXE sample position will be placed roughly 5 m from the HFM, thus delivering a minimum spot size on the order of 2–3 µm, thus fulfilling the spot size requirements in the 5–1000 µm range.*
(Source: CDR: X-Ray Optics and Beam Transport*, April 2011.)*

The SASE1 beam will be guided through a pair of horizontal offset mirrors (placed at 250 and 255 m from the SASE1 source), and a horizontal deflection mirror (at a distance of 370 m), into the experiment hall. As such, the FXE instrument will be located at the SASE1 side-branch with the SPB instrument being located at the centre line. The overall concept of the beam transport to FXE is shown in Figure 10.

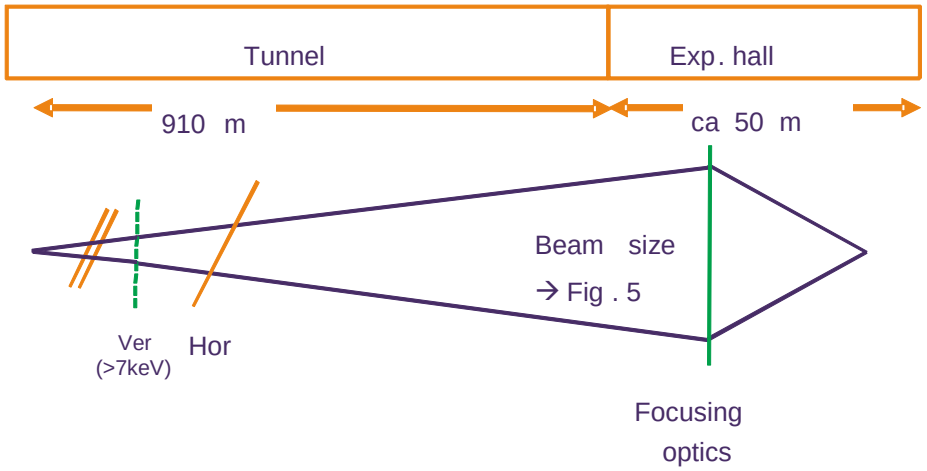

Figure 10: *X-ray beam transport and delivery scheme for FXE. Two horizontal offset mirrors suppress the hard X-ray Bremsstrahlung, and an additional deflection mirror guides the beam into the FXE station in the experiment hall. (Optional: One CRL downstream of the offset mirrors can be inserted to collimate the beam, but cannot be used for full burst-mode operation at photon energies < 7 keV). The second offset mirror can be bent in order to manipulate the horizontal beam divergence.*

For beam sizes in the experiment hall < 3 mm, acceptance of 4σ of the beam by a KB focusing optic is planned (KB angles < 3 mrad provide high reflectivity throughout the 3–20 keV range). This condition is naturally fulfilled for energies > 8 keV (see Figure 7, left), and, only for the lower energies in the 3–8 keV range, some gentle collimation may be required, possibly at reduced transmittance due to some beam clipping. One possibility for this would be to precondition the horizontal SASE1 beam size with mirror benders (deflecting mirror, leading to horizontal changes).

This concept ensures that most of the SASE beam will be usable for the experiment. It is our mission to maintain flexibility towards using the full SASE beam. The overall conceptual design from WP73 for the FXE beam transport matches the FXE concept shown in Figure 10.

SASE1 beam inside the FXE hutch

Figure 11 shows the conceptual design inside the FXE hutch. The hutch will comprise the following basic elements: A laser table will serve to manipulate (e.g. wavelength tuning) and characterize the pump laser beam for time-resolved experiments. The sample will be able to be placed either onto a sample stage positioner in air (ambient setup) or inside a vacuum chamber mounted on a laser table in the WAXS/SAXS region of the figure.

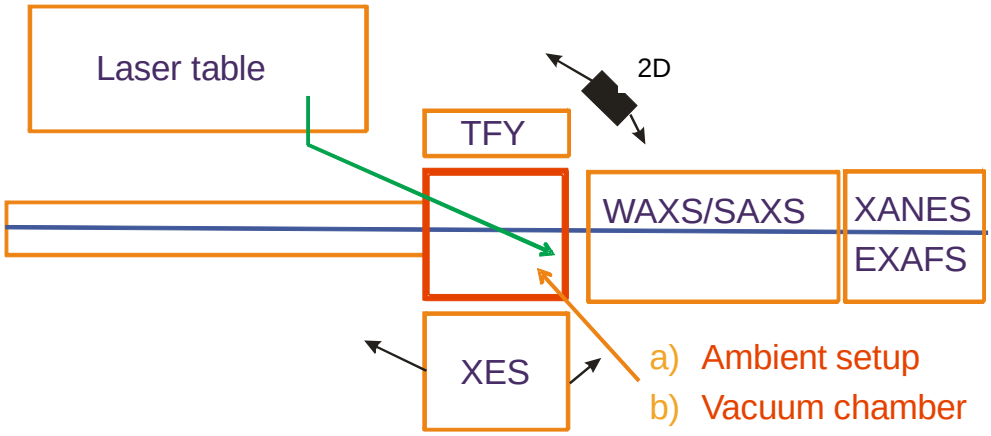

Figure 11: *FXE instrument schematic. A laser table inside the X-ray hutch will be used for laser beam treatment (e.g. wavelength tuning) and characterization. An X-ray emission (XES) setup will be mounted next to the sample position, adjacent to a total fluorescence yield (TFY) setup. These setups permit EXAFS and XANES studies with the monochromatic beam. A freely adjustable < 128 kpx detector (2D) can catch desired reflections outside the range of the 1M XRD detector. Behind the sample, there will be a large 1 Mpx area detector for WAXS with SAXS capabilities. A dispersive transmission spectrometer at the far end can permit XANES (and even EXAFS) studies in transmission mode with the pink beam. The sample environment will consist of interchangeable ambient and vacuum chamber setups.*

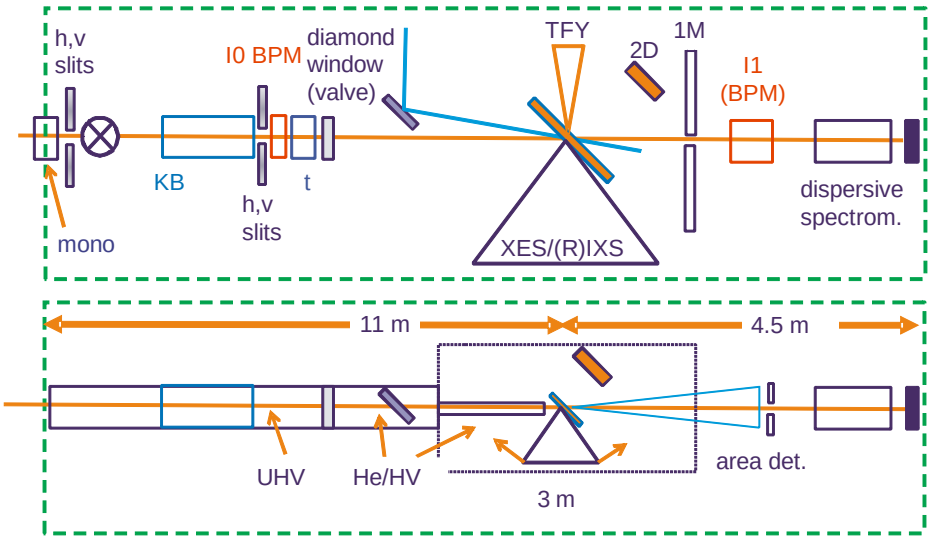

Figure 12: *FXE basic conceptual beamline design without a vacuum chamber (which can be added behind the ambient setup). The primary monochromator (mono) will be situated at the end of the tunnel section. Inside the FXE hutch will be X-ray slits for the expanded beam (see Figure 5, left), a fast valve, the KB focusing mirrors, a non-destructive I_0 monitor and beam position-sensitive device (BPM), a pulse-by-pulse timing monitor (Δt), and finally a diamond-windowed gate valve, which separates the UHV environment upstream from the rest of the beamline. The X-ray emission spectrometer (XES) and the 0D detectors for XANES/EXAFS measurements in total fluorescence yield (TFY) mode, possibly preceded with Soller slits and (Z-1) filters (unnecessary for liquid jets), and the (1 Mpx) large area detector surround the experimental sample, next to an additional small are detector (2D). The sample itself can be enclosed in a small chamber with suitable exit ports for XES, TFY, and XRD, either in protective gas (He) or in a vacuum. Behind the area detector are I_1 monitors, the dispersive transmission mode spectrometer, or both.*

Requirements for subcomponents

This chapter describes the requirements for subcomponents of the FXE scientific instrument.

Focusing optics

The requirements for focusing optics are the same as those for KB optics, as described earlier in this document (Figure 9).

Slit systems

The slit system (h, v) defines the beam size accepted onto the focusing optics and should be adjustable in the 0–10 mm range. The second slit system serves to clean up the transmitted beam.

Beam positioning monitor, possibly combined with an I_0 monitor

After the focusing optics, we need information about the beam position and the beam intensity. Intensity measurements also assess the losses through the focusing optics and clean-up slits, and the BPM assesses the actual positions and the deflected angles (e.g. via KBs). The intensity measurement behind the focusing optics and the slit system defines the experimental conditions at the sample, and this measurement needs to be as precise as possible (better than 1% desired for each shot).

Monochromator

A Si(111)-based channel-cut monochromator can be used for an energy resolution of $\Delta E/E \approx 2 \times 10^{-4}$ (in the 3–20 keV range). One problem concerns the EXAFS capability, especially in the lower energy regions below 10 keV. The displacement can amount to up to 250 µm/keV, which in consequence demands shifting all downstream optical elements, including (a) KB optics, (b) the downstream slit system, and (c) laser–X-ray interaction (the laser would have to move accordingly, and the sample possibly too). This can be avoided in (a) a four-bounce geometry (which maintains a fixed exit between pink and monochromatic beams), or (b) via a pseudo-channel-cut monochromator (fixed-exit monochromatic beam). A second monochromator, e.g. Si(333) [2×10^{-5}] or Si(311) [5×10^{-5}] in series with the Si(111), will further improve the energy resolution to the user's needs (Figure 14). Since high-resolution experiments do not require extensive scanning (within 10–30 eV is usually sufficient), beam offset corrections during the scans with both monochromators are no longer needed here.

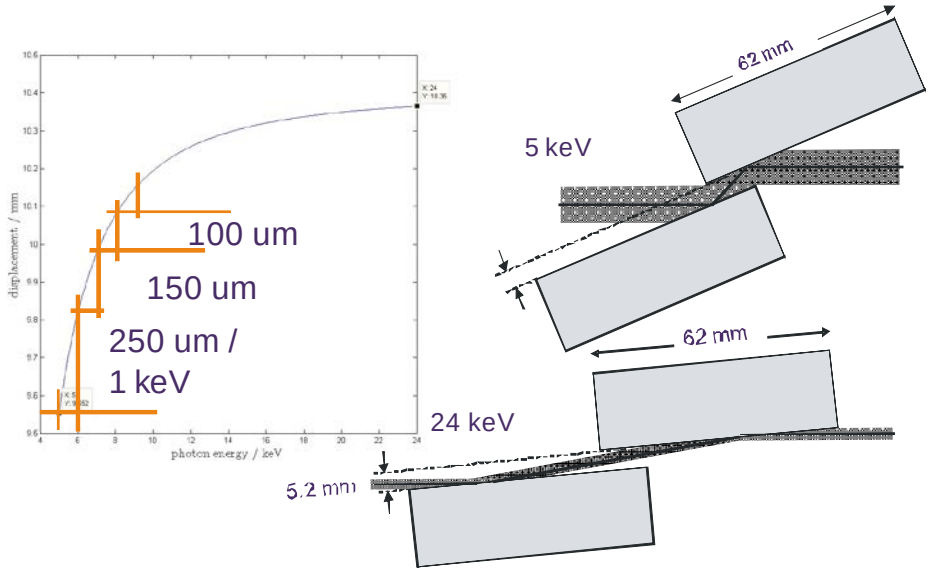

Figure 13: *Displacement of the X-ray beam as a function of X-ray energy for the primary Si(111) channel-cut monochromator*

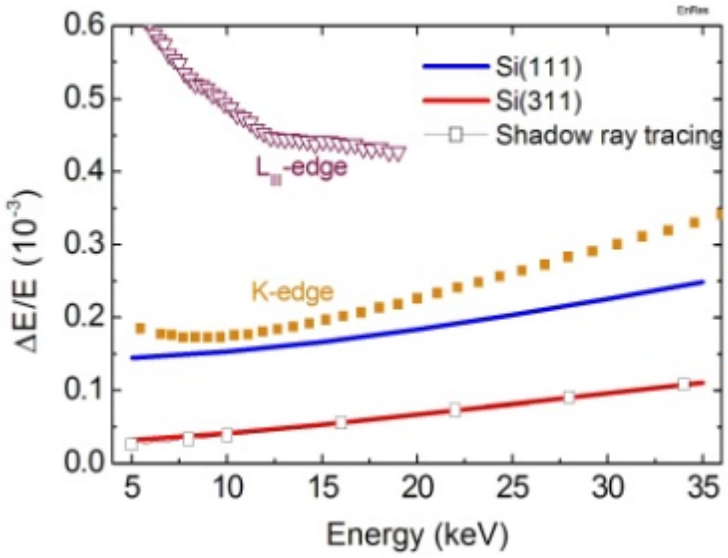

Figure 14: *The energy resolution achieved by the optics (blue or red lines) is always better than the line broadening due to the photon absorption process (core-hole lifetime of elements at relevant K- and L_{III}-edges in orange and purple). (Source: Rossendorf beamline at ESRF.)*

However, not only the beam offset needs to be accounted for in femtosecond X-ray experiments, but also the actual timing drifts themselves. The primary monochromator can be either a channel-cut or a pseudo-channel-cut Si(111), with varying beam offset during scans or fixed exit, respectively. In both cases, we experience striking temporal shifts of the pulse arrival time during energy scans (Figure 15), which can be compensated by a synchronously driven delay line stage for the laser beam. In the case of a vertical displacement of the beam (Figure 13), during scans, the arrival time is a superposition of both the beam offset and the different path lengths through the monochromator as a function of scan energy. The laser-X-ray spatial beam overlap would also be affected by the beam offset, but one can install a periscope between the laser table (fixed height) and X-ray bench (variable height) to nevertheless maintain a perfect spatial overlap between both beams during scans. It should be noted that the time delay already changes significantly over the SASE bandwidth itself (e.g. ca. 0.3% at 7 keV), thus within the XANES range, namely about 30 fs at 7 keV, and this change becomes dramatically larger when working at lower energies in the 3–7 keV region (Figure 15). Thus, we would operate the monochromator with fixed exit

in the 5–20 keV range, and with constant crystal spacing in the 3–5 keV range, to avoid excessive slopes of the different arrival times.

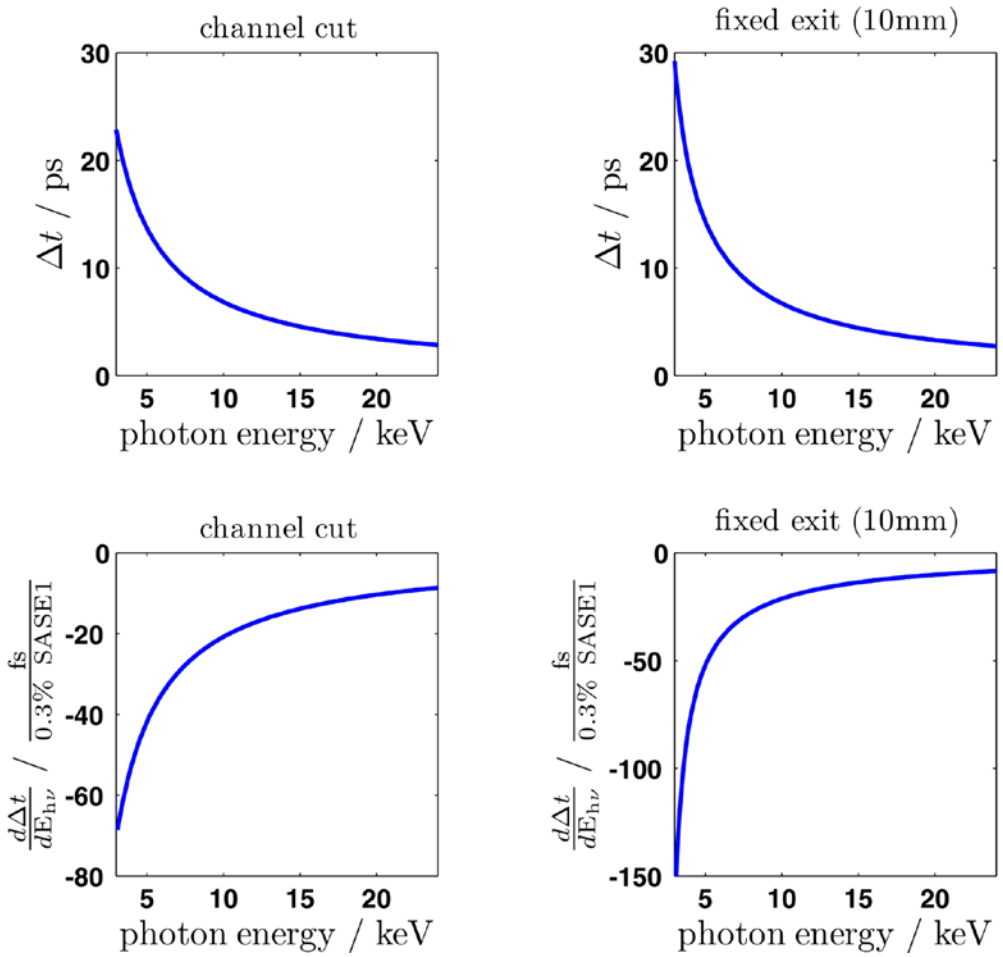

Figure 15: Top: *Temporal shift of the pulse arrival time due to the altered X-ray beam path during a monochromator scan for (a) a channel-cut (5.2 mm distance) Si(111) and (b) a fixed-exit (10 mm offset) Si(111).* Bottom: *Time-delay change within the SASE1 bandwidth of 0.3%.*

Time domain monitor

Time domain monitoring could be done similarly to LCLS via a “transient mirror” on a material that survives the full XFEL beam, and should be placed closer to the focusing optics in the large beam (e.g. the diamond window below could serve a dual purpose). The time domain monitor requires a suitable, rather small area detector, compatible with burst mode operation and single pulse readout.

Window (gate valve)

A diamond window could be used to separate the UHV conditions upstream from the ambient He atmosphere (or the HV conditions in the exchangeable vacuum chamber). The window needs to withstand burst mode operation, and thus needs to be not too close to the focus ca. 5 m downstream from the focusing optics. The window could be used as the reflective surface for the time-arrival monitor.

UV-NIR laser system

The laser system will deliver 800 nm / 15 fs pulses aiming for 0.2 mJ or more pulse energy, in burst mode (4.5 MHz). An optical parametric amplifier located inside the FXE hutch near the sample, as well as an SHG/THG box, will convert this wavelength to the desired pump wavelength throughout the UV-visible-NIR ranges (ca. 200 – 2 000 nm). The laser system itself is located inside the SASE1 laser hutch next to the FXE and SPB X-ray hutches, and will be guided via evacuated (foreline vacuum) beam transport tubes into the X-ray hutch onto the laser table (ca. 1.4 x 3 m^2), on which the NOPA is mounted. This requires broadband dielectric mirrors at 800 nm. On the optical table, there is an SHG and THG assembly, next to the OPA. The last metres to the experiment are realized with interchangeable dielectric coated mirrors (for the NOPA) and those coated for SHG (400 nm) and THG (266 nm).

Synchronization unit

The synchronization unit generates a local synchronized oscillator signal from the signal delivered from the electron source. This unit serves as input for the burst mode pump laser required here. (Source: WP78.)

Laser lab space, including the synchronization hutch, burst-mode laser, and a 30–50 m^2 laser lab for laser-only preparative studies, but also for pre-alignment of the vacuum chamber, requires altogether ca. 90–110 m^2.

Note on the required laser pulse energy: At ID26, we utilized our FXE MHz laser at 1.4 MHz (ca. 8 uJ pulse energy) on a 0.1 x 0.6 mm spot on sample, and yielded superb S/N and excitation yields on a dilute model system, Fe(bpy)3. This relates somewhat to the future FXE experiments: we no longer need to excite as much as possible (thus approaching the highest laser fluencies possible), but can rather enter the “tickle and probe” regime. This strategy has also proven very successful for our recent campaign at APS, where we also demonstrated the possibility to probe photoexcited molecules via X-ray diffuse scattering in dilute solutions.

In a next step, we seek to exploit short THz pulses for sample excitation, for which we need to generate THz pulses in the laser lab, and guide them appropriately to the sample inside the X-ray hutch.

Further laser instrumentation will include a pulse-shaper to tailor the excitation pulses according to the dynamics investigated. Auto and cross correlators will be installed on the laser table inside the FXE hutch as well.

UV-NIR laser-in (mirror)

Both options may be vital: a strict collinear geometry (dielectric mirror at ca. 45° with a tilted hole in the center for X-rays), or a tilted input (by roughly 45°) to decrease time spread through a 0.1 mm sample due to the velocity mismatch between optical and X-ray laser beams. This is easily possible due to the flexible sample environment under ambient conditions (see “Sample environment, secondary spectrometers, and imaging devices”). The mirror mount must permit easy interchanging between dielectric coatings for different spectral ranges.

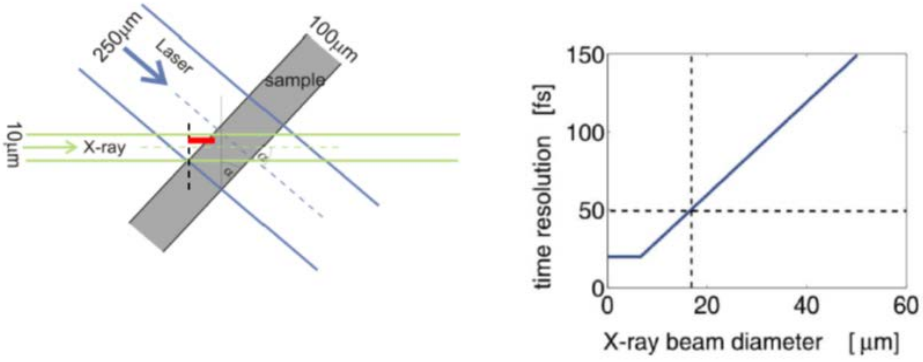

Figure 16: Left: *Top view for a laser (blue) and an X-ray beam (green) traversing a sample with n=1.34 (for the laser), and essentially n=1 (for the X-ray beam). At 41.75°, both beams propagate with the same speed though the sample depth, thus this strategy allows us to minimize the time-zero spread (which governs the instrument response function) to below 50 fs, for diameters of the X-ray beam smaller than 17µm.* Right**:** *Shows the dependence of the time resolution assuming a 20 fs laser pulse and a somewhat shorter X-ray pulse probing the sample at the optimal angle of 41.75°. The cursor position shows the needed diameter of the X-ray pulse for a time resolution better than 50 fs.*

Sample environment, secondary spectrometers, and imaging devices

This section describes the requirements for the sample environment, secondary spetrometers, and imaging devices for the FXE instrument.

Sample environment strategy

User needs are diverse and thus a single sample environment is insufficient to cover a broad user base, including vacuum, liquids, cryogenic temperatures, etc. In order to maintain maximum flexibility for the secondary spectrometer needs (including large rotations), the basic setup will permit studies on solids and liquids under atmospheric conditions, while the setup will permit further upgrades to include e.g. vacuum chambers.

The sample environment will be ambient and contain appropriate He bags for the secondary spectrometer. Thus, the SAXS/WAXS imaging 2D detector will be mounted under these conditions, possibly with a He cone to reduce air scatter from behind the sample. A 20 cm needle tube (open diameter 1 mm) upstream and He flown will reduce the air losses and scatter into the He-filled environment upstream to the diamond window gate valve. This gate valve can be opened and the He-filled tubes replaced by a vacuum pipe ending at a specially designed vacuum chamber for liquid and solid samples.

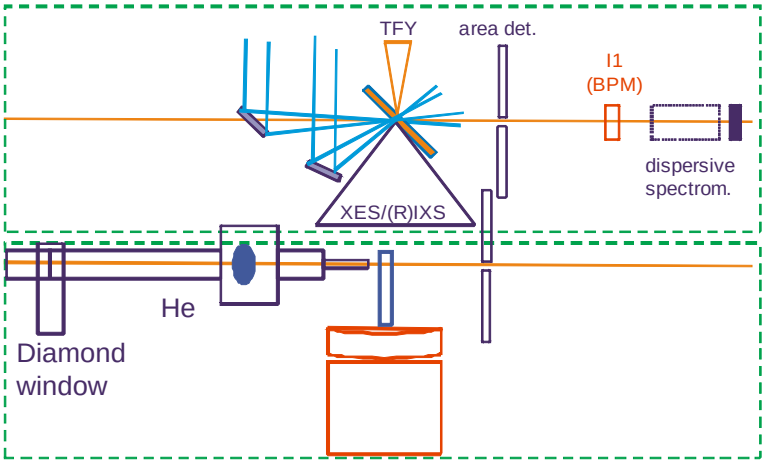

Figure 17: *Top and side view of the sample environment concept*

Two options are foreseen: a very small-sized (< 20 cm) vacuum chamber with exit windows for XES and TFY. In transmission, it will be necessary to extend the vacuum tube length until one can safely place a window towards ambient conditions. This chamber will most likely not permit WAXS studies. Another option is to increase the size of the chamber, so that at least one XES crystal and detector fit inside sideways, and a large 1 Mpx area detector can be placed and moved on rails behind the sample. The sample itself would be mounted on a fitting hexapod to permit precise angular and spatial adjustments.

Issue for the large vacuum chamber: This would demand a 1 Mpx detector, which can be equally placed in vacuum and in air (very unlikely), thus two 1 Mpx detectors would be needed to fulfil both ambient and vacuum conditions.

Sample stage

A heavy-duty sample tower with rotation, *xyz* translation, and inclination will be installed below the sample position (total height ca. 1.20 m). A laser table behind the sample position can serve as a support for rails for the SAXS detector as well as a support for the large vacuum chamber. The smaller vacuum chambers will be mounted as the ambient setup onto the diffractometer tower. Liquid samples will be flown through a free-flowing jet, and we are opting for liquid sheets a few mm wide and thicknesses of 1, 25, 100, 200, µm, etc. for which commercial and semi-commercial solutions already exist.

Secondary spectrometer for XES and RIXS

A von Hamos secondary spectrometer will be implemented for XES and resonant inelastic x-ray scattering (RIXS). It will be rotatable around a vertical axis through the sample. Curved Xtals (cylindrical) will image the XES onto an area, ca. 1–2 x 4–6 cm in size. The spectrometer will be horizontally rotatable around a vertical line through the sample, and the XES detector mounted on a *z* stage.

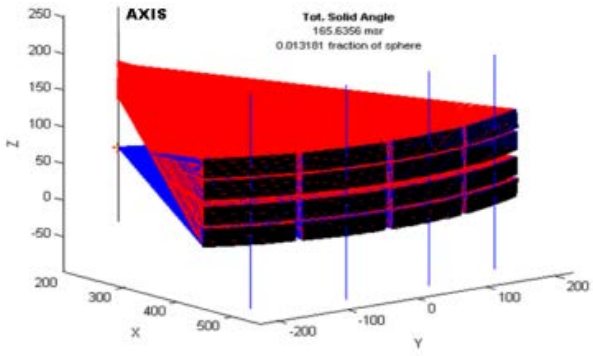

Figure 18: *Example of the imaging geometry for a dispersive XES analyser in von Hamos geometry. (Source: Roberto Mori, SLAC.)*

XES spectrometer and detector requirements

The XES spectrometer should provide an energy resolution of around 0.1 eV in the 6–9 keV range (3*d* transition metals). This can be fulfilled with appropriate curved analyser crystals in von Hamos geometry. (Figure 18 shows the simulated example for the LCLS XES spectrometer, which is adopted here.) The solid angle for the FXE instrument will lie in the 10^{-3}–10^{-2} range for analyser curvatures of 0.5 m (and single analyser elements having a 110 x 25 mm^2 active area). For example, for a solution of 0.1 mM (and 0.1 mm thick) of a Fe-containing protein, only 5 x 10^{-5} of the incident radiation is absorbed by Fe. Most of the fluorescence escapes with 0.3 yield and disperse mainly into the *K alpha* 1 and 2 lines (thus over ca. 20 eV, or over 100 resolution elements of the detector), and we yield on average a detection efficiency around 2 x 10^{-10}. An experiment at very high temporal resolution (or low incident intensity) would deliver 6 x 10^{10} photons per pulse, thus this extreme dilution case approaches the single photon case, but does not quite reach it. In return, this means that, for the majority of pump-probe XES experiments, the XES baseline detector need not have superior intrinsic energy resolution. An energy resolution of < 200 eV at 7 keV (FWHM) would be desirable only in experiments with much less sample than the case examined above, and could then further reduce the background in the Si detector by e.g. scattered light from the sample. This is possible only if the detector can be operated in single-photon-counting mode (low incident flux, concentration, or both) or if pile-up effects can be corrected for. The maximum technologically possible quantum efficiency of the sensor is desired in the energy range between 3 keV and 20 keV.

At present, we foresee two potential detector concepts to be used as XES analysers in the dispersive plane of the XES gratings: either a Si strip detector with a strip width of ≤ 0.1 mm over a length of 4 cm or a 2D Si detector with a pixel size of ≤ 0.1 mm providing a total sensitive area of at least 1 x 4 cm^2. A strip width or pixel size below 0.1 mm in the dispersive direction would provide a sufficiently high over-sampling factor of spectral lines of at least 10–100 over the entire sensitive energy range of the spectrometer.

In comparison to a 1D strip detector, a 2D detector would provide additional valuable information, e.g. to reduce systematic effects due to fluorescent background or stray light effects originating from the detector environment. To estimate the benefit of a 2D detector over a 1D strip detector, further performance studies will be made.

X-ray diffraction (XRD) setup

Ideally, an area detector with an angular coverage of at least 70° should be installed behind the sample at a minimum distance of approx. 50 mm up to 4.5 m. At a first stage of expansion, we will implement a 1 Mpx Si 2D detector with central hole, behind the sample. The size of the central hole should be adjustable in horizontal and vertical direction. The minimum and maximum possible size of the hole has yet to be defined.

A laser table-rail combination will allow one to move the detector to distances between 50 and 4.5 m from the sample interaction point. A He cone between sample and detector (especially at low energies) will ensure good transmission to and low air scattering into the detector. Since the primary startup goal is focused on liquid phase scattering, an angular resolution corresponding to pixel sizes ≤ 0.5 mm at the given distances is sufficient. The maximum technologically possible quantum efficiency of the sensor is required in the energy range between 3 keV and 20 keV.

XANES and EXAFS setup

The XANES and EXAFS will be mostly recorded in total fluorescence yield, in some cases in transmission mode (scanning the primary monochromator, but we need to deal with the beam offset during scans). Alternatively, e.g. for XANES studies, one can also analyse the transmitted radiation (without an

incident monochromator) via a dispersive spectrometer in transmission, and in this way collect an entire XANES spectrum within one burst (or up to 2 700 pulses, which deliver a smooth spectrum within the SASE1 bandwidth). This strategy would even permit one to record EXAFS over an extended energy range of 1 keV over several bursts, when tuning the electron energy accordingly. Figure 19 shows the principle idea for such a dispersive transmission detector.

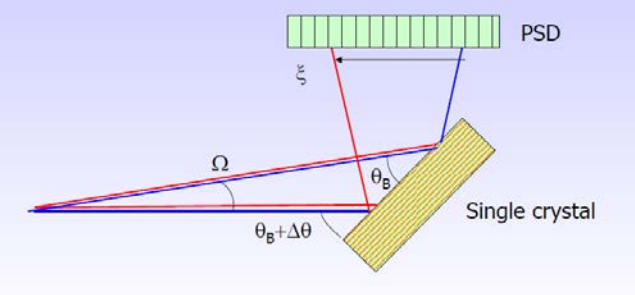

Figure 19: *Conceptual idea for a transmission spectrometer. (Source: Makina Yabashi, Spring8.)*

This spectrometer design could also be placed upstream from the sample to measure the incident spectrum from a scattering foil. Its utility in transmission depends strongly on the load onto the position-sensitive detector (PSD). For example, for 20 pC bunches we expect around 10^{10} photons/pulse. A strip detector could accept up to ca. 10^4 12 keV photons/pulse per strip and, assuming 10^3 strips, yield a total of 10^7 photons that could be processed with this device. Thus, in transmission mode, filters may need to be inserted, depending on sample transmission, but the scattering foil will be fully useful when inserted upstream for an incident I_0 spectrometer.

DAQ strategies at the FXE instrument

The burst-mode operation of the European XFEL offers new and interesting strategies for acquiring data, which are briefly sketched out here. In principle, one can distinguish between single-shot experiments and single-burst experiments. The needs for single-shot experiments are quite obvious, and even in single-burst mode, it can be very important to have single-shot capabilities (frame rate = 4.5 MHz). However, the data acquisition (DAQ) strategies can be similarly versatile as in current MHz pump-probe experiments at synchrotrons, and some examples will be presented below.

Pink beam experiments

To exploit single-burst experiments with up to 2 700 pulses, one can use the setup scheme shown in Figure 20. The single-shot SASE spectrum will produce a spiky spectrum (inset in Figure 20), which is good for probing XES, but not for probing XANES/EXAFS. Over the entire burst, the average spectrum will be much smoother, and one could also record the photoexcited spectrum and ground state spectrum each at 2.25 MHz. This requires detector and DAQ capabilities at the full 4.5 MHz burst rate.

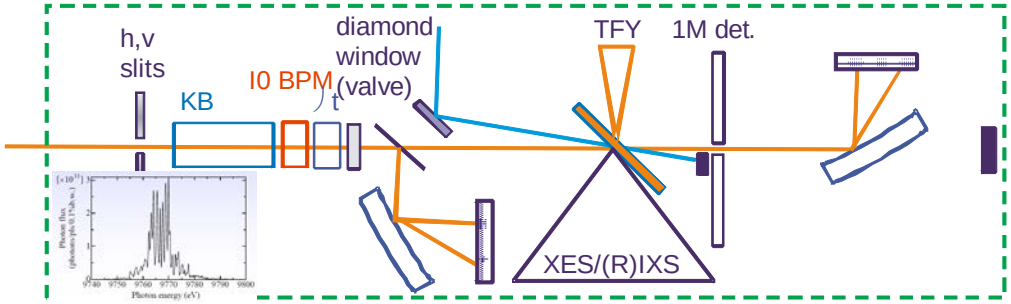

Figure 20: *Setup strategy for single-burst experiments using the pink beam. In this configuration, each SASE pulse produces the indicated spectrum, which will average to a smooth curve within the burst. Incident I_0 and I_1 dispersive spectrometers will then record the averaged spectrum after 2 700 pulses. Note that, in this configuration, there is no beam displacement.*

Detectors

Table 3: *Summary of the required detectors and relevant performance parameters. The XES detector, if the 2D version is applied, can also be used for the Bragg detector. (Thus, no XES is possible when there are e.g. reflectivity studies on the surfaces.)*

Parameter	Diffuse scattering	XES analyser	Solid state Bragg reflection	Time domain monitor
Detector type	2D Pixel	1D Strip / 2D	2D	2D
Energy range	3–20 keV	3–20 keV	3–20	UV-vis
Energy resolution	No	< 200 eV@7 keV (SPC) (or none)	No	No
Frame rate	4.5 MHz	4.5 MHz	4.5 MHz	4.5 MHz
Pixel/strip size	< 500 x 500 μm^2	100 x 100 μm^2 100 µm	100 x 100 μm^2	< 100 x 100 μm^2
Sensitive area	22 x 22 cm^2	2 x 6 cm^2	up to 10 x 10 cm^2 (2 x 6)	ca. 1 x 1 cm^2
No. of pixels	1 M	200 x 600	≥ 200 x 600	100 x 100
Sensor material	Si	Si	Si	Si
Sensor thickness	500 µm	500 µm	500	N/A

FXE hutch dimensions at the SASE1 beam port

The SASE1 tunnel exit port is offset towards the SASE3 tunnel exit, thus the three beams (for FXE, SPB, and NC) will be slightly off-centre. The total SASE1 area is 15 x 44 m^2, and this has been divided into three areas for each instrument (Figure 21). SPB and FXE each have a small (3.5 x 2.5 m^2) sample preparation lab, which is vital for the FXE startup configuration to study chemical and biological dynamics in liquids and physiological media. A large laser lab (ca. 120 m^2) will be shared between both SASE1 and SASE3 beamlines, equipped with two burst mode lasers, one synchronization oscillator, and a small area for preparative laser-only studies and pre-alignment of additional setups (e.g. chambers), which may go into the respective scientific instrument. Control rooms and rack areas are foreseen as well.

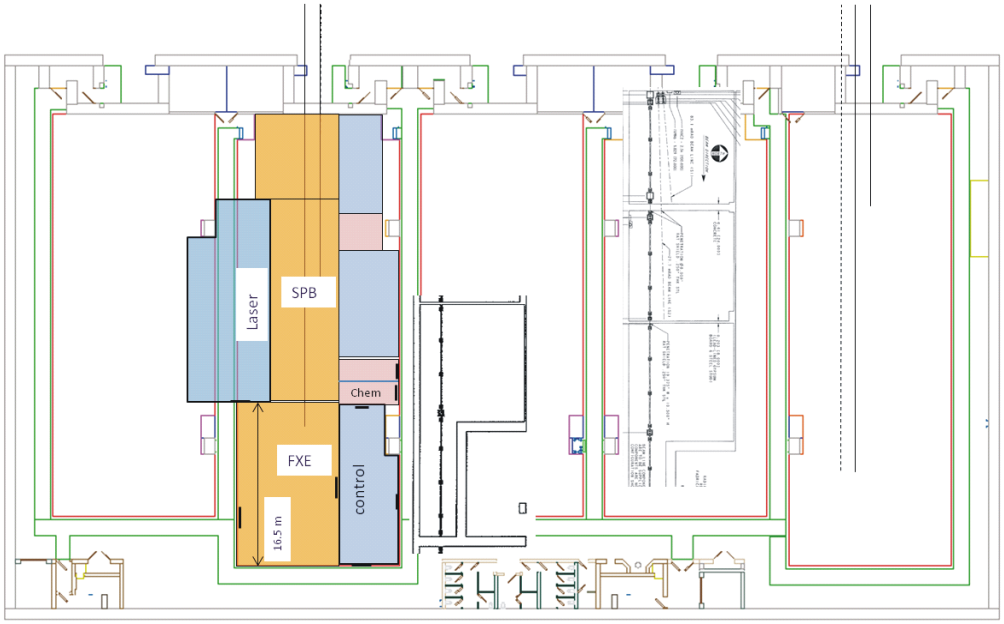

Figure 21: *Sketch of the overall instrument layout at the SASE1 beamline.* Orange boxes: *X-ray hutches (left to right: FXE, SPB, NC).* Blue boxes: *Control hutches (total: three).* Red boxes: *Joint laser lab between SASE1 and SASE3.* Red lines: *FXE beam tube.* Black lines: *SPB beam tube.*

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