

CONCEPTUAL DESIGN REPORT

Scientific Instrument SQS

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1 Introduction

This document reports on the present status of the conceptual design for the Small Quantum System (SQS) scientific instrument at the European XFEL. Within the overall European XFEL project, this instrument is one of the six experiment stations foreseen in the startup scenario. It will cover applications in the soft X-ray wavelength regime and will use the intense radiation from the SASE3 undulator. The equipment and the optical layout of the SQS instrument will be dedicated to the investigation of processes in atoms, ions, small molecules, and clusters occurring in highly intense beams using a variety of spectroscopic techniques. Scientific areas of application are atomic and molecular physics, chemical dynamics, nanoscience, and, in very general terms, investigations of matter under extreme conditions. Samples are typically prepared in gaseous form, in jets or beams, or by trapping.

In the technical design report (TDR) for the European XFEL in 2006 (DESY 2006-097), two major applications (high-resolution spectroscopy and high-flux applications) had been favored initially, leading to the request of two SQS instruments. However, due to budget restrictions, the startup scenario allows for one instrument only. The current planning does not foresee the inclusion of a monochromator. The instrument will be suitable primarily for high-field applications, non-linear processes, and time-resolved pump-probe investigations. The scientific case for the SQS instrument and the subsequent experimental requirements were developed in two international workshops, which have gathered a large user community.

The first workshop was held in October 2008 in Aarhus:

http://www.xfel.eu/events/workshops/2008/sqs_workshop_2008/

The second workshop was held in December 2010 in Trieste:

http://www.xfel.eu/events/workshops/2010/soft_x_ray_science_and_instrumentation_workshop

The presentations given at these workshops and the results of the working groups provide the principal basis for this report. Recent results and expertise obtained during experiments using the atomic, molecular, and optical (AMO) science end station at the X-ray free-electron laser LCLS (SLAC National Accelerator Laboratory), which became operational in the summer of 2009, were discussed during the workshop in Trieste and provided up-to-date contributions to further shape the specifications for the SQS scientific instrument. These contributions were possible because the photon energy range, pulse energies, and durations available at the AMO end station are very similar to the expected beam parameters at SQS. The main difference between the stations is, by two orders of magnitude, the higher repetition rate provided by the European XFEL. This unique characteristic will open up various new possibilities, in particular for “photon hungry” experiments and for applications of coincidence techniques.

Through this exchange with the user community, priorities were identified leading to the definition of the following principal requirements, which should guide the design of the SQS scientific instrument:

- 1 The vacuum chamber will provide high modularity, enabling the (parallel) use of a variety of experimental techniques.
- 2 Spectrometers and detectors will be based on state-of-the-art technology in order to provide the highest experimental standard from the start of operation of the European XFEL in 2015 and beyond.
- 3 Experimental techniques that explore the unique properties of the European XFEL, in particular its high repetition rate, will be prioritized.
- 4 The layout of the SQS scientific instrument will fully integrate a synchronized, optical femtosecond laser system operating at the same repetition rate as the European XFEL.

- 5 The use of various gaseous samples (e.g. atomic and molecular gases, clusters, ion beams, nanoparticles, and nanodroplets, as well as biomolecules) will be anticipated in the design of the experiment chamber.
- 6 An “open port” will be included in the general layout of the experiment area, allowing the installation of specific instrumentations, which are beyond the scope described here for the baseline equipment of the SQS scientific instrument, but can be brought in by interested user groups.

The present conceptual design report for the SQS scientific instrument follows these requirements and suggests a corresponding general layout. The technical realization of the instrument will be developed in a subsequent step for the technical design report (TDR). Experiment equipment, which is specified as “baseline equipment”, will be delivered and installed by the European XFEL. It represents the instrumentation available for all users to perform experiments after acceptance of their scientific proposal by the corresponding committee. Additional equipment beyond the baseline equipment (e.g. apparatus for cluster and nanoparticle beams, or ion sources and ion traps) are not included in the present budget and cannot be provided by the project in a first phase. They will therefore be presented only briefly. However, active participation of the interested user groups is encouraged, and it is anticipated that requirements for adding such instrumentation to the SQS scientific instrument will be described in the SQS TDR.

After a summary of the SASE3 parameters (Chapter 2), this document provides a short review of the scientific case (Chapter 3). The main part of the document (Chapters 4–12) is devoted to the description of the optical layout and, in particular, to the suggested layout of the SQS scientific instrument, including the additional requirements (e.g. optical laser and FEL beam diagnostics).

2 Photon beam parameters

The SQS scientific instrument will be installed behind the SASE3 undulator (Figure 1), which will deliver intense ultrashort soft X-ray pulses in the wavelength range between 0.4 and 4.8 nm, corresponding to photon energies between 260 and 3000 eV.

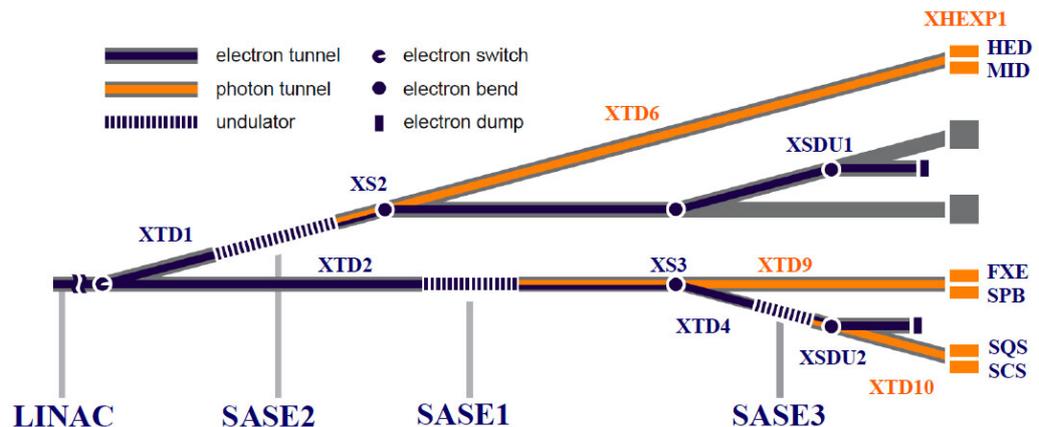


Figure 1: Schematic presentation of the undulators, beamlines, and scientific instruments of the European XFEL

The undulator will be installed about 450 m before the experiment hall and will consist of 21 segments of 5 m length each (i.e. a total length of 105 m). The gap of the undulator will be tunable in order to operate at fixed electron energies. The minimal gap of 10 mm corresponds to the minimum achievable photon energy of 260 eV and 470 eV for operation modes at electron energies of 10 GeV and 14 GeV, respectively.

The main parameters of the SASE FEL radiation, calculated for different operation modes of the accelerator, are given in Table 1. These numbers underline the exceptional performances of this soft X-ray undulator and of the corresponding radiation parameters in terms of pulse energy (up to 11 mJ), pulse durations (2–100 fs), photons per pulse (up to 10^{14}), and average photon flux (above 10^{18} photons per second), which is directly related to the high number of pulses (max. 27 000 per second) arriving in bunch trains

containing at most 2 700 individual pulses, with a repetition rate of 10 Hz. The nominal temporal separation between the individual bunches within a bunch train is 220 ns (4.5 MHz). Different bunch separation patterns are possible and interpulse periods in the microsecond range (0.1–1 MHz) down to single bunch operation (10 Hz) can be provided. In order to assure the parallel operation of different instruments, the maximum number of pulses might be reduced by a factor of 2 in standard operation, distributing an equal number of pulses to the SASE2 and the SASE1–SASE3 branch.

Table 1: Soft X-ray (SASE3) FEL radiation parameters for selected settings of the electron energy and bunch charge [1]

Photon energy	keV	0,28			0,496			1,55			3,1		
Radiation wavelength	nm	4,43			2,50			0,80			0,40		
Electron energy	GeV	10,5			14			14			14		
Bunch charge	nC	0,02	0,25	1	0,02	0,25	1	0,02	0,25	1	0,02	0,25	1
Peak power	GW	105	106	94	118	119	105	90	86	72	73	66	51
Average power	W	5	67	273	5	75	304	4	54	209	3	41	147
Source size (FWHM)	μm	51	65	79	43	56	68	39	50	60	36	46	56
S. divergence (FWHM)	μrad	33,9	29,6	26,0	23,1	20,0	17,5	9,7	8,1	6,9	5,6	4,6	3,9
Spectral bandwidth	1E-3	6,9	6,4	5,7	5,8	5,3	4,7	4,4	3,9	3,3	3,6	3,1	2,5
Coherence time	fs	1,49	1,63	1,83	1,01	1,11	1,25	0,43	0,49	0,57	0,26	0,31	0,38
Coherence degree		0,96	0,96	0,96	0,96	0,96	0,96	0,96	0,96	0,96	0,96	0,96	0,91
Photons/pulse	1E11	39	547	2240	25	347	1420	6	81	312	2	31	109
Pulse energy	mJ	0,2	2,5	10,1	0,2	2,8	11,3	0,2	2,0	7,8	0,1	1,5	5,4
Peak brilliance	1E31	7	7	7	16	17	17	49	54	53	98	104	93
Average brilliance	1E21	3	46	212	7	109	498	22	338	1520	44	654	2680

Parameter	Unit					
Bunch charge	pC	20	100	250	500	1000
Pulse duration (FWHM)	fs	2	9	23	43	107

The possibility to realize variable (linear and circular) polarization is presently under investigation by a dedicated working group. Startup scenarios involving short helical or cross-planar undulator segments could allow the delivery of, e.g., circular polarization in the second harmonic of the FEL radiation. Solutions to separate the first and second harmonics for the direct branch (without monochromator) have still to be developed.

More information is given in the technical note “Layout of the X-ray Systems of the European XFEL” [1].

References

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3 Résumé of the scientific case

Based on the expected parameters of the FEL radiation produced by the SASE3 undulator, a broad range of scientific applications has been established during the two user workshops in Aarhus (2008) and Trieste (2010). Up to the start of operation of the European XFEL in 2015, the corresponding catalogue of benchmark experiments will be regularly refined and complemented in consideration of the latest theoretical results as well as new experimental developments and ideas arising from recent experiments at LCLS in the USA, and later at SCCS in Japan. New results obtained at FLASH (Hamburg) and FERMI (Trieste) will be followed with high interest, but transfer of these applications to the short wavelength region has to be examined carefully. The scientific applications outlined in this chapter also direct the design and layout of the SQS scientific instrument, including the data acquisition modes and additional equipment needed to fully explore the potential of a soft X-ray end station for gas phase investigations at the European XFEL.

Most experiments take advantage of more than one FEL beam parameter, but a first global classification of scientific application or experimental method with respect to the most relevant photon beam parameters can be established:

High intensity ($> 10^{15}$ W/cm ²)	→ Non-linear phenomena
Short pulses (2–100 fs)	→ Ultrafast dynamics
High photon flux ($> 10^{12}$ photons/pulse)	→ Extremely dilute targets, Processes with small cross sections
Soft X-ray photon energies	→ Threshold and site-specific phenomena C(1s):290 eV, N(1s):410 eV, O(1s):540 eV
High repetition rate (27 000 pulses/s)	→ Coincidence experiments
Variable polarization	→ Dichroic effects
Spatial coherence	→ Coherent Imaging

A complete and detailed description of possible scientific applications is beyond the scope of this CDR, and only a short summary, including a few examples, of the main research topics is given below. Numerous additional examples are summarized in the presentations given at the two workshops and can be found on the corresponding websites (Chapter 1).

Non-linear processes represent the primary scientific applications defined for the SQS instrument. Intensities of more than 10^{18} W/cm² will be achieved in the focus of the XUV radiation at the SQS end station, which offer, together with the high repetition rate of the European XFEL, unique possibilities to explore and extend the limits of this novel and exciting research field. Compared to studies with intense optical lasers, which interact only with the outer valence electrons, the high photon energies of the FEL radiation efficiently create vacancies in the strongly bound, inner electron shells. For the investigation of multiple ionization and multiple-photon excitations, the fast relaxation of these core holes through Auger decay, which takes place on the femtosecond time scale, results in complex dynamics governing the sequential and direct ionization processes. The detailed understanding of these processes is not only essential for improving the theoretical models describing the photon–atom interaction, but also for the accurate analysis of scattering experiments [1].

The importance of non-linear processes was first demonstrated by ion spectroscopy on atomic Xe at FLASH [2] and later transferred to the X-ray regime with experiments on atomic Ne at LCLS [1, 3]. Although the results on Ne are in perfect agreement with theoretical predictions [4], the results on Xe are still the subject of an ongoing debate [5]. A detailed understanding of the underlying processes can be obtained only by applying more sophisticated experimental techniques, based, e.g., on electron spectroscopy [6,7] and coincidence techniques [8]. Future investigation of non-linear phenomena will go beyond these approaches and will strongly benefit from the higher repetition rate at the European XFEL (enabling higher coincidence rates and thus improved statistics), as well as from further developments in the design of electron and fluorescence spectrometers (enabling the reduction of space charge effects). Full characterization of the electronic and radiative decay will

make it possible to unravel competing sequential and direct multiple-photon processes, as well as complex relaxation cascades induced by the formation of multiple core holes. Similarly, the influence and importance of non-linear phenomena for processes in more dilute species (ions) and complex species (clusters) can be analysed in greater detail up to the complete characterization.

Time-resolved experiments combining the FEL and a synchronized optical laser will take advantage of the ultrashort pulse duration of the FEL radiation (2–100 fs) and the envisaged synchronization (10 fs) between both sources. Detailed analysis of the temporal evolution of the photoinduced fragmentation of a molecule, the “molecular movie”, will become possible. In particular, the low-charge mode enabling the production of pulses with the duration of a few femtoseconds gives access to the time scale where atomic displacements in molecules take place. Experimental verification of already-existing theoretical predictions for wave packet dynamics in innershell excitations of small molecules (e.g. NO [9]) and for proton transfer mechanisms in H₂O dimers [10] will be within reach. These short pulse durations, together with advanced detection methods, are the key ingredients for the success of these experiments. Furthermore, the ultrashort durations of the FEL pulses induce photoionization processes on the time scale of (or even shorter than) one optical cycle of the additional dressing laser (2.6 fs and 6.5 fs for 800 nm and 2000 nm, respectively). Under these conditions, extremely strong optical fields are applied during the photoionization process leading to electron “streaking” in the photoelectron spectra [11, 12]. This provides an extremely promising approach to analyse the photoionization dynamics on very short (sub-femtosecond) timescales and, eventually, to modify and control the photoionization or subsequent Auger process.

The **high photon flux** (10^{12} – 10^{13} photons/pulse or 10^{16} – 10^{17} photons/second) represents the necessary and indispensable requirement for experimental studies on very dilute ionic species (10^5 – 10^6 cm⁻³), as demonstrated in studies in the VUV wavelength regime at FLASH [13, 14]. Experiments of single trapped atomic and molecular ions will become feasible, and experimental techniques, such as electron and Auger spectroscopy, as well

as electron–ion coincidences, will become accessible, allowing the complete analysis of photoexcitation and photoionization processes. The much weaker cross sections in the XUV (compared to the VUV) wavelength regime can be compensated, enabling the extension of the experiments to higher charge states, where influences of relativistic effects are more pronounced, and to studies of innershell resonances and ionization thresholds.

The **XUV wavelength regime** (260–3000 eV) corresponds to the photon energy range necessary to excite the strongly bound core electrons of many important atomic species. For example, in biologically relevant targets, the ionization threshold of the 1s electrons in the carbon (290 eV), nitrogen (410 eV), oxygen (560 eV), phosphor (2145 eV), and sulphur (2470 eV) components are situated in this range. Due to the localization of the core electrons in the atom, element, and site, specific investigations can be performed on molecules, heterogeneous clusters, and large biomolecules. In the case of studies on atoms and clusters, which are related to applications in material science, the important 2p resonances and ionization thresholds of the 3d transition metals (550–1000 eV) as well as the excitation of the 3d shell in the rare earth metals (800–1300 eV) are perfectly covered by the radiation of the SASE3 undulator.

The **high repetition rate** of the European XFEL—providing up to 27 000 pulses per second to the experiment stations—is presently a unique feature of this accelerator. It exceeds by more than two orders of magnitude the number of pulses delivered by other FEL sources. The pulse delivery time pattern is imposed by the electron accelerator, which operates at a 10 Hz repetition rate for bunch trains containing up to 2 700 bunches each. The minimal temporal separation of the individual pulses within a train is 220 ns (i.e. a repetition rate of 4.5 MHz). This exceptional pulse rate enables various new possibilities, in particular for experiments based on single event counting, such as coincidence experiments and single-shot imaging experiments. For the full characterization of a photoionization or photofragmentation process, the simultaneous analysis of all fragments (electrons and ions, eventually photons) produced during one event is essential. As a consequence, the higher repetition rate transforms directly into higher coincidence rates and

increased statistics. Even for applications requiring larger pulse separations in the microsecond range (e.g. for the analysis of heavy ions or ionic fragments), the repetition rate still exceeds that available at other FEL sources.

Variable polarization of the FEL radiation (i.e. the possibility to perform experiments with linearly or circularly polarized light), will be important, e.g., for investigations of chiral molecules or studies on atoms, clusters, and nanoparticles with relevance for the magnetic properties of matter (i.e. on systems containing Fe, Co, or Ni components). Experimental and theoretical analysis of the linear and circular dichroism in photoionization has demonstrated the power of this approach in two-color, pump-probe experiments at synchrotron radiation sources [15]. The time-resolved application of the method, possible with the ultrashort pulse durations of FELs, is starting only now with experiments at FLASH and LCLS. Generally, the combination of two independently controllable polarized photons will provide unique insight into the photoionization dynamics enabling in certain cases the quantum mechanically “complete” experiment.

The **spatial coherence** of the FEL radiation, combined with its high flux and short pulse length, enables a range of coherent imaging experiments. For systems requiring less than the atomic resolution, the use of soft X-ray radiation enables higher cross sections and therefore increased scattering strength. Numerous studies will take advantage of this. For example, the scattering cross sections are enhanced in the XUV regime and experiments with increased contrast becoming possible. By detecting scattered radiation at larger angles, diffractive imaging with soft X-rays can approach wavelength-limited resolution. Biosamples can be studied in their native, wet environment using wavelengths in the water window (i.e. below the K-edge of oxygen, which avoids staining or otherwise modifying the sample while still providing high-contrast information. Special conditions are also provided for samples of several microns diameter, which benefit from the longer wavelengths of the XUV radiation due to higher cross sections and relaxed sampling conditions, and are not limited by these wavelengths, as the structure of samples at this scale, in general, do not need to be determined to atomic resolution to be valuable (e.g. cells and organelles). The first experiments at FLASH [16] and

recent studies on clusters and nanoparticles at LCLS [17, 18] have demonstrated the feasibility of these studies. Finally, as these experiments are intended to be performed on a single-shot basis, due to the strong radiation damage to the sample, the gain in information (i.e. the number of diffraction patterns obtained in a given time interval) will be drastically enhanced at the high repetition rates of the European XFEL, yielding a commensurate increase in the number of such systems that can be studied, or, in certain cases, improving the efficacy of the structure determination method [19].

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4 Optical layout

The optical transport of the FEL radiation from the SASE3 undulator to the experiment station is outlined in the conceptual design report for the beam transport systems (CDR-BT_2011). The resulting schematic presentation is given in Figure 2.

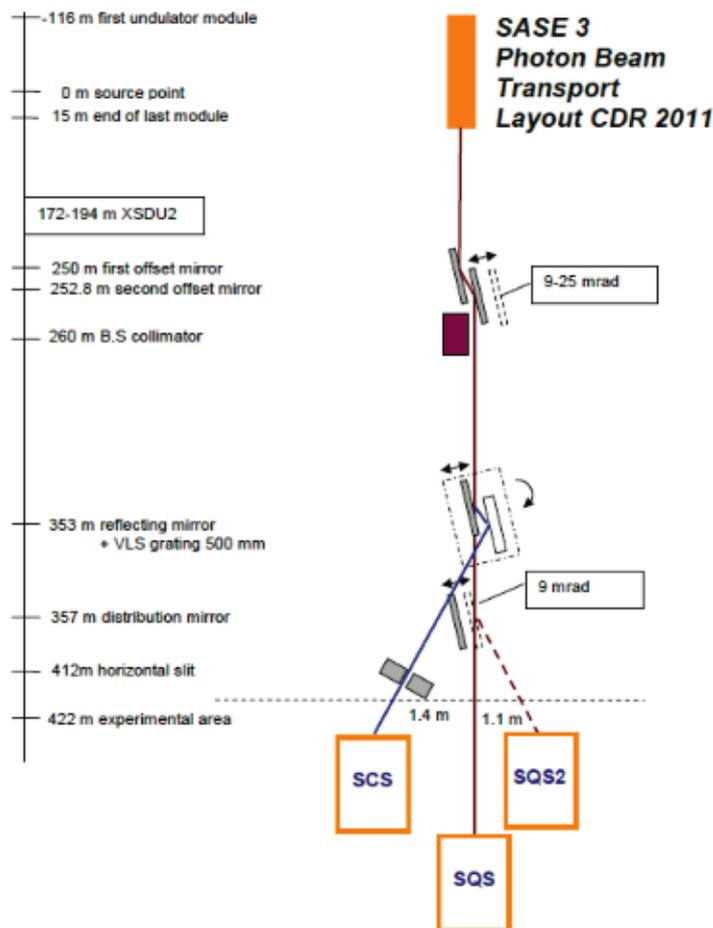


Figure 2: Optical layout behind the SASE3 undulator (from CDR-BT_2011)

The SASE3 undulator will deliver FEL radiation to three experiment stations:

- 1 The SQS scientific instrument dedicated to the study of non-linear phenomena and processes in intense radiation fields is placed in the central branch and receives, after passing the minimal number of optical elements, the direct non-monochromatized beam.
- 2 A side branch will provide an “open port” (SQS2) with relaxed focusing conditions for the non-monochromatized beam, enabling the setup of specialized experiments and equipment, which will be provided by the users.
- 3 The Spectroscopy and Coherent Scattering (SCS) scientific instrument receives monochromatic light by introducing a variable line spacing (VLS) monochromator into the direct beam. The performances of the monochromator are discussed in the CDR-BT_2011. The conceptual design of the SCS scientific instrument will be presented separately.

The important parameters for the optical elements of the SQS branches are summarized below.

Offset mirrors

About 250 m behind the SASE3 undulator, a pair of offset mirrors deviates the FEL beam in the horizontal plane by at least 35 mm in order to protect the experiment area from the intense Bremsstrahlung background. These mirrors can be operated at different incidence angles (9 mrad to 25 mrad) to ensure maximum transmission over the entire photon energy range from 260 to 3 000 eV (Figure 3). The varying horizontal displacement of the second mirror (35–60 mm) necessary to accommodate different incidence angles of the mirrors, and the resulting displacement of the FEL beam, are compensated using the angle of the second offset mirror. The high-energy cutoff of the mirror transmission can also serve as low-pass filter reducing harmonics of the FEL radiation, i.e., by choosing the appropriate reflection angle the third harmonic is efficiently suppressed for photon energies (in the first harmonic)

of more than 350 eV. In addition, the second mirror will provide prefocusing in the horizontal plane through adjustable bending in order to match the acceptance of the successive optics. The diameter (FWHM) of the FEL beam at the entrance of the experiment area (i.e. about 170 m behind the offset mirrors) is on the order of 1.5 mm and 12 mm at 3 keV and 260 eV, respectively.

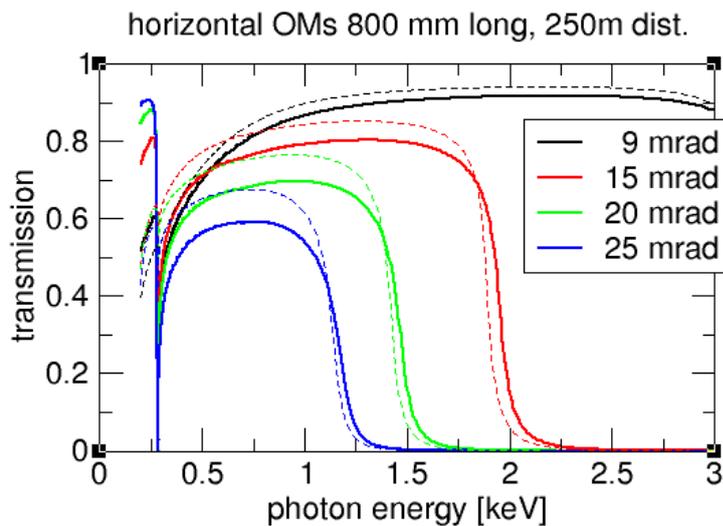


Figure 3: Transmission for the pair of offset mirrors for different incidence angles calculated for carbon (solid lines) and B4C coating (dashed lines) of the mirrors (from CDR-BT_2011)

KB focusing mirrors

The main central branch will be equipped with a Kirkpatrick-Baez (KB) mirror system, which represents the only feasible solution in the soft X-ray wavelength regime to provide the required minimal focus diameter of about 1 micron in the interaction region, while maintaining a high intensity. The KB mirrors will be optimized to assure maximal intensity in a wide range of photon energies between 500 and 2000 eV (15 mrad), while still keeping an appreciable transmission at lower photon energies, i.e., down to the Carbon 1s threshold (260–500 eV, see Figure 4). For experiments requiring photon

energies between 2 and 3 keV, a different incidence angle (9 mrad) will be used.

If required, the transmission below 500 eV can be increased by a factor of 2 by choosing larger incidence angles for the KB optics (25 mrad). Further optimization in the region of the C 1s edge is possible by using a Ni coating for the KB optics, but would result in a drastic decrease of transmission at photon energies above 850 eV.

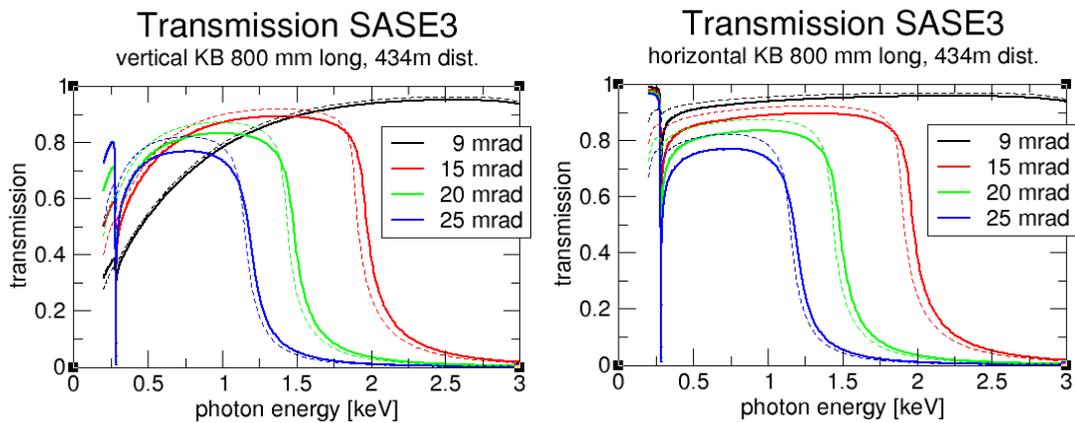


Figure 4: Transmission curves for the vertical (left) and horizontal (right) focusing mirror of the KB system calculated for carbon (solid lines) and B4C coating (dashed lines) of the mirrors (from CDR-BT_2011)

Operating the KB mirrors for the different photon energy regimes (i.e. at different incidence angles) imposes a change of the lateral focus position in the experiment chamber. For the two operation modes (i.e. 9 and 15 mrad), the focus will move by about 24 and 36 mm in the horizontal and vertical direction, respectively. This displacement has to be compensated by a realignment of the experiment chamber. The alignment procedures established for the AMO end station at LCLS have demonstrated that precise and reproducible movements in this order are feasible. The final technical solution adopted for the SQS end station will be examined in the technical design report.

In addition, an experiment station with different sections (i.e. different interaction regions along the beam propagation direction) is foreseen. In the present design (Chapter 5), two segments of the experiment stations, located

2.0 m and 3.3 m behind the second KB mirror, respectively, are under consideration. The KB setup will enable a displacement of the microfocus to the second section by ensuring an only slightly reduced minimal diameter (< 2 microns), possible due to the relative large distance (more than 400 m) to the source point. Furthermore, the possibility to adjust the focus size at a given position in the experiment chamber provides the additional advantage to optimize the spatial overlap between the FEL beam and the optical laser for two-colour, pump-probe studies.

Distribution mirror

The installation of a distribution mirror is foreseen to provide the non-monochromatized FEL beam also to the “open port” (SQS2). This plane mirror can be introduced in the beam path at a distance of 357 m from the SASE3 undulator, i.e., 150 m behind the offset mirrors (Figure 2). When using the mirror under the smallest reflection angle (9 mrad), a horizontal separation of 1.1 m is achieved between the two SQS branches, therefore representing also the maximal lateral extension of the experiment chamber used at SQS2. The plane distribution mirror provides an unfocussed beam ($2 \times 2 \text{ mm}^2$ to $16 \times 16 \text{ mm}^2$, depending on the photon energy, see above) or a horizontally prefocused beam (300 micron) to the instrument located about 8 m behind the entrance to the experiment area. The unfocused beam can serve for sub-micron focusing applications in the experiment chamber (provided by the users).

The distribution mirror, installed only 4 m behind the monochromator, also provides the option to steer the monochromatized beam into the central branch of the SQS scientific instrument. For most of the experiments planned for the SQS scientific instrument, a photon energy resolution of $\Delta E / E = 10\ 000$ is sufficient to select, e.g., a particular resonant excitation. Since an energy resolution of $> 10\ 000$ is presently under consideration for the SCS branch, even the slightly reduced performances of the monochromator, which is expected in this configuration and by adding a proper exit slit to the SQS branch, should meet this requirement. In addition, the possibility to use the beam behind the monochromator offers the possibility to separate the first and second harmonic of the circularly polarized

FEL radiation produced, as presently discussed, by short helical or cross-planar undulator segments (Chapter 2). This extremely interesting option to deliver monochromatic FEL radiation also to the main SQS end station will be further investigated and discussed in more detail in the SQS TDR.

Toroidal mirror (Option)

To obtain a smaller focus (30–50 microns) of the direct non-monochromatized beam at the SQS2 end station, the simplest (and least expensive) option is given by the installation of an additional toroidal mirror. The mirror can be installed in the side branch and will provide a fixed focus. In addition, it will enable a larger separation of both branches, as well as provide a reasonable focus size for general (not sub-micron) applications.

Split-and-delay unit (Option)

The installation of a split-and-delay unit is under consideration, but is not part of the baseline instrumentation for the SQS scientific instrument. Such a setup will enable XUV–XUV pump-probe experiments, which is one of the principal requirements of the SQS user community. A split-and-delay unit for the soft X-ray regime is currently under design using the experience of the analogue instrument built for FLASH [1].

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5 Conceptual design for the SQS end station

The layout of the experiment station, which will be installed on the central branch of the SASE3 undulator beamline, is guided by the principal goals of the SQS scientific instrument (i.e. the investigation of non-linear and time-resolved phenomena as well as studies in strong radiation fields). In the last few years, the scientific community based around SQS has developed numerous advanced experimental techniques aimed either at the characterization of specific aspects and particular relaxation channels of photoinduced processes or at the complete characterization of the complex relaxation mechanisms. Typically, experiments in the gas phase consist of probing a variety of targets (e.g. free atoms and molecules, atomic and molecular ions, clusters, nanoparticles, and large biomolecules). In general, these targets each require specific preparation techniques and different methods of injection into vacuum. To provide the users with the most advanced experimental techniques and to enable its optimal utilization, while maintaining a broad range of applications, the SQS end station will be separated into two independent experiment sections (Figure 5).

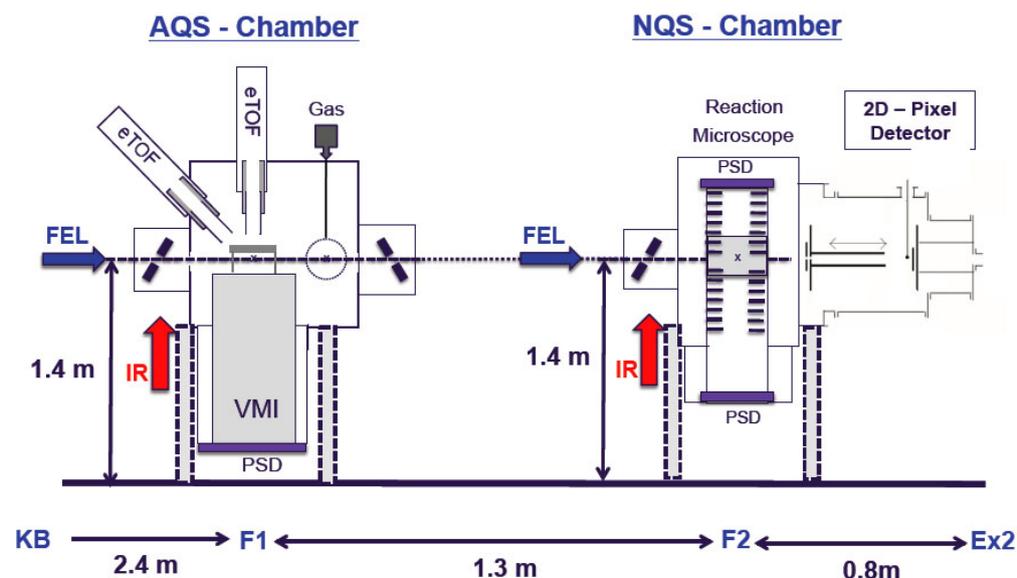


Figure 5: Schematic layout for the two experiment sections of the SQS scientific instrument. Left: Section devoted to experiments on Atomic-like Quantum Systems (AQS). Right: Section devoted to Nano-size Quantum Systems (NQS).

The AQS chamber will be optimized primarily for studies on “Atomic-like Quantum Systems” (i.e. free atoms and small molecules). Scientific applications will focus on investigations at high spectral and angular resolution, as well as time-resolved, pump-probe experiments and coincidence methods. The NQS chamber will be devoted to experiments on “Nano-size Quantum Systems” (i.e. larger gas phase targets, such as clusters, nanoparticles, and biomolecules). Dedicated equipment will enable single-shot imaging of these large species, as well as complete characterization of their fragmentation processes through coincidence and pump-probe techniques. Emphasis will be given in the design to high modularity, allowing, in principle, the use of different specialized components (analysers and detectors) in both experiment sections. However, the baseline setup and configuration of specific equipment will be prioritized for each of the two experiment chambers (Figures 5–8).

The AQS chamber will operate under ultrahigh vacuum conditions ($<10^{-10}$ mbar) and is located at a distance of approx. 2.4 m from the centre of the second KB mirror. This distance will provide sufficient space to install a differential pumping stage, a collinear focusing setup for the optical laser, and

a set of YAG screens for monitoring the FEL position. For the NQS chamber, the vacuum requirements will be slightly relaxed ($<10^{-9}$ mbar) in order to accommodate the particle beams and the imaging detector. It will be placed approx. 1.3 m further upstream. A differential pumping stage between the two chambers will house laser exit and entrance (second chamber) setups as well as an optional beam stop module. The possibility to install the NQS chamber also in the position of minimal focus size (i.e. replacing the AQS chamber for dedicated experiments) will be evaluated in the technical design report.

AQS chamber

The first section of the SQS scientific instrument will be dedicated to experiments on free atoms and small molecules, which will be introduced through a supersonic beam into the vacuum chamber. A background pressure of better than 10^{-10} mbar should be achieved in this section in order to avoid strong background signals from the residual gas, in particular for studies in the tightly focused FEL beam and with low target densities.

Focusing of the FEL radiation to a diameter of 1 μm will produce intensities of up to 10^{18} – 10^{19} W/cm^2 (i.e. intensities that will definitely induce multiple-photon processes and multiple-ionization of the target species). For the investigation of these processes, the chamber will be equipped with a set of high-resolution electron analysers, a high-resolution XUV fluorescence spectrometer, and a VMI-type analyser to measure the angular distribution of the electrons or ions. The suggested (schematic) layout is given in Figure 6.

AQS - Chamber

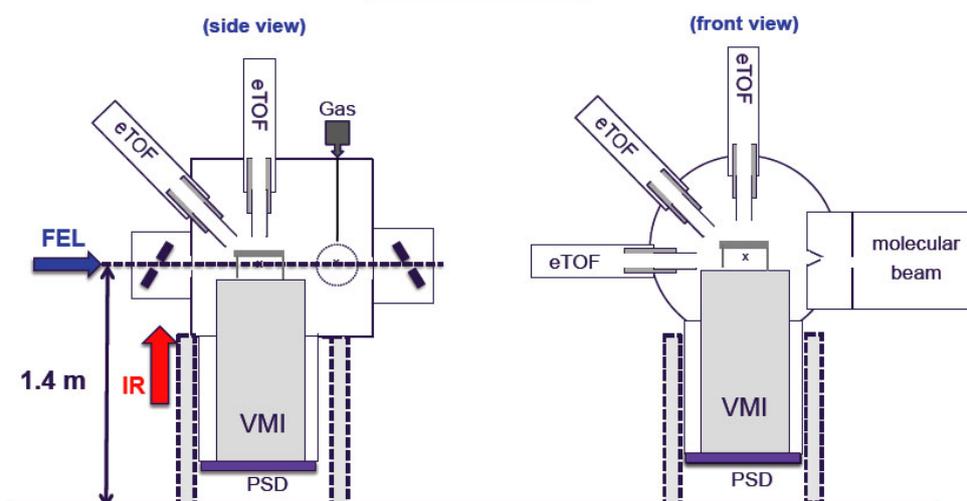


Figure 6: Suggested layout for the AQS chamber of the SQS scientific instrument

For baseline operation, five high-resolution, electron time of flight (TOF) analysers are to be installed at fixed angles around the interaction volume; three in the dipole plane (i.e. perpendicular to the beam propagation direction), and two in the non-dipole plane, are foreseen. The geometry chosen for the analysers is similar to that used at the AMO end station, which in turn was inspired by established experiment setups used at synchrotron radiation sources. For FEL experiments requiring high kinetic energy or high angular resolution, TOF analysers have demonstrated excellent performance on multiple occasions. The optimized design proposed for the SQS instrument will enhance the capabilities to achieve perfect spatial alignment of the five analysers around the interaction volume of 1 μm diameter. It will also add access possibilities for the optical laser and ease its alignment to the FEL. Furthermore, dedicated electron optics should enable the use of the TOF analysers in a “high energy-resolution mode” connected with small acceptance angles and in a “high-acceptance mode” suitable for coincidence experiments.

In addition, a velocity map imaging (VMI) analyser, which will be configurable either for electron or ion detection, can be used to measure the full angular distribution at lower energy resolution.

All these analysers can be used independently or in coincidence mode.

Several coincidence modes will be possible with this baseline configuration:

- 1 Electron–electron coincidences with the five electron TOF analysers (eTOFs) using up to a 4.5 MHz repetition rate
- 2 Electron (VMI) – ion (TOF) coincidences using up to a 4.5 MHz repetition rate
- 3 Electron (TOF) – ion (VMI) coincidences using pulsed extraction fields, i.e, operating at a lower repetition rate (up to 100 kHz) and with reduced performances for the analysis of the ions

Furthermore, the AQS chamber will host a magnetic bottle electron spectrometer (MBES) for pulse-to-pulse analysis and an XUV fluorescence spectrometer for the analysis of non-linear processes unperturbed by space charge effects. These two spectrometers will be installed independently, centred on a second interaction volume about 20 cm behind the first one (Figure 7). The FEL focus can be moved by the KB mirror optics to this second position. Optionally, the two parts can operate in parallel allowing, e.g., the use of the MBES for single-shot calibration of experiments performed with the high-resolution TOFs. The design to provide two interaction regions for one experiment chamber greatly increases the overall performance of the SQS instrument, especially because it enables modularity by keeping fixed alignments for sensitive experiment parts. Furthermore, this option has the clear advantage that different gas inlet systems adapted to these spectrometers can be used. The MBES, which is mainly used as a single-shot device, will benefit from higher local gas pressures, produced, e.g., in a conventional effusive gas jet at the outlet of a small capillary with diameters of less than 200 microns. The XUV spectrometer is often used in combination with a high-pressure gas cell, which enables compensation of the low efficiency for photon detection, but requires a separate mounting.

AQS - Chamber

(top view)

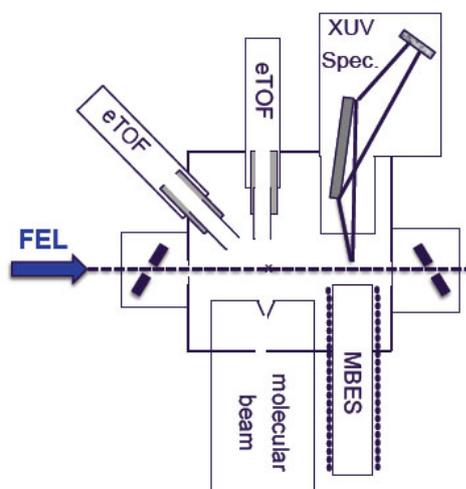


Figure 7: Suggested layout for the AQS chamber of the SQS scientific instrument

The chamber will be equipped with an appropriate setup to introduce the optical laser, to align it to the (already centred) FEL beam, and to monitor it after the interaction region. High flexibility will be provided for the access of the optical laser, enabling not only a collinear beam, but also crossed beam geometries. The alignment of the optical laser for pump-probe experiments will be controlled at the entrance, in the centre, and at the exit of the chamber. In the centre of the chamber (i.e. in the interaction volume), a special diagnostic paddle equipped with at least a fast photodiode for rough temporal alignment and a YAG screen for spatial alignment will be provided on a high-precision XYZ manipulator. Various view ports for observation of the alignment will be implemented at appropriate positions on the chamber.

The technical layout and geometry of the AQS chamber will enable high modularity, i.e., assuring that the installation of equipment dedicated to the NQS chamber (e.g. reaction microscope and cluster beam) is technically feasible.

Table 2: General specifications of the AQS chamber

AQS chamber	
Vacuum	$< 10^{-10}$ mbar
Target preparation	Molecular jet Effusive jet High-pressure gas cell
Focus diameter	> 1 micron
Analysers	High-resolution electron-TOF (x 5) Velocity map imaging spectrometer Magnetic bottle electron spectrometer XUV fluorescence spectrometer Reaction microscope (optional)
Diverse	Synchronized optical laser Alignment and diagnostics tools

HR electron TOF

High-resolution (HR) electron TOF spectrometers will be installed for the spectroscopic investigation of linear and non-linear photoionization processes induced by the intense FEL radiation. An energy resolution of $E / \Delta E > 10\,000$ is envisaged in order to obtain detailed information on the kinetic energy distribution after ionization in the soft X-ray regime (i.e. at photon energies of several hundred eV). The decay of photoinduced inner shell holes produces Auger electrons with kinetic energies of the same order (some hundred eV). In order to distinguish individual multiplet lines of an atomic configuration or vibrational states of a small diatomic molecule, this resolution is necessary and can be achieved by using suitable retardation optics, which decelerate the electrons at the entrance to the field-free drift region.

A candidate design could be similar to the setup of the AMO station at LCLS, but adapted and optimized to the requirements of the SQS instrument. The TOF analysers used at AMO are based on a design outlined in [1]. These analysers have an overall length of about 44 cm and an angular acceptance of ± 2.7 degrees, which enables also angular-resolved studies at fixed angles. This possibility will be explored by mounting three analysers at different angles (0° , 54.7° , and 90°) with respect to the horizontal electric field vector of the linearly polarized XUV radiation. Specially designed entrance optics should enable the use of these TOF analysers for experiments requiring high

energy and high angular resolution as well as for coincidence experiments requiring high transmission (at reduced energy and angular performances). Two further TOFs are mounted at 45° with respect to this dipole plane. This geometry will enable to obtain information about the importance of non-dipole effects, which, up to now, have been widely neglected, but are particularly relevant for the theoretical modelling of general photon–matter interactions in the soft X-ray regime.

VMI

The VMI analyser will provide the complete angular resolved information of electrons and ions with lower energy resolution. For these devices, a high extraction field (some kV/cm) is applied to direct all fragments of the same polarity (electrons or ions) towards the detector (i.e. full solid angle acceptance can be achieved). The use of a position-sensitive detector (e.g. a delay line detector) enables measurements of the angular distribution of the emitted fragments as well as their final kinetic energies. The complete angular distribution can be extracted almost directly (applying known image conversion techniques) from the measured two-dimensional spectra. The typical length of these analysers is on the order of 20–30 cm, which together with the high extraction fields, results in a moderate energy resolution ($E / \Delta E = 50$).

There are several references for the design of these analysers (e.g. [2–4]). The successful adaptation of the method to experiments at FEL sources was realized by Vrakking and Johnsson (e.g. [5]) and the extension to high kinetic energies (keV) is under development. The design of the VMI analyser for the SQS instrument will be developed in close contact with these groups and will take advantage of existing expertise. In particular, the extraction field needs to be adapted to the particular environment (i.e. it will be designed to enable the use of the eTOF analysers without the need for realignment and to provide the possibility of coincidences between the VMI and TOF analysers).

MBES

A magnetic bottle electron spectrometer (MBES) will provide the possibility to record electron spectra on a shot-to-shot basis, which is of particular interest

for many time-resolved, pump-probe studies combining the FEL and the synchronized optical laser. Recording spectra for each individual FEL pulse enables the post-sorting of the spectra with respect to the “actual” temporal delay, thereby overcoming limitations of the temporal resolution imposed by the relative time jitter between the two sources. The high acceptance (up to 2π solid angle) is achieved by a strong magnet, which is installed close to the interaction region. The analysis of the electron kinetic energy is given by time-of-flight spectrometry providing an energy resolution $E / \Delta E$ of about 50–100 for conventional drift lengths of 60–100 cm. The overall resolution of the device can be improved by applying a retardation voltage to the entrance of the MBES.

Most of the MBES devices currently in use are based on the design proposed by J. Eland et al. [6] and are routinely used at the AMO end station at LCLS [7] and FLASH [8]. The high collection efficiency of the MBES also represents an interesting facet for coincidence experiments, e.g., the study of either cascade processes in electronic relaxation (e–e coincidences) or molecular dissociation pathways (e–ion coincidences). Recent developments for these coincidence applications, based on a special design of the interaction region [9], will be included in the design of the MBES of the SQS instrument.

XUV spectrometer

A XUV fluorescence spectrometer will be installed for high-resolution studies of radiative relaxation pathways. The fluorescence analysis enables, in particular, overcoming space charge problems in experiments of non-linear processes, where, typically, a large number of ions and electrons are produced during one FEL pulse in a small interaction volume. Although the radiative decay is generally much weaker than the electronic decay, the analysis of the fluorescence will provide a powerful alternative and complement to the analysis of charged fragments after excitation with intense FEL radiation. As already demonstrated in synchrotron radiation work [10, 11], the technique has a high resolving power, but is often limited by low count rates. For the SQS instrument, the spectrometer will be designed to match to the small spot size of the FEL radiation and a resolution of $E / \Delta E > 10\,000$ is envisaged. The overall size of the setup should not exceed

1.5–2.0 m. The detection will be performed with a small pixel size CCD detector. Related to the reduced count rate expected for the fluorescence emission, the installation of a high-pressure cell, which will allow a substantial increase of the target density, is envisaged.

For photon energies up to about 1.5 keV, a conventional high-transmission grating spectrometer is under consideration. The general design will rely on the initial suggestion by Nordgren and Nyholm [12] and consider latest developments and improvements, in particular with respect to the layout and performance of the detector.

NQS chamber

The second section of the SQS scientific instrument will mainly be devoted to studies of larger gas phase systems, such as clusters, nanoparticles and biomolecules (Figure 8). Systems for preparing these specific targets and for introducing them into the vacuum chamber will be developed in close collaboration with interested user consortia, which will provide the necessary expertise. An essential part of the instrumentation will be a large-area 2D pixel detector, such as the DSSC detector, which is already under development and which will enable imaging experiments on these larger particles in the soft X-ray wavelength regime. Installed about 1.3 m behind the AQS chamber, the KB optics will provide a focus spot of 2–3 microns, which is essential to ensure high performance and optimal resolution in the imaging experiments. Additional baseline equipment of this section will comprise a reaction microscope, an electron or ion TOF, and a Thomson parabola, which are used for complementary experiments performed independently or, if possible, in coincidence with the imaging detector. This chamber will operate under high vacuum ($< 10^{-9}$ mbar), which is well adapted to the desired targets and especially to the corresponding introduction systems (electrospray and droplets). In addition, the large area pixel detector is presently not compatible with ultrahigh vacuum conditions. For this reason, special attention will be given to the installation, partial pumping, and spatial separation of the 2D

detector unit. Experience gained with the “CAMP” and the newly designed “LAMP” chamber at LCLS will be taken into account.

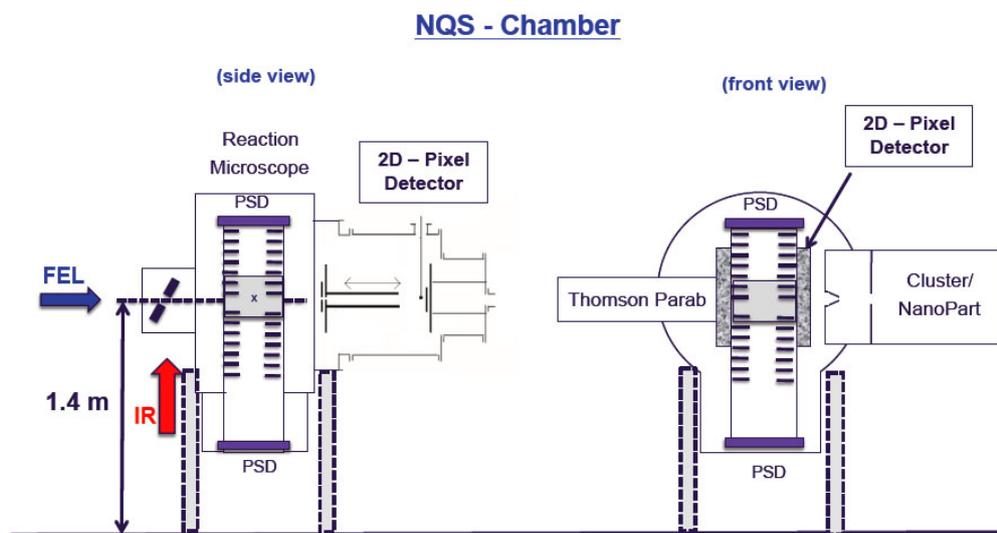


Figure 8: Suggested layout for the NQS chamber of the SQS scientific instrument

The reaction microscope will enable the complete characterization of the interaction between the FEL pulses and the target through simultaneous detection and analysis of the kinetic energies and angular distribution of both electrons and ionic fragments. This device will take advantage of the high repetition rate provided by the European XFEL, since electrons and ions are detected in coincidence. For experiments requiring higher spectral resolution, an additional electron or ion TOF and a Thomson parabola can be used. These devices will be installed, if technically possible, parallel to the reaction microscope or will replace it.

To assure high flexibility of the SQS instrument, the design of the reaction microscope will be such as to allow its installation in the AQS chamber. Likewise, the NQS chamber should be able to accommodate the XUV fluorescence spectrometer and the magnetic bottle electron spectrometer.

Similar to the AQS chamber, the imaging section will be equipped with appropriate modules for introducing the optical laser and enabling its precise alignment in the chamber for pump-probe experiments or for experiments on laser-aligned molecules. A dedicated diagnostic paddle equipped with at least

a fast photodiode for rough temporal alignment and a YAG screen for spatial alignment will be provided on a high-precision XYZ manipulator. In addition, various view ports for observation of the alignment will be implemented at appropriate positions on the vacuum chamber. For the mounting of the 2D detector, dedicated mechanics are under consideration for its precise alignment with respect to the FEL beam. These mechanics will include a variable aperture for the central hole in the detector area and variable distance to the sample. Particular care will be taken to separate the detector area from the sample area in order to avoid contamination of the detector.

Table 3: General specifications of the NQS chamber

NQS chamber	
Vacuum	< 10 ⁻⁹ mbar
Target preparation	Cluster source Nanoparticle beam Liquid jet
Focus diameter	> 2 micron
Analysers	Reaction microscope Thomson parabola Electron or ion TOF 2D pixel detector (DSSC) XUV fluorescence spectrometer (optional) High-resolution eTOF (optional)
Diverse	Synchronized optical laser Alignment and diagnostics tools

Reaction microscope

The reaction microscope is used to obtain the complete characterization of the molecular fragmentation process. By means of combined electric and magnetic fields, the electrons and ions are directed on well-defined trajectories to position-sensitive detectors. Since all electrons and ions are extracted from the interaction volume, this device is ideally suited for coincidence spectroscopy. The analysis of the coincidence patterns provides detailed information on the angular distribution of the electron emission for well-defined orientations of the molecule with respect to the polarization vector of the FEL radiation. The power of this analyser has been demonstrated in many experiments at synchrotron radiation facilities as well

as FEL sources. In particular, the high repetition rate available at the European XFEL (up to 27 000 pulses per second) will be extremely beneficial for these measurements, since it allows an increase of the coincidence rate by more than two orders of magnitude compared to other FEL sources operating at 10 Hz (FLASH) up to 120 Hz (LCLS).

The design will be adapted to the particular conditions at the SQS end station, but will be inspired by the design proposed for the CAMP chamber, which was successfully used at LCLS. For the final layout, the expertise of the research groups in Heidelberg (Ullrich, Moshhammer) and Frankfurt (Dörner) will be requested in order to optimize and to match all parameters to the characteristics of the SQS instrument.

2D pixel detector

Scattering experiments on large structures (e.g. clusters, nanoparticles, biomolecules, and small cells) requires spatial resolution of better than 10 nm, aiming to achieve 1–2 nm. For a typical 2-micron object, this would require measuring diffraction patterns with an angular opening of up to 45° for 500 eV photons, sampled at more than 800 points in each direction perpendicular to the beam propagation direction. Ideally, the detector should provide a frame rate of 4.5 MHz (i.e. full XFEL burst mode capability). Single photon counting capability at high scattering angles and the maximum technologically possible quantum efficiency of the sensor is required in the energy range between 0.26 and 3.0 keV.

Presently, a large area, 2D, 1 megapixel detector optimized for the photon energy range 0.5–4 keV is under development (WP75), and is expected to be available for users in 2016. The detector module will consist of four quadrants of 512 x 512 pixels, with a hexagonal pixel geometry of approx. 236 to 272 μm in diameter. The detector will provide single photon sensitivity and will be capable of recording with a 4.5 MHz repetition rate up to 512 images within one bunch train of the European XFEL. When mounted 40 (200) cm from the interaction region, a resolution of about 5 (25) nm can be achieved for a 1 (5) μm object. An increase of the detector size would directly and linearly improve the resolution. The possibility to vary the distance to the

object, to adjust the position with respect to the FEL beam, and to adapt the centre opening of the detector to beam dimensions enables numerous studies on a variety of targets of different sizes. In addition, the fast readout offers the option of recording in coincidence electron or ion spectra (i.e. providing full information about the photon–matter interaction). The implementation of a DSSC-like detector, combined with the high photon flux delivered at the SQS end station and the higher repetition rate available at the European XFEL, will provide unique possibilities for performing imaging experiments in the soft X-ray regime.

As a complementary solution to a DSSC system, a CAMP-like pnCCD detector could be implemented in the station to cover the energy range between 200 eV and 1 keV. This type of detector has been extremely successful at FLASH and at LCLS operating with a maximum readout rate of up to 200 Hz [13–15]. The limitations due to the low frame rate in comparison to the XFEL burst mode will be studied in detail. Such a detector system could be made available for users at the start of operation of the European XFEL in 2015 and could therefore close the time gap related to the delivery of the DSSC detector in 2016.

Thomson parabola

For investigations on large molecular fragments or larger clusters, the installation of a Thomson parabola ion spectrograph is under consideration. The device will enable simultaneous determination of charge state and kinetic energy of the different ionic fragments released in the photoinduced process.

eTOF

An additional electron TOF (eTOF) analyser with moderate energy resolution ($> 1\,000$) will enable the characterization of the broader structures in the electron spectrum of clusters and large molecules. Important information about the energy transfer and the dynamics of the processes can be deduced from these spectra. The installation of the eTOF should be compatible with the mounting of the other devices.

A schematic summary of the various components of the SQS instrument is given in Figure 9. The components dedicated for the FEL beam diagnostics are discussed below.

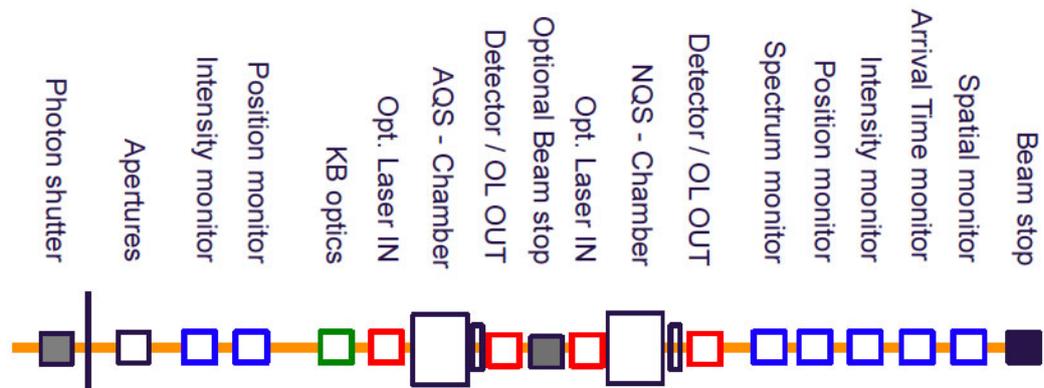


Figure 9: Overview of the optical elements and vacuum components of the SQS scientific instrument

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6 Floor plan of the SQS scientific instrument

In the experiment hall of the European XFEL, 15 x 36 m² of floor space will be dedicated to the instrumentation behind the SASE3 undulator (i.e. the SQS and SCS scientific instruments). A possible layout for the SQS scientific instrument is presented in Figure 10. The main SQS scientific instrument is located at the central branch with the longest distance to the undulator (about 450 m). This location provides enough space on both sides of the FEL beam, i.e., with no space constraints by the other branches (SQS2 and SCS). Furthermore, it allows the installation of the optical laser close to the experiments, avoiding, in this way, a long beam transport and the minimization of beam instabilities. Two lasers tables will be located close to the experiment chamber, which will serve for the final match of the optical laser parameters (wavelength, intensity, polarization, pulse duration, etc.) to the requirements of the specific experiment. The grey shaded areas define the working areas around the experiment stations. At present, it is assumed that no radiation protection is required for the soft X-ray end stations, and access to the experiment is provided during FEL operation. However, for experiments using the optical laser, controlled access based on laser safety requirements should be foreseen. Finally, the green shaded areas mark the control room for the electronic racks, which are located outside the experiment area.

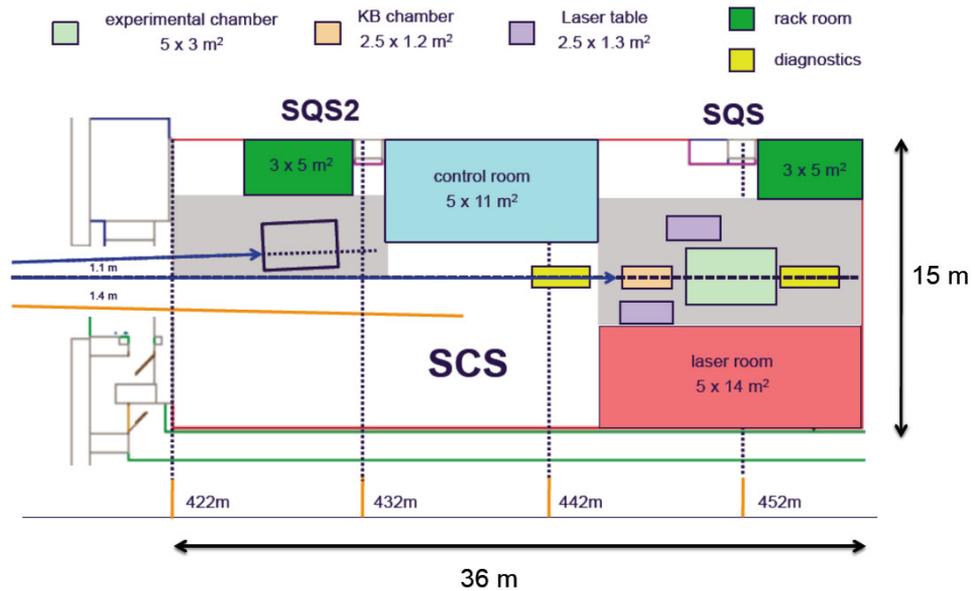


Figure 10: Layout of the SQS scientific instrument in the experiment hall

The SQS2 side branch will occupy the space close to the entrance of the FEL beam to the experiment hall. In this area, no dedicated SQS instrumentation is foreseen, since it is reserved for installation of user experiments (“open port”). In addition, space will be made available for the possible installation of an ion storage ring, which is not included in the baseline layout of the SQS instrument, but could be provided by an interested user consortium. The technical feasibility of such an installation, as well as the additional infrastructure requirements, will be examined for the SQS TDR.

The control room of about $5 \times 11 \text{ m}^2$ will be placed between the two experiment stations (SQS and SQS2) and will serve for both experiment stations. It will host all computer controls for the beamline optics (offset mirrors, deflection mirror, KB optics), detectors, and analysers, as well as for data acquisition.

7 Data acquisition modes

The SQS scientific instrument will contain many eTOF and iTOF detector components, as well as a reaction microscope, requiring the DAQ system to handle data from multiple digitizer channels simultaneously. Basically, the DAQ system should be capable of recording an electron TOF spectrum over the entire bunch train (600 μ sec) with a resolution of 100 ps (i.e. transferring 6×10^6 data points with a 10 Hz repetition rate).

The DAQ system capable of handling these data would therefore require that:

- Data from up to ~16 channels can be acquired.
- Channels are sampled at 2–8 GS/s with 10-bit resolution.
- 10-bit digitization result is stored in 2-byte words.
- Sampling is performed over the entire 600 μ s train period.

These requirements result in a data volume per digitizer channel per train for one eTOF component of 9.6 MB (8 GS/s). For one iTOF component, the load per train will be 2.4 MB (2 GS/s). The reaction microscope requires 12 digitizer channels at 2 GS/s for determination of position plus two at 8 GS/s for flight-time determination (48 MB per train). Note that the maximum value is a worst-case scenario as it simply assumes digitizing over the entire acquisition period of train delivery and does not take into account any effects that could shorten this, like quick arrival time of eTOFs and delay-line signals. Reducing the amount of data taken should be aimed for once the experiment is understood.

A DAQ system for acquiring multiple-channel data is shown in Figure 11. Data from digitizer channels are multiplexed together into a CPU and transferred to the train builder during the inter-train period of 99.4 ms using 10 Gbps network links. The train builder is being developed for the readout of imaging detectors and aggregates all input data into one block before transferring it, during following intertrain periods (data aggregated from four

inputs require four intertrain periods to send the data on one output link) to blades in the PC layer through a network switch. Monitoring of the data and transfer to the disk cache are performed by the blades.

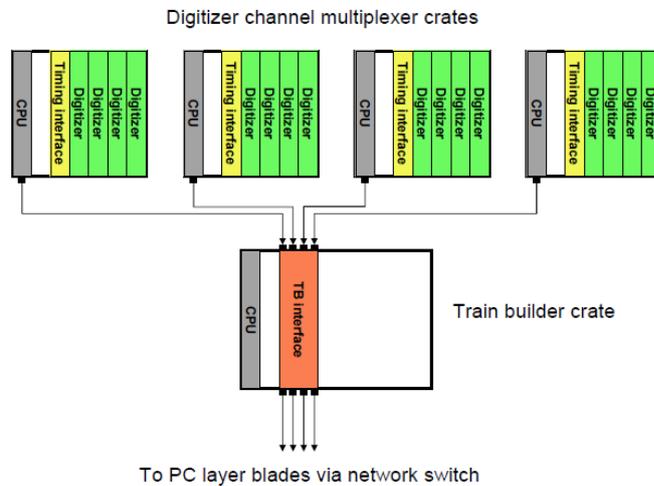


Figure 11: Schematic presentation of a DAQ system for the SQS scientific instrument

The 10 Gbps network links used can transfer 100 MB during one intertrain period and the baseline train-builder design foresees processing 64 MB of data per input, the later determines the maximum amount of data that can be handled per digitizer multiplexer crate. The maximum number of 9.6 MB/train payload digitizers per crate is 6, when overheads are ignored.

The number of digitizer channels combined in the multiplexer crate is also driven by digitizer-to-CPU readout performance. Digitizer crate solutions currently available (e.g. Acqiris, RoentDek, etc.) are relatively slow (≤ 100 MB/s) and limit the number of digitizers per crate to one. RoentDek is developing a crate system using PCIe with higher bandwidth (300–500 MB/s), which could increase the number of digitizers per crate to 3–4, thus reducing cost.

The baseline train-builder design for use with 1 megapixel image detectors foresees 16 inputs, 8 in and 8 out. The prototype TB demonstrator board will have inputs, 4 in and 4 out, and this board would be sufficient for the 3–4 crate solution.

The amount of data produced by 16 channels digitizer as described above can produce up to 12.6 TB per day. These data should be further reduced before storing it in the archive. This can be done already in the online mode on the PC layer or just after the data is temporarily stored on the DAQ data cache. The data processing will be performed using the framework provided by the DAQ and Control Systems group (WP76), which allows for experiment-specific software module integration.

The raw data from unsuccessful experiments or from the tuning phase should not be stored in the archive. The summary information can be put to the catalogue for further reference. The reduced good quality data will be transferred to the archive and to the highly accessible disk servers for further analysis on site in the offline mode.

The DAQ system outlined can, on paper, satisfy the maximum readout requirements of multiple channel digitizer systems. It has the advantage of reusing readout hardware being developed for the imaging detectors. To prove the design testing is required.

8 Optical laser

Many experiments are based on the combination of the ultrashort and intense FEL pulses with an additional synchronized femtosecond optical laser. Ideally, the laser operates at the same repetition rate as the FEL pulses (i.e. in a 10 Hz burst mode and a 4.5 MHz intraburst repetition rate). Pulse durations and energies of the optical laser, which are required for pump-probe experiments at the SQS scientific instrument, should be in the order of 10–100 fs and 1 mJ, respectively. These values match the duration of the FEL pulses, which is an important criterion for time-resolved studies, and open the access to the non-linear high-field regime also for the optical laser. Synchronization and temporal stability of the optical laser pulses with respect to the FEL pulses should be better than the pulse durations (i.e. less than 10 fs). Additionally, the possibility to align or to orient small molecules in the laser field should be available requiring pulse energies of more than 10 mJ at the highest possible repetition rate (≥ 100 kHz.)

A laser system capable of fulfilling these requirements is presently under development at the European XFEL (WP78). Based on non-collinear optical parametric amplification (NOPA), a first demonstrator, operating continuously at up to 100kHz, was shown at DESY in collaboration with the University of Jena and the Helmholtz Institute Jena, delivering in excess of 60 μ J, sub-10fs pulses in 2009 [1,2]. The further development aims at scaling the pulse energy and repetition rate to the mJ, MHz level respectively, with a timing structure matched to that of the European XFEL (10Hz burst operation). For the start of operation of the European XFEL in 2015, it is envisaged that WP78 will provide optical (800 nm) burst-mode lasers with pulse durations of 10–100 fs and pulse energies of 1 mJ at 1 MHz intraburst repetition rate. At the maximum XFEL repetition rate of 4.5 MHz, a pulse energy of 200 μ J is expected, while the system should also be able to deliver up to 10 mJ at 100 kHz with an acceptable degree of configuration change.

Synchronized to the XFEL timing distribution system (WP18), the laser timing jitter will be around 10 fs (rms) with respect to the XFEL machine clock, ensuring the best possible synchronization with the FEL pulses. This, in turn, is a basic requirement for time-resolved, pump-probe experiments as well as studies of laser-oriented molecules. As a particularly interesting option for adiabatic laser-induced molecular alignment, 1030 nm radiation can be extracted, delivering up to 250 mJ within a 1 ns pulse duration at a repetition rate of 100 kHz.

The pump-probe and molecular alignment laser system and its synchronization unit will be located in a laser room close to the experiment area dedicated to the SQS scientific instrument (Figure 10). For additional specific applications, requiring a broader variation of laser beam parameters, the adaptation of these parameters to the particular experimental needs will be undertaken in the experiment area.

The following possibilities will be part of the baseline instrumentation of the SQS instrument:

- 1 Tuneable wavelength (400–3000 nm) using optical parametric amplifier (OPA). The repetition rate is identical to that of the 800 nm pump laser operating in burst mode (i.e. delivering up to 4.5 MHz as intraburst repetition rate).
- 2 Frequency up-conversion using optical crystals to obtain 400 nm and 266 nm radiation at the 4.5 MHz repetition rate.
- 3 Production of THz radiation with the 800 nm radiation using appropriate crystals and optics.
- 4 Variable polarization (i.e. linear and circular polarization as well as rotatable linear polarization) will be provided using the appropriate optics (quarter and half wave plates, Fresnel rhomb, etc.).
- 5 Pulse stretcher allowing the controlled variation of the pulse duration between 10 fs and several picoseconds (chirped).

In addition, pulse and beam characterization methods such as auto-correlation, optical spectrum, and CCD will be provided.

References

- [1] F. Tavella et al., Opt. Express 18, 4689 (2010).
- [2] J. Rodthardt et al., Opt. Express 18, 12719 (2010).

9 FEL diagnostics

Precise knowledge of the photon beam parameters is essential for the quantitative analysis of the experiment results. In particular, the strong shot-to-shot variation of certain parameters caused by the non-linear, self-amplified stimulated emission (SASE) production process of the FEL radiation requires that some quantities are available for each individual pulse.

The following photon beam parameters will be provided “online” and can be integrated directly in the data acquisition system:

1 Pulse energy

The pulse energy will be measured with a relative precision of $\pm 1\%$ using a gas monitor detector (GMD) adapted to the XUV wavelength regime. This detector is routinely implemented in the beamlines at FLASH [1] and was also successfully tested at LCLS for higher photon energies. At the SQS instrument, measurements should be performed at the entrance of the experiment area (Figure 9) to monitor the intensity delivered by the SASE3 undulator as well as behind the focusing optics and the instrument chambers of the SQS instrument to monitor the intensity actually used for the experiment. The absolute calibration of the GMDs is foreseen, although, for most of the experiments, only the variation of relative intensity between the individual pulses is the relevant parameter.

2 Wavelength

The wavelength stability of the FEL radiation is expected to be on the order of 1%. For a precise attribution of single-shot spectra to the “actual” wavelength, a relative precision of 0.1% should be obtained. One possibility consists in the careful calibration of the electron bunch parameters, which will be available “online”. Additionally, a wavelength monitor based on the measurement of photoelectron spectra, similar to the one used at FLASH [2], will be developed by WP74, aiming to provide the “centre of gravity” of the photon energy distribution for each photon

pulse. This device will be located upstream of the SQS instrument, before the distribution mirrors.

3 Arrival time

All time-resolved pump-probe experiments require the precise knowledge of the relative arrival times of the pulses from the FEL and the optical laser at the interaction region in the experiment chamber. A setup for transmissive online monitoring of this relative arrival time for individual soft X-ray pulses is presently under development at the LCLS. The experimental approach is based on the measurement of XUV-induced reflectivity on a semiconductor surface [3]. Since a full 2D image is recorded for each photon pulse, the repetition rate of the device is limited at present to 10 Hz. In addition, a promising alternative approach to determine the arrival time by the measuring the streaking of photoelectrons in a superimposed THz field has been proposed for experiments at LCLS [4]. The outcome of the corresponding experiments will be followed very closely and, if successful, applied for the diagnostics at the SQS instrument.

Further photon beam parameters can be measured only by intercepting the photon beam or by averaging over many pulses. The determination of these parameters is nevertheless foreseen for the complete characterization of the FEL beam as well as for alignment purposes.

1 Spectral profile

For many experiments, in particular for investigations of resonant processes, it will be important to obtain information about the spectral distribution of the XUV radiation. A high-resolution variable line spacing (VLS) monochromator with a spectral resolution $\Delta\lambda / \lambda = 10^{-4}$ can provide such information. The monochromator could be installed behind the experiment chamber and the measurements would not affect the experiments performed in the SQS chamber. Recording of “online” spectra would be possible.

2 Pulse duration

Up to now, measurements of the pulse durations are dedicated experiments and no practical concept for “online” monitoring of the pulse

duration exists. A split-and-delay unit (e.g. an autocorrelator), which is under discussion for the realization of particular scientific applications, could be used for the determination of the overall pulse duration as well as of the coherence time [5]. This device is presently not part of the baseline instrumentation of the SQS instrument.

3 Beam position

For the precise alignment of the experiment chambers, the beam position will be monitored in front of the KB mirror optics and behind the experiment chambers. A combination of YAG screens surrounding the optical path of the FEL beam, in combination with the corresponding visual monitoring, will serve for this purpose.

4 Spatial profile

The spatial homogeneity of the FEL beam, relevant for the studies of non-linear processes, can be monitored in regions of an extended beam profile. Appropriate imaging of the beam onto a CCD detector with small pixel diameters will enable the monitoring of spatial fluctuations on a sub-micron scale. Such a device can be installed behind the experiment chamber, but will allow recording only with a 10 Hz repetition rate.

5 Temporal profile

A method that is capable of measuring the temporal profile of the FEL pulses directly is not yet known. Possible developments in this direction, such as the streaking of photoelectrons in a strong THz field [4], will be followed up and eventually integrated in the final design of the SQS scientific instrument.

References

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- [2] M. Wellhöfer et al., JINST 3, 02003 (2008).
- [3] C. Gahl et al., Nature Photonics 2, 165 (2008).
- [4] A. Cavalieri et al., beam time proposal LCLS 2011/2.
- [5] R. Mitzner et al., Opt. Express 16, 19909 (2008).

10 Add-on equipment

All instrumentation outlined and described above is considered as “baseline” instrumentation of the SQS scientific instrument. Due to the broad range of applications, the various experimental methods, and the different target preparation techniques, it is not possible to provide the required equipment for all possible experiments. It is expected that interested user groups will provide additional equipment, which is important for certain classes of experiments and which, furthermore, might require specific expertise. This add-on equipment will be defined in close collaboration with the corresponding user groups and could be integrated in the final layout of the SQS instrument and the experiment area, but it is not included in the budget for the SQS instrument.

The following instrumentation was already identified as important “add-on” equipment for the SQS scientific instrument. Other equipment might be defined in the next months and years.

1 Pulsed cluster source for the production of mass-selected clusters

Substantial expertise in handling these sources in combination with the FEL radiation has already been gathered by a broad collaboration involving various research groups. A new apparatus is under construction for experiments at FERMI. After validation of the CDR by the Scientific Advisory Committee (SAC), concrete discussions with the user community have to be undertaken in order to organize the possible integration of the cluster source into the SQS scientific instrument.

2 Nanoparticles beam

Numerous applications are devoted to the investigation of large particles and biomolecules that can be introduced into the vacuum by a liquid jet or the technique of electrospray. Similar to the situation for cluster beams, the corresponding equipment has to be provided by interested users who

will be involved in the discussion about the final technical layout of the instrument.

3 Ion storage ring

Particular attention will be given to a proposal by H. Pedersen (Aarhus), A. Wolf, and J. Crespo (Heidelberg). The collaboration suggests a permanent installation of an ion storage ring (2.7 x 4.4 m²) into the SASE3 beamline. The storage ring could be used in parasitic mode and would be transparent for other users. A possible installation could be in the area close to the entrance to the experiment hall. Since a prototype of the ion storage ring is presently under construction in Aarhus, a very detailed discussion can be undertaken during the development of the TDR in order to explore practical solution for the installation of the storage ring.

4 Fluorescence spectrometer

For experimental studies using high-resolution fluorescence spectroscopy in the photon energy range above 1.5 keV, which is not covered by the VLS spectrometer described above, the use of a crystal monochromator similar to the one described by [1] could be envisaged. However, this type of spectrometer is at present not foreseen in the baseline instrumentation of the SQS instrument.

References

- [1] Journal et al., Rev. Sci. Instrum. 80, 093105 (2009).

11 Time line

The construction and installation of the SQS scientific instrument is scheduled to follow this (rough) time line:

Delivery of the conceptual design report (CDR-SQS)	April 2011
Consultation of the user community for the elaboration of the TDR	> April 2011
Delivery of the technical design report (TDR-SQS)	April 2012
Start of sending out the orders for equipment	mid 2012
Definition, organization, and scheduling of the “add-on” equipment	> mid 2012
Reception, test, and assembly of equipment	2013
Start of installation of the SQS instrument in experiment hall	2014
Ready for beam	end 2014

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29–31 October 2008, Aarhus (Denmark)

John Bozek	AMO Science at the LCLS – Instrumentation and First Experiments
Thomas Möller	Ultrafast processes of clusters in intense X-ray beams
Robert Moshhammer	Atomic and molecular fragmentation in intense XUV laser fields
Michael Meyer	Pump-probe experiments in the XFEL regime
Henrik Stapelfeldt	Laser aligned molecules as sample holders for FEL experiments
Daniel Rolles	Multi-particle correlation measurements on atoms, molecules and nanoparticles
Kiyoshi Ueda	Atomic, molecular and cluster science using X-ray FELs
Stefan Schippers	Photon-Ion experiment with hard X-rays: From PETRA III to the XFEL (Merged-beam technologies)
Andreas Wolf	Photon induced fragmentation in molecular systems studied with fast beam imaging
Mats Larsson	Experiments with stored ion beams
José R. Crespo López-Urrutia	Soft x-ray laser spectroscopy
Alexander Dorn	Tracing ultra-fast many-electron processes in the super-brilliant light of the XFEL via high-resolution MOTRIMS
Todd Ditmire	Strongly coupled ion plasmas probed with the XFEL

Working Group I: Gas Phase Instrumentation

Chairs: Th. Möller, M. Meyer

E. Rühl	Experiments on Nano-Particles
T. Laarmann	X-ray Femtochemistry on small molecular systems
T. Ditmire	Studies on Clusters
D. Rolles	X-Ray Fluorescence
J. Costello	Time-resolved Pump-Probe experiments
J. Marangos	Non-linear Processes in the X-ray regime
H. Stapelfeldt	Molecular Alignment and Orientation
M. Vrakking	Velocity-map Imaging
R. Moshhammer	COLTRIMS and Multi-coincidences

Working Group I: Dilute Ion Targets

Chairs: H. Pedersen, S. Schippers

Lutz Lammich	Fast Ion Beams
Andreas Wolf	High energy ion beams and cryogenic storage rings
José R. Crespo López-Urrutia	Electron Beam Ion Traps (EBITs)
Reinhold Schuch	Penning Ion Traps
Michael Drewsen	Trapped ion-XFEL interactions
Jean-Marc Bizau	Ion beam-XFEL interactions
Ottmar Jagutzki	Detection of electrons and heavy fragments
Andreas Schwarz	Detection of Photons
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D. Rolles Recent Results from the AMO Beamline at LCLS T

Th. Möller “Aarhus” WG 1 Updated Report

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A. Wolf Results of Soft X-Ray Studies with Atomic and Molecular Ion
Targets at Free Electron Lasers

O. Gessner Exploring New Regimes of X-Ray Multiphoton Processes at
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