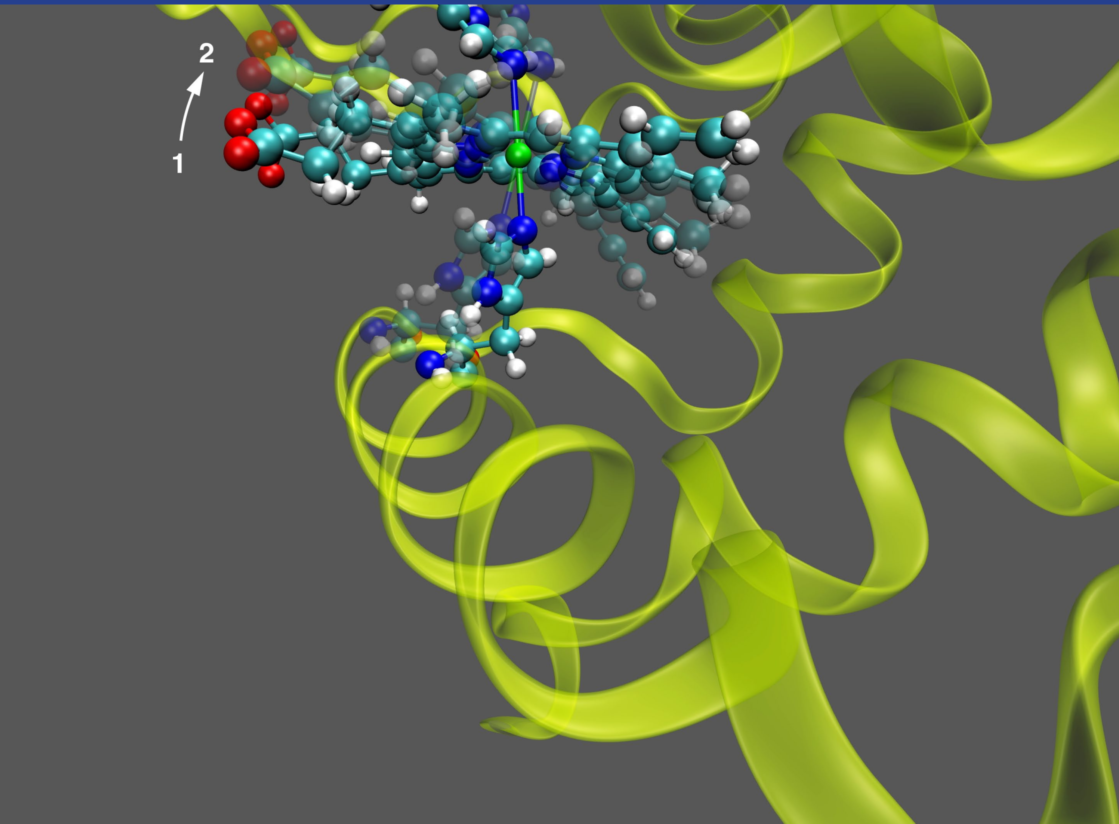
PAUL SCHERRER INSTITUT

SwissFEL X-ray Free Electron Laser

Workshops on Hard X-Ray Instrumentation at the SwissFEL
12.9.11 and 21.11.11
University of Bern



Information for Workshop Participants

Content

Cover figure:
Courtesy of M. Meuwly, University of Basel

1 Motivation

The Paul Scherrer Institute (PSI) is planning the construction of an X-ray Free Electron Laser (SwissFEL) close to the existing PSI facilities in Würenlingen (Figure 1a). The present design foresees the injector, three accelerating sections and two beamlines (Figure 1b).

The hard X-ray beamline ARAMIS (0.1 – 0.7 nm wavelength) will begin commissioning mid 2016, with user operation in 2017 in two experimental areas. A third area will go into operation at a later time, and the soft X-ray beamline ATHOS (0.7 – 7.0 nm wavelength) will come online in 2019.

The design of the building is close to being definitive, and a first draft of the X-ray beam optics for the ARAMIS beamline has been realized. The SwissFEL photonics group requests the input of potential users to implement their requirements into the design of the beamline and the experimental stations, and therefore announces two user workshops on

HARD X-RAY INSTRUMENTATION AT THE SwissFEL

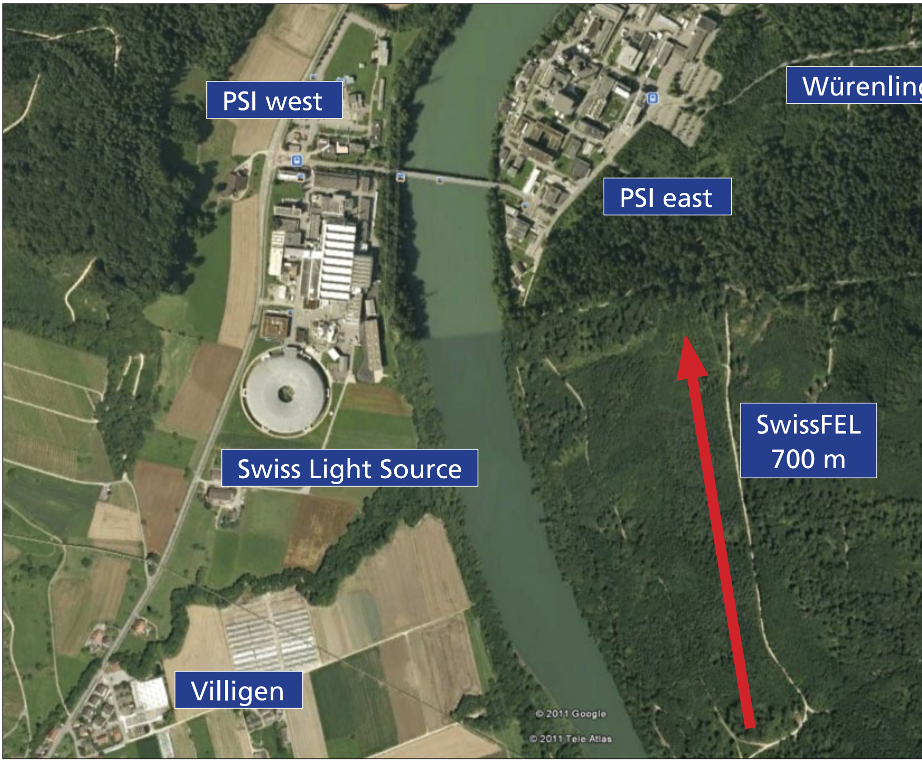
Workshop 1: September 12, 2011:
Spectroscopic experiments
Workshop 2: November 21, 2011:
Scattering and Diffraction experiments

2 Goals of the Workshops

The main goal of the workshop is to assess the interests of the potential SwissFEL users, and to identify their **requirements to the X-ray beam optics and to the experimental infrastructure.** The focus of the workshops discussion will be on the specific needs of the experimental groups and on the necessary pieces of equipment.

In parallel, other important aspects are:

- **Space:** in the planning of the experimental areas, it will be important to reserve sufficient space and to account for the presence of nearby X-ray beam transport pipes.
- **X-ray beam diagnostics:** the beam diagnostics scheme is starting to be planned in detail, and it will be important to know which X-ray beam parameters should be measured, eventually shot by shot, for a given experiment.



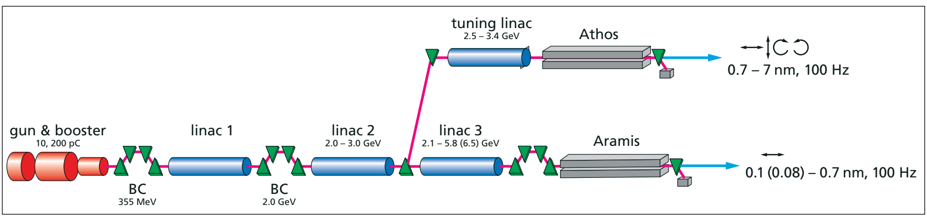


Figure 1. (a) Map of the planned location for the SwissFEL, in the forest close to the present PSI-east facilities. (b) Schematic view of the planned SwissFEL machine, which includes the injector, three accelerator sections and the two X-ray undulators ARAMIS and ATHOS.

3 ARAMIS layout

3.1 X-ray beam parameters at the ARAMIS undulator exit

The ARAMIS undulator will provide X-ray pulses at a repetition rate of 100 Hz with linear horizontal polarization. Estimates of X-ray beam parameters at the ARAMIS undulator exit are given in Table 1.

3.2 General layout

In the present layout (Figure 2), the section of the SwissFEL following the ARAMIS undulator exit is divided into the front end (0 – 45 m), the optics section (45 – 100 m) and the experimental area (100 – 144 m). The last is 6.6 m wide and 44.3 m long, and will be divided into three hutches. The positions of the separating walls have not yet been fixed.

3.3 Preliminary beamline layout

In the optics section, a system of mirrors positioned approximately 50 m from the undulator exit will filter away the gas Bremsstrahlung and deflect the direct X-ray beam towards the different sample locations in the experimental area. In the present concept, the optics covers the photon energy range 2 – 12 (15) keV.

The direct beam will be deflected by 4 – 7 mrad, resulting in the potential sample position areas shown in Figure 2a. Three

Parameter	Unit	λ = 0.1 nm	λ = 0.7 nm
Photon energy	keV	12.39	1.770
Pulse energy	mJ	0.0724	0.143
Photons per pulse	#ph/pulse	$3.6 \cdot 10^{10}$	$5.1 \cdot 10^{11}$
Effective peak power	GW	2.2	3.3
Pulse length, RMS	fs	13.1	15.7
Beam radius, RMS	µm	24.5	43.0
Beam divergence, RMS	µrad	1.5	5.3
Bandwidth, RMS	%	0.044	0.096
Peak spectral flux	#ph/pulse/0.1%bw	$8.2 \cdot 10^{10}$	$5.3 \cdot 10^{11}$
Peak spectral brightness	#ph/pulse/µm2mrad2/0.1%bw	$7.4 \cdot 10^{31}$	$1.0 \cdot 10^{31}$
Average brightness per pulse	#ph/pulse/µm2mrad2/0.1%bw	$2.4 \cdot 10^{18}$	$4.1 \cdot 10^{17}$
Weight of first coherent mode	%	82	

Table 1. X-ray beam parameters at the ARAMIS undulator exit, extracted from numerical simulations at different photon wavelengths. The electron bunch charge is 200 pC.

possible beam usages are foreseen: freely propagating beam; 1:1 focusing scheme with 30 µm spot size; beam focused down to a few hundred nanometers (“microfocus”). For the last, preliminary calculations of the focusing system in Kirkpatrick-Baez geometry have been performed, and the results concerning the working distance and the angular beam acceptance are given in Figure 3.

Included in the present design is also the possibility, shown in Figure 2b, of inserting large offset monochromators (LOMs) which would, in the energy range 4 – 12 keV, reduce the bandwidth to 10^{-4}, and at the same time

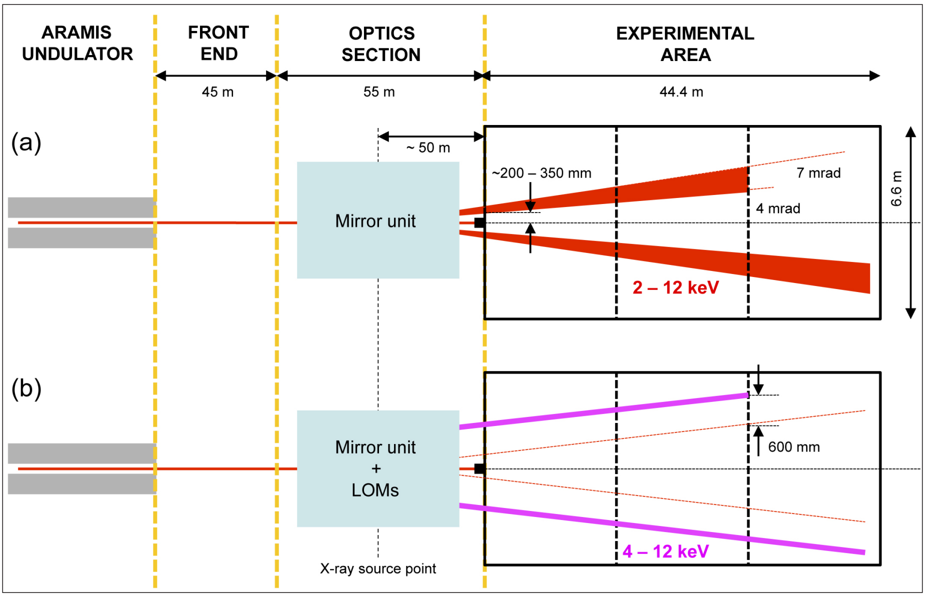


Figure 2. Preliminary layout of the ARAMIS beamline. The space following the exit of the ARAMIS undulator is divided into front end, optics section and experimental area. Note that within the experimental area building, the positions of the walls separating the three hutches have not yet been fixed. (a) is the arrangement without monochromators; the raw beam will be deflected laterally to either side by 4 – 7 mrad. The areas drawn in red show the possible sample positions. (b) corresponds to the arrangement with large offset monochromators (LOMs) inserted after the deflecting mirrors. The monochromated beam, drawn in magenta, will be offset laterally by typically 600 mm with respect to the beam in (a).

laterally shift the potential sample positions by 600 mm.

3.4 End station equipment

Based on the information collected at the workshops, a list of standard instrumentation (in particular sample chambers and detectors) to be provided by the SwissFEL will be established. Special instrumentation, not included in such list, will then be the responsibility of the user.

3.5 Pump laser

It is foreseen to make synchronized high-power laser light for sample pumping available in each hutch. The source will be a Ti:Sapph laser working at 800 nm with 100 Hz repetition rate, providing 20 fs pulses of 20 mJ of energy. Different wavelengths in the visible and perhaps in the UV will be obtained by frequency up-conversion, while infrared and THz wavelength may be generated by parametric down-conversion. In the CEPS mode, few-cycle pulses of 5 – 6 fs duration will also be available.

3.6 Beam diagnostics

At the present stage of planning, a preliminary X-ray beam diagnostics concept has been developed. Table 2 summarizes the parameters that are planned to be measured.

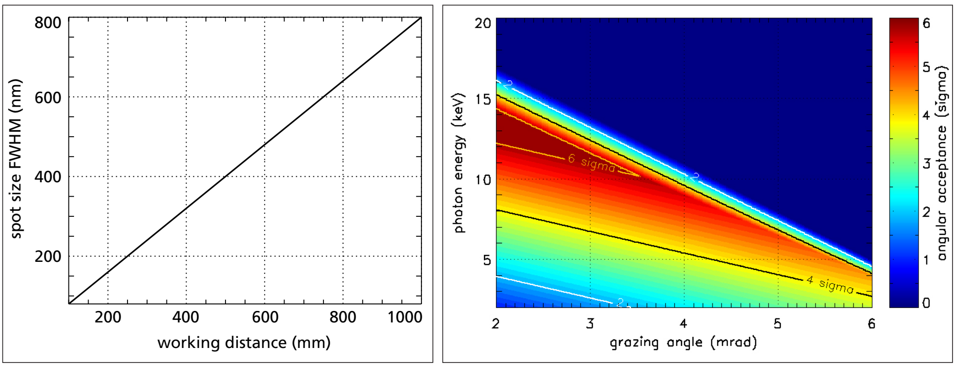


Figure 3. Beam parameters after two focusing mirrors in Kirkpatrick-Baez geometry. (left) Minimum focus spot size as a function of the distance between the sample and the end of the KB focusing system. (right) Contour plot displaying the beam acceptance as a function of the photon energy and the grazing incidence angle of the KB mirrors (linear approximation).

4 Expected input from the workshop participants

Besides a general description of typical experiments, we strongly encourage the workshop participants to provide us with the **requirements on the X-ray beam parameters** at the experimental station, listed in Table 3, and with a **sketch of the experimental setups** which indicate the key equipment pieces, as shown in the example in Figure 4. In particular, this should provide answers to the following questions of fundamental importance:

- Is a **monochromator** necessary?
- Is **photon energy scanning** required? If yes: which range/rate/step?
- Is focussing required? If yes: are **changes in the focus size** required? If yes: which range/rate/step?
- If a **sample chamber** is necessary, what size would it have, and which parameters have to be controlled?
- What kind of **sample holder/injector** will be necessary?
- What kind of **detectors** are required? And what would have their size and their position with respect to the sample be?

We also encourage the participants to answer additional questions regarding the implementation of the proposed experiments:

- Is a synchronized source of pump radiation required, and if yes, of which type (wavelength, pulse length, pulse energy)? If not available on site at the SwissFEL, how much space will it occupy?
- Is there any other bulky equipment necessary?
- Which additional beam parameters must be monitored on average or shot by shot?

Parameter	Resolution	Range	Single shot
Intensity	10^{-3}	0 – 10^{12} ph	yes
Beam position	1 µm	± 100 µm	yes
Beam width	5 µm	0 – 300 µm	no
Pulse duration	5 fs	0 – 200 fs	no
Arrival time, coarse	200 fs	± 500 ps	no
Arrival time, fine	2 fs	± 500 fs	yes
Mean energy	10^{-3}		yes
Energy spectral width	10^{-3}		no
Longitudinal source point	1 m	± 20 m	no

Table 2. Measured X-ray beam parameters, according to the present beam diagnostics concept.

- Is there a preference for one of the three experimental areas?
- Are there particular requirements on auxiliary facilities (storage / setup / ...)?

We expect that each experiment has particular requirements.

Parameter		Unit	Requirement	Motivation / Remarks
Beam parameters				
Energy		keV	6 – 12	Diffraction at biomolecules
	stability		0.1 %	
Bandwidth		%	0.1	0.5 nm resolution at 11.2 keV
	stability		< ±10 % bw	Stable incoming beam wished
Beam position	stability		< 1 µm	
Beam size		µm	< 0.5 (microfocus)	< 40 x 40 unit cells illuminated
Photons per pulse		#ph	$> 10^{10}$	Maximal flux wished
	stability		< ±10 %	Stable incoming beam wished
Pulse length		fs	< 20 fs	Diffract and destroy regime required
	stability		---	Pulse length should remain < 20 fs
Pulse arrival time	stability	fs	---	Not an issue
Beam parameter changes during experiment				
Energy	range/step	eV	---	Energy adjusted only during setup
	rate	eV/min	---	
Beam size (microfocus only)	range/step	µm	---	Focus size adjusted only during setup
	rate	µm/min	---	
Pulse length	range/step		---	Pulse length adjusted only during setup
	rate		---	
Beam geometry				
Beam slope	max. tolerable	µrad	---	Not an issue
Working distance	min. required	mm	100	Allow sample rotations and translations
Other				
Transverse coherence			full	Required for coherent diffraction at extended object

Table 3. Example of table of "at the sample X-ray beam parameters", expected to be completed by the workshop participants for each suggested experiment (entries in red). The given parameters are specific for an example experiment involving coherent diffraction on 2D membrane protein crystals.

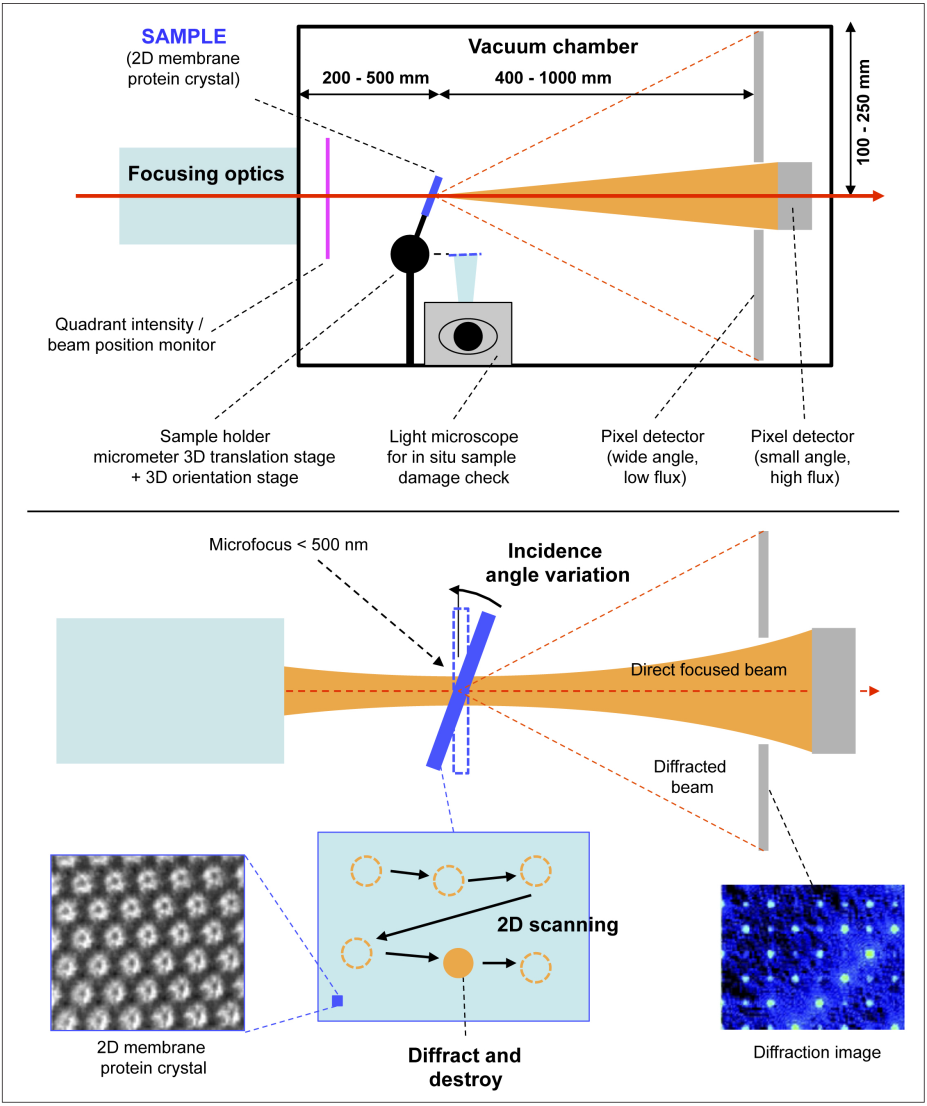


Figure 4. Example of a sketch of an experimental setup, expected from the workshop participants for each suggested experiment. The experiment shown is based on coherent diffraction by 2D membrane protein crystals.

5 Organization of the Workshops

The workshops will be held at the University of Bern, and will be scheduled to allow single day train travel from all of Switzerland. They will be based on poster contributions from potential national and international user groups. Following overview talks by the SwissFEL team, short oral presentations will be made of each poster. Several posters are welcome from a single research team. The workshop will conclude with an open discussion of controversial issues.

For documentation purposes, the posters will be collected and distributed electronically prior to each workshop. A large-size copy will be printed directly at PSI, and transported to the workshop. Young researchers, including PhD students and postdocs, are particularly encouraged to submit innovative and unconventional posters. The schedule is as follows:

Deadline for workshop registration and poster submission:

Workshop 1: September 1, 2011
Workshop 2: November 7, 2011

Distribution of collected posters:

Workshop 1: September 7, 2011
Workshop 2: November 14, 2011

Registration:
Details are available at the SwissFEL homepage **http://www.psi.ch/swissfel/** or from **silvia.bacher@psi.ch**

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