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## Progress in Physics (58)

### The SwissFEL X-ray Laser

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*Part of the SwissFEL accelerator complex: accelerating structures for ARAMIS (right) and extraction towards ATHOS (left). More on p. 7.*

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## The SwissFEL X-ray Laser

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### Introduction

X-ray free electron lasers have become in the last years routinely available for researchers worldwide – a dream has finally come true 50 years after the invention of the optical laser and 40 years after the first theoretical work on FELs. In contrast to optical lasers, free electron lasers employ relativistic electron beams to amplify light, and the FEL concept works for the entire spectral range from the far infrared (IR) to hard X-rays, generating coherent, ultra-short pulses with extremely high peak power. FELs are bold examples of disruptive technologies: revolutionary instruments that expand the scope of what can be achieved in a field of science.

Several laboratories around the world are currently operating, constructing and developing Free Electron Lasers (FELs), currently the world's brightest sources of UV and X-ray radiation. In the hard X-ray regime, three facilities are in operation: LCLS (USA), SACLA (Japan) and PAL-XFEL (Korea) while two others have entered the commissioning phase: EuXFEL (Germany) and SwissFEL (Switzerland). In the ultraviolett and soft x-ray range FERMI (Italy) and FLASH (Germany) are running successfully since many years.

A list of XFEL facilities worldwide that provide hard x-ray radiation is given in the following Table 1. The most relevant parameters in the Self Amplified Spontaneous Emission (SASE) operation mode are presented. The values are taken from the webpages describing the instruments [1, 2, 3, 4].

The research applications of the ultra-short and intense pulses produced by these sources range from condensed matter and materials research, to femto-chemistry, molecular biology, atomic spectroscopy, and many more.

The Paul Scherrer Institute has built during the last four years the SwissFEL whose start of commissioning was officially inaugurated in December of this year, and which will begin user operation in the fall of 2017 [5, 6]. The facility consists of a high-brightness electron gun, a 5.8 GeV linear accelerator, permanent magnetic undulators and a variety of photon beamlines to several experimental stations.

The SwissFEL (Fig. 1) uses a low-emittance electron beam in conjunction with short-period in-vacuum undulators to generate hard X-rays at the relatively low electron energy of 5.8 GeV. These specifications can be realized with a relatively short facility, which is 740 m long. The concept foresees two undulator lines for different wavelength regions. The first beamline, ***ARAMIS***, is designed for wavelengths between 0.1 and 0.7 nm. The second undulator beam line, ***ATHOS***, is designed for wavelengths in the range 0.6 nm to 7 nm, and will offer the option of circularly-polarized radiation. It will be built in a second phase in the years 2017 - 2020. By virtue of the acceleration of double electron bunches and fast-switching magnets, X-ray pulses will be simultaneously available at both ARAMIS and ATHOS with a 100 Hz repetition rate.

| FEL, Institution | Location | Start of operation | Rep. rate (Hz) | Photon energy (keV) | Pulse length (fs) (FWHM) | Pulse energy (mJ) |
|---|---|---|---|---|---|---|
| LCLS, SLAC | Palo Alto, USA | 2009 | 120 | 4.0 – 10.0 | 10 - 300 | 0.2 - 3 |
| SACLA, RIKEN | Harima, J | 2012 | 30 (60) | 4.9 – 15.0 | < 10 | < 0.3 |
| PAL_FEL | Pohang, KOR | 2016 | 60 | 5.0 - 12.0 | < 100 | < 2 |
| SwissFEL, PSI | Würenlingen, CH | 2017 | 100 | 2.0 – 15.0 | 5 - 50 | 0.2 - 1.4 |
| EuXFEL | Hamburg, D | 2017 | 10 x 2700 | 3.0 – 25.0 | 2 - 100 | 0.06 - 2 |

*Table 1. Worldwide hard X-Ray facilities*

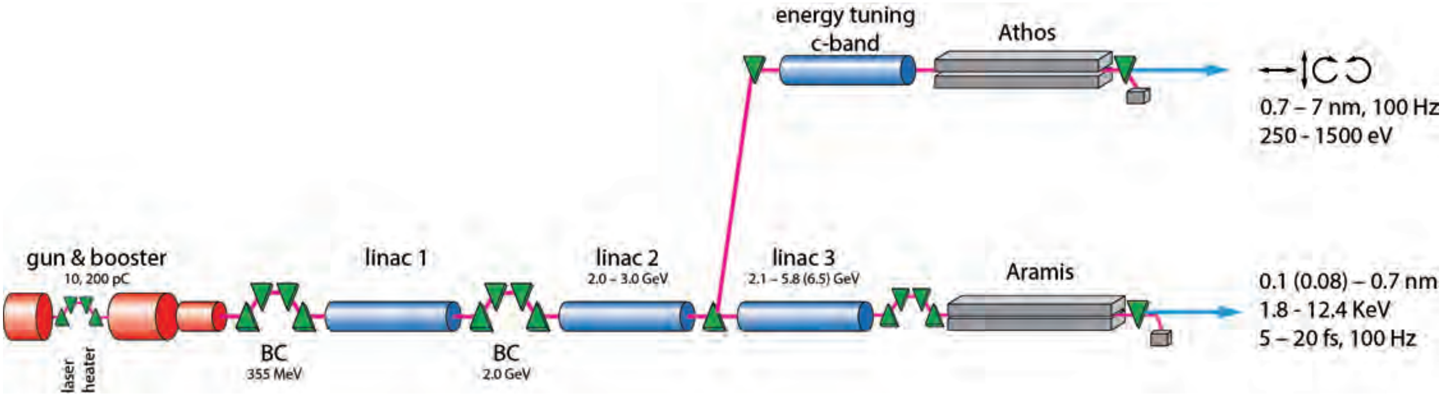

*Fig. 1. Schematic plan of the SwissFEL facility, including the hard and soft X-ray beamlines ARAMIS and ATHOS (undulators in grey).*

The hard X-ray beamline ARAMIS [7] is designed for photon energies in the range 2.0 – 13.0 keV. With a possible future accelerator upgrade, the upper limit may be shifted up to 15 keV. In the standard SASE operation mode, the duration of the pulses will be 5 - 50 fs full width at half maximum (FWHM), the relative bandwidth will be of the order of $2.0 \cdot 10^{-3}$, and the pulse energy for the long pulse mode is predicted to be around 1.4 mJ.

A system of offset mirrors directs the x-ray beam along three different beamline branches, to either one of the three subsequent experimental hutches downstream. The first two hutches will host the experimental stations ESA [8] and ESB [9], which will host pilot experiments by fall 2017. A third branch with an additional station named ESC is currently in the conception phase and will be realized in the years 2019 - 2020. Each experimental station will be served by an optical pump-laser system to perform time-resolved experiments.

Specialties foreseen for the SwissFEL facility include: nearly transform-limited "self-seeded" pulses, a mode with up to 7% FWHM "broad-bandwidth" wavelength range, a pump-probe time resolution of approximately 10 fs FWHM, optics, instrumentation and detectors for the strategically interesting photon energy range 2-4 keV and in-house developed 2D X-ray detectors with single-photon sensitivity, large dynamic range and virtually zero dark noise.

## Science opportunities

### *Photochemistry and Biology*

*Conceptual design*

Experimental Station A (ESA) is envisioned as a pump-probe X-ray spectroscopy station, for investigating processes in biology and chemistry that can be triggered with light. ESA will have three significant advantages, which it plans to exploit:

1. SwissFEL will generate X-rays in the range from 2-5 keV, which is a photon energy range that is difficult to access at the facilities commonly used by the XAS/XES community. This energy range includes elemental absorption edges of P, Cl, S, K, and Ca which are relevant to biology, and of Ti, which is relevant to both sustainable energy sources and photocatalysis.
2. SwissFEL will have the ability to tune the photon energy easily courtesy of the variable-gap undulator design, which greatly facilitates X-ray spectroscopy measurements.
3. There is significant expertise in Switzerland in time-resolved X-ray absorption and emission spectroscopy, on both solid and liquid samples, providing a strong local base of expert users.

### *Pump and Probe in Condensed Matter*

*Conceptual design*

The proposed station ESB dedicated to perform pump and probe experiments in condensed matter combines time-resolved laser spectroscopic methods and X-ray scattering techniques to study the dynamics of cooperative interactions in crystalline materials that exhibit long-range electronic and magnetic order. Important representatives are the strongly correlated electron systems or "quantum materials" that exhibit competition between lattice, charge, orbital and spin degrees of freedom. From the correlations of the atomic, electronic and magnetic constituents, new phases or states of condensed matter emerge. Recent examples include materials with high temperature superconductivity, colossal magnetoresistance, metal-to-insulator transition, electron fractionalization and novel quantum-critical states. Multiferroics, materials combining several functional properties, hold promise for future device applications. Characterization and control of such materials - especially when they are not in strict thermodynamic equilibrium - is ideally done in the time domain where the coupled excitations can be distinguished on account of their different response and relaxation times. Photon-in/photon-out scattering allows the direct correlation of the electronic, magnetic and structural dynamics.

## Opportunities in structure determination

### *Using a non-monochromatic microbeam for Serial Snapshot Crystallography*

The SwissFEL facility will provide a broad-band pass mode with an energy bandwidth of about 4%, which has important implications for structural studies. By exposing a small crystallite (from nano- to a few micrometers in size) to a single ultrafast pulse, a diffraction pattern can be obtained before the crystal is damaged. If such single-pulse diffraction patterns, collected sequentially on many randomly oriented crystallites, are combined, it is possible to determine the structure of the material accurately [10]. Performing such an experiment with a strictly monochromatic beam has a serious drawback: only a single position of the Ewald sphere is accessed in each pattern and, because reflections have a finite width, the diffraction condition is not satisfied completely for any of the reflections recorded. By using the 4% energy range of the SwissFEL beam, a new option for structural studies of crystalline materials may become possible. The use of such an 'extra pink' beam in a diffraction experiment with stationary crystallites should not only increase the number of reflection intensities that can be collected in a single shot, but also overcome the problem of 'partial reflection' measurement that is inherent to the monochromatic experiment. In a recent proof-of-concept study, a new approach, inspired by the Laue single-crystal (micro)diffraction technique was examined [11].

### *Protein Crystallography Possibilities*

The requirements for jet-based protein crystallography experiments have been taken into account in the design of the ESA experimental chamber with a suitable photon energy range, beam size and sample atmosphere. The chamber is designed to host injectors delivering crystals with liquid or viscous jets.

While the original concept of SwissFEL did not include instrumentation for fixed-target protein crystallography, the promising results from fixed-target experiments at running facilities reported in the last years have triggered the initiative to offer the fixed-target approach as a standard method at SwissFEL. Several possibilities have been considered, but it soon became clear that beam parameters and the infrastructure foreseen at the ESB station are best suited. In March 2015 the ESB-MX project [12] started with the goal of building a fully dedicated instrument to be first installed at the ESB station for measurement campaigns of 5 – 6 days. Because it is easily mountable and flexible, the instrument is also suitable for operation at the future experimental station ESC. Fixed-target protein crystallography has been thoroughly developed during the last decades at synchrotron X-ray sources, and the applications to XFELs require their adaptation of sample handling and data collection methods.

## Opportunities in the soft x-ray range: ATHOS extension

In the following years 2017 – 2020 the second undulator line of SwissFEL, ATHOS [13], will be constructed. The photon energy region covered by ATHOS extends from 240 eV to 2000 eV. This region covers absorption edges for the light elements oxygen, carbon and nitrogen, that play an important role in surface catalysis, as well as those of the transition metals manganese, iron, cobalt, nickel and copper, which are prominent components in magnetic and correlated electron materials. The opportunities for scientific research opened up by ATHOS well reflect important challenges to be faced by industrial societies in the near future. ATHOS is an important complement to ARAMIS both in terms of measurement technology and of scientific goals. The scientific opportunities have been discussed with Swiss research groups and have been compiled in a scientific case around the areas: studies of photochemical transformations on the molecular level, the role of complexity in materials properties, and non-linear X-ray interactions that unravel coherent electronic excitations in matter.

Several proposals have been made to improve the properties of XFEL pulses towards the femtosecond regime, while keeping a high radiation power level as in facilities in operation [14]. In a recent study [15], a new method has been presented in order to generate short pulses with a high power in a very efficient and flexible way. In this method practically all the electrons in a bunch can contribute to the XFEL process and the scheme can be used to achieve either a minimum pulse length or the maximum pulse energy. The authors based their scheme on superradiance and the use of a transversely tilted beam: by suitably compensating the trajectory and delaying the electron beam between selected undulator sections, all the electrons in a bunch can be used to enhance the pulse in the superradiance regime.

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*The undulators of the ARAMIS beamline.*