Coherent science at the SwissFEL x-ray laser

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New Journal of Physics 12 (2010) 035012 (16pp)
Received 14 October 2009
Published 31 March 2010
Online at http://www.njp.org/
doi:10.1088/1367-2630/12/3/035012

Abstract. The Paul Scherrer Institute is planning the construction of a hard-x-ray free-electron laser, the SwissFEL, by 2016, which will produce intense, ultrashort pulses of transversely coherent radiation in the wavelength range 0.1–7 nm, with future extensions to cover the range 0.08–30 nm. Special design considerations include (a) a compact construction, compatible with the status of a national facility, (b) a uniform 100 Hz repetition rate, well suited to sample manipulations and detector readout, (c) flexible wavelength tuning by the electron beam energy and undulator gaps, (d) soft x-rays at approximately 1 nm wavelength, with circular polarization and Fourier-transform-limited pulses, (e) hard x-rays of pulse duration 5–20 fs and (f) an independent source of high-energy, half-cycle terahertz pump pulses. The science case for the Swiss FEL project, which emphasizes the dynamics of condensed matter systems and the damage-free imaging of nanostructures, includes novel considerations that make optimal use of these features.

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1. Introduction

The SwissFEL will be a compact and economical hard-x-ray free-electron laser (XFEL) source in a national facility. It will be a significant extension of the capabilities of the existing spallation neutron (SINQ) and synchrotron radiation (SLS) sources at the Paul Scherrer Institute (PSI). Special features of the SwissFEL include the following.

- Minimization of the electron beam energy required for producing hard x-rays, via a low-emittance electron beam and short-period undulators.
- A constant 100 Hz repetition rate, simultaneously delivered to two experimental stations, to permit compatibility with 1D and 2D imaging detector readout, wavelength tuning, and sample and delay adjustments.
- At $\lambda \approx 1$ nm: gap tuning of the wavelength, variable polarization and transform-limited pulses.
- At $\lambda \approx 0.1$ nm: 5–20 fs pulse duration.
- An independent source of THz pump pulses.

The scientific case for the SwissFEL project [1] emphasizes studies of ultrafast condensed matter dynamics and the damage-free coherent imaging of nanostructures. Following the priorities of the prospective user community, the case includes the following themes.

- Ultrafast magnetization dynamics on the nanoscale
- Catalysis and solution chemistry
- Coherent diffraction by nanostructures
- Ultrafast biochemistry
- Time-resolved spectroscopy of correlated electron materials.
2. The SwissFEL machine

The SwissFEL machine (see figure 1) consists of an electron gun and booster, a three-section, 5.8 GeV linear accelerator with two bunch-compressors, and two undulator beamlines, Athos and Aramis. The soft-x-ray line, Athos, is seeded by the d’Artagnan undulator. An independent 30 MeV electron accelerator produces energetic, half-cycle pulses of terahertz radiation for non-ionizing pump signals.

2.1. The injector

The baseline electron source relies on an RF gun photo-injector: a photo-cathode placed in a high-field RF cavity is illuminated with a short-pulse laser. The timing of the laser pulses is synchronized such that photo-electrons are emitted when the RF field reaches its optimum value. For the past two decades, RF gun technology has been the subject of intense R&D worldwide; the present state-of-the-art allows the production of electron pulses of 200 pC with a normalized emittance below 0.4 mm mrad [2]. An improved FEL performance could be achieved with an injector which provides an even smaller emittance. Therefore, PSI is also investigating an alternative electron gun design, in which the photo-cathode forms the positive electrode of a pulsed diode, with a high extraction field [3]. In addition, a concept is being developed where the cathode is a field-emitter array [4], structured on the nanometer length scale (see figure 2). Such an arrangement should allow the emission of electrons with very high current density and very small momentum spread, thus providing an electron beam with very small emittance.

2.2. The linear accelerator

The SwissFEL linear accelerator (linac) must fulfill two functions: acceleration of the electron pulses from the injector to the nominal energy of the FEL, and time compression of the electron pulses from 5 ps to <25 fs (rms). Requirements of compactness and economy dictate the use of a normal-conducting, pulsed RF system for acceleration, with high accelerating fields. Use of normal-conducting accelerator technology instead of a superconducting RF system implies a considerably lower average beam current and, as a consequence, a reduced average photon flux to the experiments. This reduction is partly compensated for a uniform time-distribution of pulses, compared to the pulse trains from a pulsed superconducting linac, such as the European XFEL. Such a time structure will be a major advantage for experiments with complex detectors and/or requiring mechanical adjustments between pulses.

In order to produce the peak current of several kA required for FEL operation, the initial electron pulses, with a duration of several ps, must be compressed longitudinally to a final length
of a few tens of fs. For this purpose, two magnetic-chicane bunch compressors are located in the linac, at the 450 MeV and 2.1 GeV energy positions. The pulse is accelerated in the linac slightly off the crest of the RF wave, introducing a time-energy chirp, and the energy dependence of the electron path-length in the chicane leads to time compression.

During each RF pulse in the linac, the SwissFEL design foresees the acceleration of two electron pulses, one for each of the undulator beamlines—thus allowing the simultaneous operation of two experimental stations at the 100 Hz repetition rate. Electron extraction will occur at the end of section 2 and section 3 of the linac (see figure 1). The electron energy in linac section 3 will be varied, for wavelength tuning of the hard-x-ray line.

The nominal maximum electron energy of the SwissFEL linac is 5.8 GeV, which, when injected into the Aramis undulator, will produce saturated FEL radiation at 0.1 nm wavelength (12.4 keV photon energy). Among the advanced design options under consideration is an increase to 6.5 GeV, which would allow fundamental FEL operation down to 0.08 nm wavelength. Regarding the charge of the accelerated electron pulses, two modes of operation are foreseen at the SwissFEL: a high-charge mode (200 pC) for maximum flux and a low-charge mode (10 pC) for very short (5 fs) hard and soft x-ray pulses.

A special configuration of the bunch compressor will allow for overcompression of the bunch, leading to an inverted energy chirp, which is further enhanced by the wake field in the following linac section. With a chirp of 0.6%, the output of the FEL will have a relative bandwidth of 1.2%, which is very attractive for use in Laue crystallography and energy-dispersive spectroscopy.

2.3. Undulators

2.3.1. Aramis and Athos. Transversely coherent x-ray pulses will be generated in two undulator beamlines (see figure 1) [5]: the hard-x-ray line, Aramis, operating in the self-amplifying spontaneous emission (SASE) mode, and the soft-x-ray line, Athos, which will be

Figure 2. A prototype of the PSI-produced, double-gate field-emitter array [4]. The voltage on the first gate allows adjustment of the extraction field on the metal tips, and the second gate controls the collimation of individual extracted beamlets.
Figure 3. The novel symmetric undulator support (brown), possibly fabricated of cast mineral, shown here with the APPLE II *Athos* undulator.

seeded to produce transform-limited pulses. Both undulators will have variable magnetic gaps, which will permit selected modules to effectively be removed and will allow for module-specific tapering, to account for the change in resonant condition due to energy loss.

*Aramis* is a planar in-vacuum undulator with a period $\lambda_u = 15$ mm and a minimum gap of 4 mm, producing a peak field strength $B_0 = 1$ T. Very recent developments in permanent magnet technology allow the use of highly coercive NdFeB material at room temperature, thus avoiding a costly liquid nitrogen cooling system. A total of 12 modules, each 4 m long, must be aligned within tight tolerances to reach saturation in the SASE mode. The resonant wavelength of undulator radiation is given by

$$\lambda = \left(1 + \frac{K^2}{2}\right) \frac{\lambda_u}{2\gamma^2},$$

where the undulator $K$-value is $K = eB_0\lambda_u/2\pi mc$. The low $K$-value of *Aramis* (0.9–1.4) limits its tuning range, and hence the wavelength will be varied by changing the electron energy of linac section 3; only small adjustments in the resonant condition will be made with gap tuning.

The *Athos* undulator has a 40 mm period and a minimum magnetic gap of 6.5 mm, allowing the permanent magnet arrays to be situated outside of the vacuum chamber. The modules will have the so-called APPLE II configuration, which allows for full control of the FEL polarization and wavelength by adjusting the mechanical position of the magnet arrays—a feature of particular importance for studies of magnetization dynamics. Movements with micron accuracy must be performed in the presence of strong magnetic forces, making the mechanical design particularly challenging. Six modules, 4 m each, are needed to reach seeded saturation.

Novel developments are being undertaken by PSI for the support structures of the *Aramis* and *Athos* undulator modules (see figure 3). The symmetric ‘O-form’ of the support, which surrounds the undulator magnet array, can be much less massive than the conventional asymmetric ‘C-form’, and strategically placed openings provide access from both sides. Fabrication out of cast mineral material is being considered, for reasons of cost and weight.
Figure 4. An echo-enabled seeding simulation of the longitudinal phase space over one seed wavelength, for electron pulses injected into the d’Artagnan undulator. The principal microbunching, at 0.016 fs, corresponds to the 50th harmonic of the titanium-sapphire seed pulse. Energy spreading has been eliminated for clarity.

2.3.2. Seeding. In order to improve the longitudinal coherence and to produce approximately Fourier-transform-limited pulses down to 1 nm wavelength, seeding the Athos FEL using an optical laser system is anticipated. The most promising seeding scheme for these x-ray wavelengths is believed to be the echo-enabled approach [6, 7]. In our simulation (see figure 4), 3.1 GeV electron bunches are seeded with third-harmonic Ti–Sa light ($\lambda = 265$ nm) in a resonant undulator–modulator, compressed in a magnetic chicane, seeded again in another resonant structure, and finally compressed again. The resulting bunches then pass the d’Artagnan undulator, resonant at the 50th harmonic of the seed laser ($= 5$ nm), and are finally injected into Athos, where the fifth harmonic ($\lambda = 1$ nm) is resonantly amplified.

The ambitious goal at the SwissFEL is to have 3 GW photon pulses at 1.2 keV, with variable polarization, a duration of 10 fs and a bandwidth of 2 eV. Besides improving the coherence properties in lensless imaging experiments, such pulses could allow novel soft x-ray heterodyne and frequency-resolved optical gating (FROG) spectroscopy techniques to be realized in the time domain [8]. Using the d’Artagnan undulator without Athos, at 2.1 GeV electron energy, will in addition extend the longest wavelength of the SwissFEL to approximately 30 nm (40 eV), which is of interest for time-resolved core-level photoemission experiments and high-resolution absorption spectroscopy in low-Z materials.

2.4. X-ray beamlines

As discussed above, the basic design of the SwissFEL facility includes a hard (Aramis: 0.1–0.7 nm) and a soft (Athos: 0.7–7 nm) beamline. The experimental hall (see figure 5) will accommodate three experimental areas, approximately $15 \times 7$ m$^2$, per beamline. Also included
in the hall is a clean room for the IR and optical pump lasers and a shielded bunker for the electron accelerator-based terahertz pump source (see below). The experimental techniques foreseen for the six experimental areas are summarized in table 1.

### 2.5. Half-cycle THz pump source

Energetic half-cycle pump pulses of terahertz radiation, synchronized to the XFEL emission, hold great promise for novel classes of pump–probe experiments. Since a 1 THz photon carries the energy $4 \text{ meV} = k_B \times 48 \text{ K}$, compared to $1.6 \text{ eV} = k_B \times 18 000 \text{ K}$ for an optical laser at $\lambda = 800 \text{ nm}$, a THz pulse is non-ionizing and can be thought of as transient magnetic and electric fields. The intensity of an electromagnetic pulse, in terms of the peak fields $B_0$ and $E_0$, is given by

$$ I = \frac{B_0^2 c}{2 \mu_0} = \frac{\varepsilon_0 E_0^2 c}{2}. $$
Figure 6. (a) Production of THz radiation from a pulsed electron beam in a bending magnet. The single-particle spectrum (black) cuts off near $\omega_c$, the critical frequency for synchrotron radiation, which is proportional to the cube of the electron energy. In addition, sufficiently short electron pulses radiate coherently, up to a cutoff given by the inverse pulse duration and with a power proportional to the square of the pulse charge. (b) A schematic of the THz pump source planned for the SwissFEL facility. With a compressed electron pulse length of 0.3 ps, 17 mJ are radiated per pulse, of which 0.12 mJ lie above 1 THz in frequency [11]. Studies are underway to produce, by increased compression (requiring the use of lower charge), an emission spectrum that extends up to several THz.

A 1 mJ pulse of 1 ps duration, focused to 1 mm$^2$, produces the peak field strengths $B_0 = 3$ T and $E_0 = 9 \times 10^8$ V m$^{-1}$. This magnetic field pulse is 300 times stronger and 1000 times faster than that produced by a laser-switched strip-line and is hence well suited for initiating ultrafast magnetic phenomena. The electric field is comparable to that exerted on an atom adsorbed on a surface by a scanning tunneling microscope tip [9], and offers the possibility of controlling chemical reactions via the dynamic Stark effect [10].

Since the THz pump pulse must precede the XFEL pulse by a variable delay up to approximately 1 ns, it cannot be generated in the XFEL itself. The SwissFEL design therefore foresees the emission of coherent terahertz radiation by an independent electron accelerator (see figure 6) [11], hence allowing for an arbitrary choice of time delay.
Table 2. Comparison of XFEL projects.

| Project          | Length (m) | Max. electron energy (GeV) | $\lambda_{\text{min}}$ (nm) | Peak brightness (at $\lambda_{\text{min}}$) | Machine pulse structure |
|------------------|------------|----------------------------|-----------------------------|-----------------------------------|------------------------|
| LCLS (US)        | 1500       | 13.6                       | 0.15                        | $1 \times 10^{33}$ ph s$^{-1}$ mm$^{-2}$ mm$^{-2}$ mrad$^{-2}$ (0.1%bw)$^{-1}$ | 120 Hz                |
| SCSS (Japan)     | 1000       | 8                          | 0.1                         | $0.5 \times 10^{33}$ ph s$^{-1}$ mm$^{-2}$ mm$^{-2}$ mrad$^{-2}$ (0.1%bw)$^{-1}$ | 60 Hz                  |
| Europ. XFEL (Germany) | 3100  | 17.5                       | 0.1                         | $5 \times 10^{33}$ ph s$^{-1}$ mm$^{-2}$ mm$^{-2}$ mrad$^{-2}$ (0.1%bw)$^{-1}$ | 3250 micropulses       |
| SwissFEL (Switzerland) | 700    | 5.8                        | 0.1                         | $0.5 \times 10^{33}$ ph s$^{-1}$ mm$^{-2}$ mm$^{-2}$ mrad$^{-2}$ (0.1%bw)$^{-1}$ | $\times 10$ Hz         |

2.6. X-ray detectors

One- and two-dimensional array detectors are required in order to collect as much data as possible during a single XFEL shot. The Paul Scherrer Institute is a world leader in developing array detectors for hard x-rays. The MYTHEN detector [12], originally developed for powder diffraction, is a 1D micro-strip detector with strip separation as small as 10 µm. The PILATUS detector [13], a 2D area detector with up to 6 million $170 \times 170$ µm$^2$ pixels, is the preferred choice today for synchrotron-based protein crystallography and coherent diffraction. Both of these PSI developments provide single-photon counting, with basically zero dark noise, and frame rates in excess of 100 Hz. They will, however, be overwhelmed by the large number of simultaneous counts from an XFEL pulse, and hence PSI is participating in the development of analog 1D and 2D devices with variable gain, but which still have single-photon sensitivity.

2.7. Comparison with other XFEL projects

Although it is not the purpose of this paper to review the status of the various other XFEL projects worldwide, an approximate comparison can be made from numbers obtained from the literature [14]–[16] (see table 2). For reference, the average brightness from a U19 undulator at $\lambda = 0.1$ nm at the Swiss Light Source is approximately $1 \times 10^{19}$ ph s$^{-1}$ mm$^{-2}$ mm$^{-2}$ mrad$^{-2}$ (0.1%bw)$^{-1}$. The principal differences between the European XFEL and the SwissFEL projects are (a) the higher peak brightness and (b) the large number of micropulses per macropulse at the European XFEL. These are a result of (a) the higher electron energy (and hence longer facility length) of the European machine and (b) the fact that the Swiss machine is based on normal-conducting accelerator technology, while the European XFEL uses superconducting RF cavities. Both of these features contribute to a much higher cost for the European XFEL, and they determine to a large degree the types of experiments that are best suited to each facility. Whereas the European XFEL, with its extreme peak brightness and high frequency of micropulses, is well suited to the study of highly dilute samples, such as plasmas and atomic and molecular beams, the moderate, uniform pulse rate of the SwissFEL is better suited to studies of condensed matter in the liquid and solid state. Within a pulse train at the European XFEL, the micropulse interval will be 200 ns, which will cause significant cumulative local heating of a condensed sample, will make the efficient readout of large 2D array detectors difficult and will prevent micropulse-to-micropulse alterations in FEL wavelength, pump–probe delay or sample position. The SwissFEL Athos APPLE II undulator will allow the production of
circularly polarized soft x-rays; this scheme is not included in the baseline design of either the LCLS or the European XFEL. Finally, an alternative method to the FEL to produce short pulses in the soft x-ray region, albeit of low intensity, is laser-plasma-based high-order harmonic generation [17].

3. Experiments at the SwissFEL

3.1. General considerations

The SwissFEL will emphasize three basic types of measurement.

- **Diffract-destroy** lensless imaging of, for example, biomolecules and their complexes. For sufficiently short x-ray pulses (≤10 fs), scattering data are recorded prior to the Coulomb explosion of the sample. Although a high transverse coherence of the x-rays is sufficient to image thin samples at small \( Q \), thick samples and large scattering angles will require in addition significant longitudinal coherence. Particularly promising approaches are ‘ptychographic’ measurements on 2D protein crystals [18], multiple-detector measurements of spatio-temporal correlations in systems lacking long-range order [19] and the coherent sorting of single-shot scattering data from randomly oriented molecules using generative topographic mapping [20].

- **Pump–probe** measurements of triggered dynamics. Possible pump signals are optical, IR and THz pulses and heavy-ion implantation. Possible x-ray probes are absorption and emission spectroscopy, including spin-resolved time-of-flight photoelectron spectroscopy, and scattering, including small- and wide-angle scattering and Laue diffraction from crystals. Reproducible conditions must be created for successive shots, implying that if the sample is locally destroyed, it must be repositioned.

  For pump–probe spectroscopic investigations, it will be necessary not only to vary the pump–probe delay, but also to scan the x-ray wavelength. An extreme example is EXAFS, where x-ray absorption must be measured over an interval of typically 800 eV, requiring rapid changes in the electron energy or the undulator gap. At the SwissFEL, it is anticipated that this will be possible between successive pulses. For investigations close to an absorption edge, such as XANES and RIXS, one can make use of the full wavelength spectrum of a single shot. The intrinsic bandwidth of the SwissFEL, approximately 0.1%, or 1 eV at 1 keV, will be sufficient for some of these investigations, and with the energy-chirp mode of operation, this can be increased by a factor of 10. Ideas for single-shot x-ray emission (XES) and RIXS spectrometers are shown, respectively, in figures 7 and 8.

- **Multiple-probe** measurements of equilibrium or triggered dynamics. Since multiple (generally two) x-ray probe pulses are used, these must be sufficiently expanded or attenuated that the sample perturbation is acceptable. The pulses will be produced with split-delay units, with maximum delays of ~20 ps for soft x-rays [21] and ~3 ns for hard x-rays [22]. The standard probe–probe experiment will be split-pulse x-ray photon correlation spectroscopy (XPCS) [24], in which two speckle patterns, taken in rapid succession, are superimposed. An analysis of the speckle contrast as a function of interpulse delay and scattering angle then yields the intermediate scattering function \( S(Q,t) \). For sufficiently small scattering angles, it may be feasible to incline the split pulses with respect to one another and to collect the individual speckle patterns in two different area detectors, thereby simplifying the extraction of \( S(Q,t) \).
One can imagine extensions of the probe–probe method which in addition include a pump pulse. Two possible realizations are shown in figure 9. In the probe–pump–probe experiment (figure 9(a)) a chemical species, e.g. in a liquid jet, is probed both before and after the optical pump. The difference spectrum, unfalsified by pulse-to-pulse fluctuations, measures only the photo-excited molecules. Figure 9(b) shows a differential pump–probe–probe experiment (in this case, with a grating-based soft-x-ray split-delay unit [25]), where the difference signal, over the small time interval $\delta t$, measures the ‘velocity’ of the perturbation at the pump–probe delay $\tau$. Since the change in the perturbation may be more reproducible than the perturbation itself, this could reduce the sensitivity to inequivalent shot-to-shot conditions. A possible application is the repeated switching of magnetic nanostructures by THz pulses.

As stated above, an advanced design option for the SwissFEL foresees increasing the electron energy to 6.5 GeV, which would allow fundamental FEL operation at the ultra-narrow $(3 \times 10^{-8}$ eV) Mössbauer resonance of $^{57}\text{Fe}$ at 14.4 keV. An advantage for the SwissFEL to work at this resonance is given by the relatively long lifetime of the excited nuclear state (140 ns), which would permit (photon-hungry!) measurements of sample fluctuations [27] on ‘long’ time scales inaccessible with split-pulse techniques.

3.2. Research areas

The primary areas of application for SwissFEL research were selected based on the interests of the local scientific community and on physical and financial limitations. The result is a concentration on (a) ultrafast processes in condensed matter and (b) damage-free imaging of nanostructures. The first is championed by groups in chemistry, biochemistry,
Figure 8. A proposed spectrometer which produces a complete 2D-RIXS spectrum, as a function of both $h\nu_{in}$ and $h\nu_{out}$, from a single XFEL shot [26]. The ‘VLS’ grating has variable line spacing, and ‘KB refocusers’ refer to Kirkpatrick–Baez mirrors.

Figure 9. Schematic diagrams of (a) the probe–pump–probe and (b) the pump–probe–probe experimental geometries.

materials science and solid-state physics, and the second by investigators in structural biology and nanotechnology. Implications for the machine design include: (a) flexibility in photon wavelength, wavelength tuning and photon polarization, as well as a time structure that is compatible with 2D detector readout and on-line mechanical adjustments, and (b) x-ray pulses of duration <20 fs, for sample integrity during a diffract–destroy experiment, and a high longitudinal coherence down to the shortest possible wavelengths. Based on a series of scientific workshops and discussions with future user groups, the scientific case for the SwissFEL has
been summarized in a dedicated document [1], which includes the following sections.

- **Ultrafast magnetization dynamics on the nanoscale.**
  Using circularly polarized resonant soft x-rays and a reference-beam holographic method, it has been demonstrated [28] that a magnetic structure can be coherently imaged. The dichroic magnetic scattering can be very strong, corresponding to up to 40 electrons! With sufficient longitudinal coherence, it thus appears feasible to perform single-shot imaging close to the diffractive limit. Since a single shot will destroy the sample, a movie of the switching of magnetic nanostructures will require repeating many closely similar experiments. Half-cycle THz pump pulses, transform-limited, circularly polarized soft-x-ray pulses, a 100 Hz repetition rate and the pump–probe–probe measurement technique could make a ps/nm-scale magnetic movie a reality.

  Of particular interest to the local magnetism community are the spatial and temporal correlations of fluctuating spins. For example, low-dimensional systems such as spin chains and spin ladders, although failing to show long-range order, may exhibit an unusual dynamical mesoscopic phase coherence known as ‘hidden quantum order’ [29], with a correlation length of up to 20 nm. Cross-correlation analysis [19] of coherent, resonant, magnetic scattering patterns at the SwissFEL holds the promise of providing a more detailed picture of such quantum correlations than is possible with conventional inelastic neutron scattering.

- **Catalysis and solution chemistry.**
  Using the 100 ps time structure of the Swiss Light Source synchrotron, and the 30 fs resolution of its FEMTO beamline, solution chemists have determined the rate constants and geometrical changes in photo-triggered conformational modifications of molecules in a liquid jet [30, 31]. The SwissFEL will dramatically improve such experiments and extend them to shorter time scales. And with the availability of single-shot XANES or XES, making use of the broadband chirped mode and a dispersive detector, the SwissFEL will allow surface chemistry groups to determine the electronic and geometrical structure of short-lived intermediate states during heterogeneous catalysis.

- **Coherent diffraction by nanostructures.**
  There is a strong tradition in coherent diffraction at the Swiss Light Source [32], and plans are being made to image nanostructures using the excellent transverse (and longitudinal) coherence of the SwissFEL. Diffract–destroy experiments with ultrashort (down to 5 fs) pulses will effectively avoid the radiation damage problem. Principal applications of coherent diffraction are foreseen in biomaterials: on mesoscopic samples (imaging subcellular structures at 10 nm resolution), in sub-micrometer samples (with the synchronized 100 Hz injection of nano-protein-crystals into the XFEL beam), on 2D membrane-protein crystals (using the ptychography technique pioneered at PSI [18]) and hopefully on individual biomolecules [20].

  It has further been proposed to use time-resolved coherent diffraction to study the generation and evolution of radiation-induced crystal defects, e.g. in the structural materials used in nuclear reactors. The process would be triggered by a synchronized ion-implanter, and important physical correlations, such as the average size and density of vacancy clusters or the diffusion rate of interstitials, will be extracted and compared with simulations [33]. The fact that the length and time scales currently accessible to molecular dynamics calculations (∼100 nm, ∼1 ns) fit very well to those accessible with
the SwissFEL will allow experimental validation of the approximations and parameter values used in the calculations.

- **Ultrafast biochemistry.**
  Interested user groups foresee a wide variety of pump–probe measurements of biochemical dynamics at the SwissFEL. An optical laser pump pulse may be used to directly initiate an ultrafast photoreaction, such as those involved in vision, photosynthesis, photolyase-based DNA repair, cryptochrome-based biological clocks and photochrome-controlled processes in plants. A more general method of photo-initiation of bio-reactions is via the UV activation of ‘caged’ molecules, such as coumarin-caged ATP [34]. Methods of x-ray probing include small-angle x-ray scattering in a liquid jet, and Laue crystallography using the broadband energy-chirp mode of FEL operation.

  Of great interest to biochemists is the issue of protein folding. How do linear chains of amino acids manage to find the complex 3D shapes that minimize their energy and that allow them to carry out their biological functions? It has been suggested that time-resolved x-ray scattering experiments at an XFEL can help elucidate the rapid, subtle ‘tier 2’ changes [35, 36] in protein structure, as the folding reaction proceeds along a hilly, higher-dimensional energy surface. In order to determine the overall shape of the energy surface, it will be important not only to measure populations of intermediate local structures but also to record the correlations among these structures: if amino-acid number \( n \) has bond-angle \( \alpha \), with what probability does number \( m \) have the angle \( \beta \) [35]?

  On the theoretical side, it is interesting to note that the field of thermodynamics is undergoing progressive development toward the description of non-equilibrium states at the molecular level. ‘Mesoscale non-equilibrium thermodynamics’, an intrinsically nonlinear, microscopic treatment of transport, accounts for fluctuations among a multiplicity of local minima separated by potential barriers [37] and has as its principal domain of application the fast and short-range processes that lend themselves to XFEL investigation.

- **Time-resolved spectroscopy of correlated electron materials.**
  Strongly correlated electron materials, showing effects such as metal–insulator transitions, high-temperature superconductivity and colossal magnetoresistance, have great promise for novel functionality. In spite of decades of work by a large fraction of the condensed matter science community, a microscopic theory is still lacking. However, there is widespread agreement that many important effects arise from the interplay in these materials of the four degrees of freedom: charge, spin, orbital and lattice. A thought-provoking picture of these elements is the chimera, a beast from Greek mythology, whose body (lattice) has three heads: lion (charge), goat (spin) and snake (orbital) [38]. Determining the hierarchy of interactions within the chimera may best be performed with a time-resolved pump–probe experiment: e.g. one feeds the lion and records the time delay until the goat reacts. Elegant examples of such studies, which offer promising areas of study for the SwissFEL, are charge-pump/lattice-probe [39] and lattice-pump/charge-probe [40] studies of the electron–phonon interaction. As pump signal, the SwissFEL will offer optical production of hot electrons, IR excitation of lattice vibrations and half-cycle THz switching of a magnetic field. Probing of possibly short-lived ordered phases will be performed by non-resonant and resonant crystal diffraction, and details of the electronic structure will be visible via single-shot x-ray absorption and emission spectroscopy and possibly resonant inelastic x-ray scattering (RIXS).
The presence of nanoscale inhomogeneity and glassy dynamics has been established in many correlated electron systems [41]. Using contrast from, for example, x-ray magnetic circular dichroism or the valence-dependent core-level shift in resonant scattering, it may be feasible to perform split-pulse XPCS measurements of $Q$-dependent correlation times out to the maximum possible soft x-ray split-delay of 10 ps. In this way, one could directly observe, for example, dynamic polarons or spin-charge stripes in correlated electron materials.

4. Project milestones and schedule

The preliminary schedule of the SwissFEL project is as follows. The 100-page SwissFEL Scientific Case is now available online at the project web page (www.fel.psi.ch), and the machine-oriented Conceptual Design Report will follow soon. These documents will form the basis for the request for funding to the Swiss parliament in early 2011. Assuming a positive decision, construction will begin in early 2012, based on the highly detailed Technical Design Report. Turn-on of the machine is then scheduled for early 2016, with user operation beginning a year later.

5. Summary

The SwissFEL hard XFEL at the Paul Scherrer Institute will use innovative design features and quality craftsmanship to produce a versatile, high-performance facility with a relatively small footprint. The machine design has been developed in close cooperation with highly interested prospective user communities; principal areas of application are ultrafast magnetization dynamics on the nanoscale, catalysis and solution chemistry, coherent diffraction by nanostructures, ultrafast biochemistry and time-resolved spectroscopy of correlated electron materials. User operation is foreseen beginning early in 2017.

Acknowledgments

We acknowledge the many contributions of our colleagues on the SwissFEL team: A Adelmann, R Bakker, P Beaud, B Beutner, C David, M Dehler, J Duppich, C Escher, T Feurer, H-W Fink, H-R Fitze, T Garvey, J Gobrecht, C Gough, B Haas, C Hauri, G Ingold, R Ischebeck, B Jakob, G Janzi, K Jefimovs, M Kenzelmann, R Krempaska, S C Leemann, J Lehmann, F Le Pimpec, K Li, M Luethy, P Ming, B Oswald, M Paraliev, P Pattison, P Pollet, C Quitmann, J-Y Raguin, U Schaer, T Schietinger, T Schilcher, V Schlott, L Schulz, W Tron, M van Daalen, J F van der Veen, D Vermeulen, T Vogel, H J Weyer and J Wickstroem.

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