FREE-ELECTRON LASERS IN THE SOFT X-RAY REGIME*

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Abstract

X-ray science in imaging, structure determination, and spectroscopy, as well as diffraction/scattering, requires intense ultrafast pulses in the soft X-ray range, uniquely provided by free electron lasers (FELs). In addition to operational soft X-ray FEL facilities, there are FEL construction projects under way that include soft X-ray laser capabilities, and planned facilities with novel capabilities. This paper provides a review of the exciting field of existing and planned soft X-ray FELs with emphasis on new schemes and new technologies to achieve better performance.

SCIENCE NEEDS FOR SOFT X-RAY FELS

scientific innovation expected from The the construction and operation of X-ray FEL facilities lies in their ability to provide tools that offer extreme spatial, temporal, and energy resolution. Properties of FEL sources are expected to include the ability to reach to the ultrafast timescales of atomic motion (about 100 fs), spin motion (down to about 1 fs), and electronic motion (down to attoseconds), the spatial scale of the atomic bond (down to Angstroms), and energy resolution on the scale of the bond that holds electrons in correlated motion with near neighbors (~10 meV and greater). X-ray FEL sources offer unique capabilities to combine information on atomic length scales with data on full-scale functional systems under realistic operational conditions. In addition, these sources have an intensity and brightness needed to observe the subtlest of nature's secrets at these frontier space, time, and energy scales, and with elemental specificity.

Critical X-ray science in imaging, structure determination, and spectroscopy needs new capabilities in the soft X-ray range, accessing K- and L-edges of the earth-abundant elements, as well as diffraction/scattering in the few to several keV photon energy range. These scientific requirements give rise to the following desirable FEL performance features:

- X-ray time structure
 - Control of longitudinal phase space, with Fouriertransform-limited pulse structure extending from ~100 fs pulses with ~10 meV bandwidths to subfemtosecond pulses with ~10 eV bandwidths
 - Control of longitudinal pulse shape, amplitude and phase
 - Synchronization and full integration with conventional pulsed laser sources
 - High repetition rate with regularly spaced pulses
- Full transverse coherence
 - Requirements set by real-space imaging, diffractive imaging, and photon-correlation spectroscopy

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- Optical systems to preserve and exploit transverse coherence
- High peak flux and brightness
- Requirements set by non-linear effects in materials
- High average flux and brightness
 - Short-pulse sources with high repetition rates (100 kHz or greater) providing average flux and/or brightness substantially beyond existing sources
- Tunability, polarization control, and extended photon energies
 - Tunability throughout the transition-metal L-edges and polarization control and modulation
 - Two-color capability for non-linear spectroscopies and X-ray pump/X-ray probe
- High degree of amplitude and wavelength stability
- Multiple simultaneous users

SOFT X-RAY FEL OVERVIEW

High-gain single pass FELs at wavelengths in the EUV and shorter have been operating as photon science user facilities for almost a decade - the TESLA Test Facility (TTF) became the Free Electron Laser in Hamburg (FLASH) in 2003, and user operations began in 2005 with lasing at 25 nm [1]. FLASH now operates at wavelengths in the water-window (~4 nm) and longer. The LCLS at SLAC is the world's first hard X-ray FEL [2], and also operates in the soft X-ray regime with wavelength ~4.5 nm and shorter [3]. Both of these facilities currently operate in SASE mode in the soft X-ray range (although the LCLS also offers a hard X-ray self-seeded mode [4]). FERMI@elettra is a seeded FEL facility, offering improved temporal coherence, with tunable user beam currently offered down to 20 nm [5]. The SACLA facility currently operates the shortest wavelength FEL, in SASE mode [6].

Upgrades of these facilities are planned or are in progress and include development of soft X-ray capabilities, in capacity (adding FEL beamlines), and also in capability by extending the tuning range, seeding (either self-seeding or external laser-seeding) and offering tunable undulators and new operating regimes of pulse duration and time structure. The FERMI team is now commissioning a 2-stage harmonic cascade to reach into 🚔 the water window [7]. Upgrade plans at SACLA include 🛬 the re-location of the SCSS test facility as a soft X-ray FLASH-II will add variable-gap FEL driver [8]. undulators in a separate beamline driven by the existing linac, and seeding. LCLS-II is planned to provide selfseeded capability from 0.25-5 nm, using a new CW superconducting linac.

The European XFEL [9], SwissFEL [10], and Korean PAL-XFEL [11] facilities are under construction, and plan for soft X-ray capability, in SASE or in self-seeded mode.

The FLASH and FLASH-II, European XFEL, and LCLS-II projects are based on superconducting RF technology, and offer very high repetition rate (up to \sim 100 kHz at each FEL) providing high average photon beam brightness and coherent power. Other facilities and projects use normal conducting accelerators and provide relatively low repetition rate (up to \sim 100 Hz). Use of normal conducting accelerators operated at high gradient is attractive in allowing for a small facility footprint.

Design studies elsewhere are developing concepts for soft X-ray FELs, including SXFEL (Shanghai), IRIDE (INFN-Frascati), and LUNEX5 (SOLEIL). Other soft Xray FEL facility design studies have recently come to an end, including the NGLS at Berkeley Lab, and the NLS in the UK.

In addition to facilities, projects, and design studies, there are important R&D facilities contributing to understanding of FEL science and technology. Currently operating single-pass FEL R&D facilities are NLCTA (at SLAC), SPARC (at INFN Frascati), SDUV (Shanghai Institute of Applied Physics), and MAX-Lab (Lund, Sweden). Proposals for single-pass FEL R&D facilities include CLARA (STFC Daresbury).

OPERATING FACILITIES, AND THEIR UPGRADES AND EXPANSION PLANS

FLASH

The FLASH facility is a high-gain single pass SASE FEL driven by a pulsed superconducting L-band (1.3 GHz) linac based on TESLA technology, with maximum beam energy 1.25 GeV [12]. The time structure is a burst mode with up to 3 MHz bunch rate in an 800 µs macropulse, 10 Hz repetition rate, delivering up to 5000 pulses per second. Photon pulses in the wavelength range 4.2–44 nm, with 10–400 µJ per pulse, and duration in the range <50-250 fs, are produced in fixed-gap permanentmagnet undulators of period 27.3 mm. A Cs2Te photocathode provides electron beam in a normalconducting L-band RF gun, with charge per bunch 0.02-1 nC. Peak current at the FEL is typically 1-2 kA. Photon tuning is provided by adjusting the electron beam energy, and RF and beam-based feedback systems are used to enhance stability of beam energy, bunch compression, and timing. Development plans include production of shorter pulses, and enhanced temporal coherence through laserseeding using XUV pulses from an HHG laser, as well as high gain harmonic generation (HGHG) using a UV seed [13].

FLASH-II

FLASH-II adds a second FEL beamline in a new undulator tunnel and a new experimental hall added to the facility at DESY. Driven by the same superconducting linac, both FLASH-I and FLASH-II are to be delivered electron beam in bursts at 10 Hz repetition rate by a beam kicker that will distribute bunches from within each

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macropulse [14]. Two photocathode lasers are used to generate sub-trains in a macropulse, allowing flexibility in intra-train repetition rate, number of pulses per train, longitudinal pulse shape, and pulse energy for both FELs. The bunch spacing for beam to FLASH-II is $1-25 \, \mu$ s. The undulators are 31.4 mm period, with variable gap, and allow tuning from 4–13.5 nm in SASE mode at beam energy of 1.2 GeV, and longer wavelengths at lower beam energy. Construction is under way, and commissioning with beam is expected to begin in early 2014. Seeded FEL operation is planned, using single-stage harmonic generation from a UV seed laser, and initially radiating in the range 20-40 nm.

LCLS

LCLS demonstrated the first hard X-ray laser operation in 2009, with an S-band (2856 MHz) photocathode gun and 14 GeV linac driving an FEL with 3 cm period fixedgap permanent magnet undulators [2]. The facility provides photon wavelength from 4.5 nm to 1.2 Å, in pulses of ~3–500 fs, ~2–6 mJ per pulse, at a repetition rate of 120 Hz. Charge per pulse is typically ~250 pC to optimize brightness. Hard X-ray self-seeding at ~8.2 keV results in a factor ~50 reduction in bandwidth compared to SASE, and a brightness increase currently limited to a factor ~3. LCLS upgrade plans include development of capabilities for fs-scale pulses, hard and soft X-ray selfseeding, two-color generation, synchronized THz, multiple-bunch operation, and polarization control [3].

LCLS-II

LCLS-II is a major expansion of the FEL capabilities at SLAC, and plans are being developed to build a new 4 GeV superconducting L-band (1.3 GHz) linac based on ILC/XFEL technology developed for CW operation. The linac will drive two FELs, each an adjustable gap permanent magnet undulator design. Both FELs will be self-seeded, and one tunable over the range 1-5 nm (undulator period ~ 40 mm), the other 0.25–1.2 nm (undulator period ~26 mm). The latter will replace the existing LCLS undulator, and designed to be driven be either the new linac, or the existing S-band linac (for harder X-ray and higher per-pulse energy capability, at repetition rate). Bunch rate from lower the superconducting linac may be as high as 1 MHz, and each FEL will typically provide ~100 kHz X-ray pulses with uniform spacing, with energy per pulse up to ~ 2 mJ. A high-brightness, high repetition rate injector such as being developed at the APEX project may be used as an electron source [15]. The facility takes advantage of existing SLAC infrastructure in housing the injector, linac, RF power systems, beam transport, undulators, Xray beamlines and endstations. This approach offers cost savings, and upgrade paths both in capacity by adding FELs, and capability by implementing new FEL designs. The construction project is estimated to complete in 2020.

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The first seeded FEL user facility has been operational for users since 2012, and currently provides continuous tunability from the FEL-1 harmonic cascade over the range 20-65 nm (and longer wavelengths to 100 nm possible with specific machine setup). A UV seed laser is used to modulate the electron beam from a 1.2 GeV Sband (2998 MHz) GeV linac operating at 10 Hz, radiating at up to the 13th harmonic of the seed in 55 mm period variable-gap APPLE-II type undulators with polarization control. Peak current is ~500 A, as opposed to ~kA used in SASE FELs. Pulse energy of up to ~100 µJ can be delivered, and relative bandwidth as low as 0.05% (close to the Fourier transform limit), wavelength stability $\sim 7 \times 10^{-5}$, and amplitude variations $\sim 10\%$ (measured in the EUV) [16, 17]. An upgrade to 50 Hz is under way, by implementing a new RF photocathode gun and klystron modulators.

FEL-2 is currently being commissioned, and uses a beam of energy ~1.5 GeV (by activating SLED cavities in the RF power systems) driving a two-stage harmonic cascade using a fresh-bunch approach. The two stages are each high gain harmonic generation FELs. The first stage is seeded by a UV pulse (~260 nm, the 3rd harmonic of a Ti:Sa laser system), and lases at the 4th-6th harmonic. The output of this first stage is used to seed the second stage modulator, using a chicane to delay the electron bunch such that the seed pulse overlaps and modulates an unperturbed ("fresh") part of the electron bunch. The final FEL output is obtained at up to ~65 harmonic of the initial UV seed. Tuning range is nominally 4-20 nm although coherent FEL emission with wavelength as short as 3 nm has been observed [18].

SACLA

SACLA opened to users in 2012 and is currently a hard X-ray facility, producing photon pulses in a range 5-15 keV, with 100-400 mJ per pulse in a duration of ~10-15 fs, at a repetition rate of 10 Hz (60 Hz maximum). The undulators are in-vacuum variable-gap, with period 18 mm. The machine uses an 8.5 GeV, C-band (5.7 GHz), linac, with a novel single-crystal CeB₆ thermionic cathode and combination of VHF, UHF, L-, S-, and C-band RF systems in the injector. Bunch charge is ~100-300 pC, and peak current >3 kA. SASE central wavelength stability is $\sim 3x10^{-4}$, and pulse energy variations $\sim 10^{-4}$ 20% [6,8].

Upgrades are being pursued to provide additional FEL beamlines (up to 5 and including one soft X-ray), a bunch-by-bunch beam distribution system, hard X-ray self-seeding, higher beam energy (to 9 GeV), and relocation of the SCSS (SPring-8 Compact SASE Source) test accelerator and increasing it's energy to 450 MeV (and potentially 1.4 GeV) to drive a EUV to soft X-ray FEL [8]. The soft X-ray FEL uses in-vacuum undulators with period 18 mm (same as hard X-ray undulators), and initial tuning range is ~15-60 nm, with 50-100 µJ per pulse. First operation of the soft X-ray FEL is planned for autumn 2015. The SCSS was built in 2005 to demonstrate

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the SACLA concept with a 250 MeV test accelerator, and successfully lased at 50 nm, with HHG seeding at 61.5 nm [19].

CONSTRUCTION PROJECTS

European XFEL

The European XFEL is under construction in Hamburg, Germany, and consists of a 17.5 GeV pulsed L-band (1.3 GHz) superconducting linac serving three initial SASE FELs, delivering photons from 0.05-4 nm in pulses of $\sim 1-100$ fs. The time structure is 2700 bunches per 600 µs macropulse, at a repetition rate of 10 Hz (average bunch rate 27 kHz, and a rate of 4.5 MHz within the macropulse). Kickers will provide flexible beam distribution with simultaneous operation of three experiments. Bunch charge is 0.02-1 nC, and average beam power over 500 kW. The injector is a normalconducting L-band photo-cathode RF gun of the same type in operation at FLASH. The soft X-ray FEL is downstream from a hard X-ray FEL, using the same beam, and has 68 mm period permanent magnet undulators with adjustable gap; the tuning range is extended by adjusting the electron beam energy. Average soft X-ray power is greater than 100 W [20].

SwissFEL

Under construction in Villigen, Switzerland, SwissFEL is an X-ray laser facility with two FEL lines covering the wavelength range from 0.1-0.7 nm and 0.7-7 nm, respectively. An S-band injector delivers beam at 100 Hz to a normal-conducting C-band (5.72 GHz) linear accelerator. Two bunches of charge 10-200 pC are accelerated per RF pulse; one is extracted at 3 GeV for soft X-ray generation, while the other continues to be accelerated to 5.8 GeV for hard X-ray production. The soft X-ray FEL is self-seeded and uses 40 mm period APPLE-II type variable gap undulators with polarization control, and delivers per-pulse energy of ~100 µJ. Commissioning of the linear accelerator and the hard Xray FEL will start in 2016; funding for the soft X-ray component requires additional approval and construction is planned to begin in 2018 [10]. *PAL X-FEL* The PAL-XFEL is under construction, and designed to have three hard X-ray undulator lines at the end of a 10

GeV S-band (2856 MHz) linac, and a branch line at 3.15 GeV for two soft X-ray undulator lines. Initially, one hard X-ray and one soft X-ray FEL will be built. The injector uses an S-band photocathode gun which delivers two bunches of 20–200 pC charge at 60 Hz, bunch delivery to the soft X-ray beamline is to be controlled by a kicker system. A passive wakefield "dechirper" will be used to remove the correlated energy chirp following extraction from the linac [21]. The soft X-ray undulators are planned m to be permanent-magnet adjustable-gap devices with $34 \gtrsim$ mm period, and APPLE-II type for the final few gain i lengths to provide polarization control. Photon 🚊

wavelength is in the range 1–4.5 nm (longer wavelengths using lower beam energy), with \sim 90 fs pulse duration. FEL experiments are planned to begin in late 2016 [11].

PROPOSALS AND DESIGN STUDIES

NGLS

The LBNL-led NGLS collaboration developed design concepts for a multi-beamline soft x-ray FEL array powered by a superconducting linear accelerator, operating with a high bunch repetition rate of ~1 MHz. The CW L-band (1.3 GHz) 2.4 GeV superconducting linear accelerator design is based on developments of TESLA and ILC technology, and is supplied by a highbrightness, high repetition rate VHF-frequency photocathode electron gun under development at the APEX facility [15]. 300 pC, 500 A peak current, ~300 fs electron bunches from the linac are distributed by RF deflecting cavities to the array of up to nine independently configurable FEL beamlines with nominal bunch rates of ~100 kHz in each FEL, with uniform pulse spacing, and some FELs capable of operating at the full linac bunch Undulators are ~ 20 mm period. rate. Nb₃Sn superconducting planar devices to provide optimal performance, and are being developed in an R&D program [22]. Individual FELs may be configured for different modes of operation, including self-seeded and external-laser-seeded, and each may produce high peak and average brightness x-rays with a flexible pulse format, including multiple approaches to deliver twocolor X-rays with wide tuning range for each color, and with pulse durations in the range $\sim 0.1-100$ fs. RF and beam-based feedback systems, integrated with fiber-based timing and synchronization systems, would provide exceptional photon-beam stability and synchronization control in a high-rate, CW machine [23]. The effort is now stopped.

SXFEL

Baseline technical design studies for the Shanghai soft X-ray FEL (SXFEL) proposal have been completed. The initial configuration is planned to use a 10 Hz normalconducting linac using S- and C-band technology and would deliver 840 MeV beam energy, driving a laserseeded harmonic cascade to reach a wavelength of 8.8 nm. Upgrade to 1.2–1.3 GeV would provide photon wavelength down to 3 nm. The facility would be built at the Shanghai Synchrotron Radiation Facility, in collaboration with Tsinghua University [24].

LUNEX5

LUNEX5 is a multi-institution proposal coordinated by SOLEIL, for R&D and demonstration of advanced FEL concepts, including both RF linac and laser wakefield accelerators. Seeded FEL techniques, using in-vacuum cryogenically cooled PrFeB undulators with 15 mm period, would be developed with a 400 MeV superconducting linac, and a 0.4–1 GeV laser-plasma beam. HHG and EEHG seeding schemes would be

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explored to produce 4-40 nm FEL output in pulses of ~ 10 fs duration. A conceptual design report is completed, and the project is in an R&D stage [25].

IRIDE

The IRIDE concept under development and based at INFN Frascati [26] is a high brightness particle beams factory based on high duty cycle superconducting linacs. The design concept includes FEL oscillators and SASE and seeded FELs, operating over a very broad spectrum from IR to hard X-ray.

NLS

The NLS team in the U.K. developed a conceptual design for a 1 kHz coherent light source with FELs operating to wavelengths in the range $\sim 1-25$ nm, using a 2.25 GeV CW superconducting L-band (1.3 GHz) linac. The pulsed L-band photocathode gun would deliver 200 pC at 1 kHz, driving HHG-seeded FELs to provide temporal coherence and increased brightness. Three initial FELs were conceived, using harmonic cascade schemes and generating ~ 20 fs pulses. Upgrade paths to higher repetition rate (MHz), shorter X-ray pulses, higher energy photons (to 2 keV), and additional FELs and endstations were identified [27].

WiFEL

A concept for a Wisconsin FEL (WiFEL) has been developed based on a CW superconducting L-band (1.3 GHz) linac fed by a superconducting photocathode gun delivering bunches at MHz rate. A staged approach is suggested that includes incremental build-out of the accelerator and multiple seeded FELs, using harmonic cascades and covering a wavelength range down to \sim 1 nm, with \sim 10 fs pulses [28].

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