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THE CHALLENGE OF 4TH GENERATION LIGHT SOURCES*

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Abstract

We present results from the operation of X-ray free-electron lasers (FELs), the 4th generation sources of high brightness, coherent photons, with femtosecond pulse duration, high peak power and narrow line-width. We discuss how the experimental and theoretical progress in the electron beam -the lasing medium- generation and manipulation, can be used to further improve the source characteristics, and design optimized X-ray FELs.

INTRODUCTION

X-ray free-electron lasers (FELs) are the fourth generation light sources, operating in a wavelength range from nanometers to Ångstroms. They are the only sources of coherent electromagnetic radiation with a wavelength as small as 1Å and pulse duration as short as 1 femtosecond (fs), characteristic length and time scales of atomic phenomena. The brightness of X-ray FELs is 7 to 10 orders of magnitudes larger than any other source, giving us new, unprecedented capabilities to study the structure and dynamics of atomic and molecular systems. X-ray FELs are characterized by a very large degeneracy parameter, more than 10^9 photons in a coherence volume, compared to about 1 for spontaneous undulator radiation, allowing studies of coherent diffraction imaging, multi-photons excitations, non-linear science.

Four FELs, operating in a wavelength range from the hard X-ray to soft X-rays and UV, are now in operation. FLASH at DESY [1] operates from about 50 to 4 nm, and LCLS at SLAC [2] from about 2.2 to 0.12 nm. In 2011 SACLA at Spring 8 lased at a wavelength as short as 0.08 nm [3] and Fermi@Elettra, started operation at 40 to 30 nm [4].

Novel and unique experimental results have already been obtained using X-ray FELs [5]. Very recent LCLS results include atomic physics [6] and coherent diffraction imaging of protein structures in nano-crystals [7], and a virus [8].

New FELs are under construction in Europe and Asia. The European XFELm [9] at DESY, a hard X-ray FEL, is expected to start operation in 2015. Other FELs are being designed in the USA, Asia, Europe and Japan. A complete list of the projects can be found in the proceedings of the 33rd International FEL Conference, Shanghai 2011, published at www.JaCoW.org.

LCLS results show that the X-ray pulse duration and intensity can be changed varying the electron bunch charge from 250 to 20 pC, from about 100 to a few femtosecond, over the full wavelength range of 2.2 to 0.12 nm [10]. This flexibility is very important to tailor the X-ray pulse to the experiment being done.

Results from FLASH and LCLS show that we can generate very high brightness electron beams to drive X-ray FELs, thus making possible new developments: sub-Ångstroms wavelengths, attosecond pulses, peak/average brightness larger than present values.

The paper reviews the present state of the art of X-ray FELs physics and technology, discusses the electron beam phase space density scaling laws and other results that will lead to further developments.

PRESENT STATE OF THE ART

Many FELs are in operation around the world in the IR, visible, near UV wavelength, configured mostly as oscillator. In the soft and hard X-ray region FEL amplifiers, in the seeded or SASE configurations are the preferred choice. An oscillator configuration has been studied recently to generate very narrow bandwidth radiation [11] at 1Å.

Table 1: LCLS Radiation and Electron Beam Properties at a 250 pC Charge

Charge/bunch, nC	0.25	0.25
Beam energy, GeV	13.6	3.5–6.7
Slice emittance, μm	0.4	0.4
Projected emittance, μm	0.5–1.2	0.5–1.6
Peak current, kA	2.5–3.5	0.5–3.5
Wavelength, Å	1.5	6-22
FEL gain length, m	3.5	1.5
Photons/pulse x 10^{12}	1.0–2.3	10–20
Peak X-ray power, GW	15–40	3–35
Pulse duration (FWHM), fs	70–100	70–500
Bandwidth (FWHM), %	0.2–0.5	0.2–1.0

The results of FLASH [1] and LCLS [2] show good agreement of the high gain FEL theory and experiments. Powerful simulation tools – Start-to-End simulations [12, 13] - have been developed to evaluate and design X-ray FELs, from the generation of electrons on the cathode, to the acceleration, bunch length compression, propagation through the undulator and the emission of electromagnetic radiation.

The electron beam and X-ray properties of LCLS, are summarized in Table 1 for operation at 250 pC bunch charge. Another mode of operation with the electron bunch charge reduced from 250 to 20 pC has also been successfully implemented. The normalized emittance at 20 pC is about 0.15 μm, the pulse length is as short as a few femtosecond, with 60 GW peak power at 1.5Å and saturation [10].

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High Gain FEL Amplifier Scaling

A single pass FEL amplifier, operating in the seeded or SASE mode, is characterized by the dimensionless FEL parameter [14],

$$\rho = \left(\frac{K}{4} \frac{\Omega_p}{\omega_U} \right)^{2/3} \tag{1}$$

where $\omega_U = 2\pi c / \lambda_U$ is the frequency associated to the undulator period, $\Omega_p = (4\pi c^2 r_e n_e / \gamma^3)^{1/2}$ is the beam plasma frequency, n_e is the electron density, r_e the classical electron radius, γ the beam energy in rest mass units. The instability growth rate, or gain length, is, in a 1-D model,

$$L_G = \frac{\lambda_U}{4\sqrt{3}\pi\rho} \tag{2}$$

The saturation power, reached after about 20 gain length, is the FEL parameter times the electron beam power, $P_{sat} = \rho E_{beam} I_{beam}$. For LCLS we have: λ*=1.5Å*, I_{beam} *~ 3 k A*, E_{beam} *~ 14 GeV* , ρ *~ 5x10*$^{-4}$*.*P_{sat} *~ 20 GW*, N_{coh}*~10*^{12} *, pulse duration~100fs*. Typically ρ~10^{-3}-10^{-4} for soft and hard X-ray FELs.

The number of coherent photons/pulse scales almost linearly with pulse duration -~10^{12} at 100 fs, 10^{11} at 10fs for 8keV photons- and inversely with the photon energy.

These results are valid a 1-D model and are a good approximation to the 3-D case if three conditions, requiring a large 6-D phase space density, are satisfied: 1. Phase-space matching of the electron beam and the radiation field; 2. Radiation wavelength within the FEL gain bandwidth; 3. Losses due to diffraction less than the FEL gain.

Electron Beam Phase Space Density Scaling

To obtain a gain length not longer than a few meters for an X-ray FEL the electron beam must satisfy the requirements needed for the 1-D model to be applicable.

The beam properties in a linac based FEL are mostly determined by the electron gun, the acceleration and compression processes can only dilute the 6-D phase space density. The most commonly used electron gun is a radio frequency (RF) photo-injector, consisting of a photo-cathode illuminated by a laser and immersed in a RF field of about 50 to 150 MV/m [15]. The photoinjector scaling with frequency, voltage and other parameters has been studied in ref. [16].

Photo-injectors in S-band, operating at about 100 Hz, as used at LCLS and other FELs, are well understood and tested [17]. Lower frequencies photo-injectors, operating at a much higher bunch repetition rate, have been developed for FLASH and other FELs using superconducting linacs,

Very useful scaling laws and simulation codes, as a function of frequency and electron charge, have been developed for these systems [18] to evaluate in detail the electron dynamics. An alternative approach is an injector based on a high voltage, pulsed thermionic cathode, as developed at Spring8 [19] for the Japanese X-Ray FEL.

LCLS results show that RF photo-injectors generate beams with small transverse and longitudinal emittance and large peak current, giving a few meters long gain length at 1 Å. The transverse emittance can vary along the electron bunch. What is important for FEL lasing is the slice transverse emittance and energy spread, defined as the average value over one FEL cooperation length [20]. This quantity varies along the bunch but it can remain small, even after the bunch compression, over most of the bunch. An example of variation of beam characteristics along the bunch is given in Figure 1.

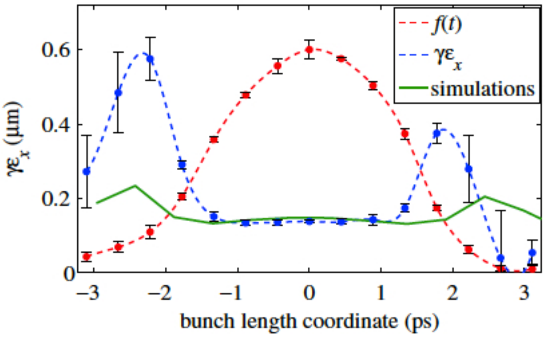

Figure 1: Normalized electron transverse emittance along the bunch length at a charge of 20 pC, from ref. [10]. The dots are measured values and the curves are the results of simulations. The curve *f(t)* is the bunch temporal distribution on an arbitrary scale. results of simulations. The curve *f(t)* is the bunch temporal distribution on an arbitrary scale.

Extensive radio frequency photo-injector simulations [21] show that, for operation near to the Ferrario working point [22], the normalized slice transverse emittance scales with charge as

$$\varepsilon_N = 1.4\sqrt{0.111Q^{2/3} + 0.18Q^{4/3} + 0.18Q^{8/3}} \tag{3}$$

where the emittance is in μm and Q in nC. The three terms describe the thermal, space charge and radio frequency contributions. The scaling includes emittance compensation [23], and assumes that the laser pulse length and spot radius are scaled with charge. The factor 1.4 is empirical and describes some uncertainty on the thermal emittance value. The emittance given by (3) is in good agreement with LCLS results.

Longitudinal Emittance Scaling

The longitudinal emittance determines the electron bunch current and energy spread, two important quantities for the gain length. Minimizing the longitudinal emittance requires proper shaping of the laser pulse at the photocathode [22, 24], depending critically on the operating condition.

The longitudinal emittance at low charge has been studied at LCLS and UCLA. Results for LCLS at 20 pC [10], shown in Figure 1, estimate a longitudinal emittance with an approximate value of 1-2 ps keV. It is interesting that the electron, and thus the X-ray, pulse shape can be changed in the compression process. In the over-compression case the bunch length is quite short, about 1μm, or 3fs.

An experiment by a UCLA group studied the transverse and longitudinal emittance of an electron beam from an S-band RF gun operating in the "blow-out " regime [25, 26], measuring a longitudinal emittance smaller than 1 ps keV.

In the blow-out scheme, a short (< 100 fs) laser pulse, as opposed to the picosecond long pulses used at LCLS, illuminates the cathode. The space charge forces change the charge distribution from its initial pancake-like shape to a nearly ideal uniformly filled ellipsoidal distribution. In the final state the beam self-fields are approximately linear in the three coordinates, and the beam dynamics and phase space are also almost linear.

Magnetic and Velocity Bunch Compression

In a single pass high gain X-ray FELs a peak electron bunch current in the kA range is necessary to obtain a gain length of a few meters. Since the current at the electron gun is much lower, magnetic compression of an energy chirped electron beam is used during the acceleration process, to reduce the bunch length, and thus increase the current, up to 100 times. LCLS uses two chicanes to compress the beam, the first at about 250 MeV, the second at about 4 Gev.

Bunch compression can dilute the beam phase space density because of collective and nonlinear effects. One damaging effect is the emission of coherent synchrotron radiation (CSR) [27], as the very short electron bunch radiates coherently in the chicane bending magnets at wavelength longer than that of the bunch density structures. CSR effects measurement agree with computer codes [28].

The two compressors in LCLS minimize CSR and other wakefield effects. However they limit the maximum compression that can be used before emittance blow up, as seen in the measurements of bunch length and transverse emittance at a charge of 250 pC after the second LCLS compressor [28]. The effect is much reduced at 20 pC [10].

An alternative method to achieve some bunch compression at low beam energy, without bending the beam in a magnet, and with emittance preservation is velocity bunching demonstrated recently by the SPARC group [29]. A combination of this technique and magnetic compression at higher beam energy can increase the maximum compression attainable without emittance blow-up.

Undulator and Linacs

Sub-centimeter period undulators can reduce the FEL size and cost in the low charge, short pulse case. Undulators with a 1.5 cm period are in use in several synchrotron radiation sources. A 1.5 cm period, 3.5 mm gap undulator is used at SACLA. One with the same period, K=1 and 5 mm gap was used for a UCLA SASE FEL experiment [30].

Several groups are working on sub-centimeter period undulators, using permanent magnets cooled to low temperature or superconducting materials. A high field, 9 mm period undulator based on a cryogenically cooled Pr-SmCo-Fe hybrid and field larger than 2 T/m has been designed and tested [31]

An LBNL group is using Nb3Sn superconducting material [32] for sub-centimeter period undulators with an undulator parameter of one and a gap of 4 to 5 millimeters. Another possibility to develop small period, large gap undulators is offered by X-band microwave undulators [33].

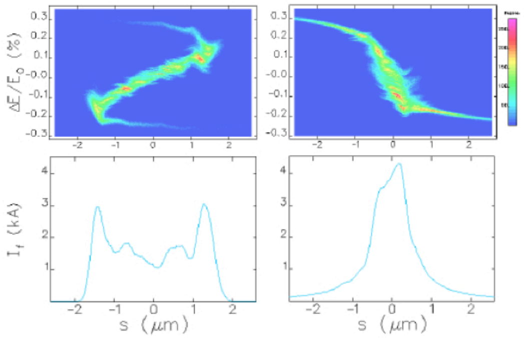

Figure 2: LCLS longitudinal phase space measurements at 20 pC after the second bunch compressor and before the final acceleration. The plots show under-compressed (top left) and over-compressed (top right) longitudinal phase space and the corresponding current profiles. The two cases correspond to different linac rf phases. Beam energy about 4 GeV. Bunch head to the left. From ref. [10].

In another development for very high repetition rate FELs, a radio frequency electron gun is being developed at LBNL [34], with the cathode inserted in a low frequency, 75MHz, normal conducting cavity. The gun repetition rate is 0.1 to a few MHz. Simulations show an emittance comparable to that of the LCLS gun.

A high frequency, C-band linac, with high accelerating gradient, is being used at. X-band linacs are also being considered. C band or X-band linacs, operated at low accelerating field, 10 to 20 MV/m, can be used to increase the linac repetition rate to 1-10 kHz, with limited input average power.

Laser/plasma/dielectric wake-field based accelerators are being developed. In the future they could decrease the accelerator length to a small fraction of its present size. One example is the aalready mentioned project at Berlin [31]. Other projects to develop high gradient laser/plasma accelerators to drive light sources are being developed at Berkeley by Wim Leemans and coworkers [35], at SLAC/UCLA by C. Joshi and coworkers [36], and in Europe within the framework of the European Extreme Light Infrastructure [37].

X-RAY FEL DEVELOPMENTS

The unique capabilities of X-ray FELs to explore atomic and molecular phenomena can be further enhanced. A list of desired performance improvements is given in Table 2.

Regimes of interest are: ultra short pulses, femto- to atto-seconds, to explore matters in the time domain; very small line-width for the exploration in the frequency domain; very high power for single molecule, single shot, coherent diffraction imaging.

The number of coherent photons per pulse is an important parameter. For single-shot experiments the number is very large, 10^{12} or more, and the sample is destroyed or damaged by the X-rays pulse. A short pulse duration is required, ten femtosecond or less for biological structures imaging, to obtain data before the structure changes. For multi-shot experiments, the number of coherent photons per pulse is small, the sample is not damaged, a high pulse repetition rate is desirable.

It is likely that different FELs will be needed to implement all the advanced parameters of Table 2. We consider here three cases.

Example 1. An X-ray FEL oscillator is a candidate to produce pulses with a line width a small as 10^{-6}-10^{-7} [38] well beyond the capability of an amplifier. The oscillator generates a small number of coherent photons in a long pulse, 0.1 to 1ps, at MHz, repetition rate, using a CW superconducting linac and low emittance, low charge, 50 pC, bunches. Main challenges are the development of low loss mirrors in the Ångstroms region and the development of high repetition rate, one to a few MHz, electron guns.

Example 2. Single molecule, single shot imaging with few Å resolution, a great scientific breakthrough, requires 10^{13} of energy 8 keV, or larger, in 10 fs or less, about 1 TW peak power, leading to very different FEL optimization. Measurements are single shot, blowing up the sample. Matching the sample preparation time and the FEL repetition rate is important.

Example 3. In the femto/attosecond region the number of photons per pulse is small, the sample is not destroyed and the amount of data/shot is limited. A high FEL repetition rate, up to MHz, is desirable. Using low charge, low emittance bunches the beam energy can be reduced.

The desire for longitudinal coherence is widespread. The X-ray pulse from a SASE FEL has full transverse coherence, but a spiky time structure [20]. The line-width is determined by the cooperation length and not by the bunch length. The UCLA/SPARC groups have shown that single-spike, ultra-short SASE pulses can be generated using a few pC bunches at nm and sub-nm wavelength [39]. In other cases an external coherent signal is needed to seed the FEL process. The seed can be a laser at the same wavelength of the FEL fundamental, or a laser at a lower harmonic, or a combination of two laser at wavelengths longer that of the FEL, as proposed by Stupakov [40].

Table 2: Requirements for the Development of X-ray FELs (* brightness in photons/s/(mm mrad)^2/0.1bw)

Photon energy, keV	0.1-100
Pulse repetition rate, Hz	10^2-10^6
Pulse duration, fs	<1-1000
Coherence, transverse	Diffraction limited
Coherence, longitudinal	Transform limited,
Coherent photons/pulse	10^9-10^{14}
Peak (Average) brightness *	10^{32}-10^{36} (10^{21}-10^{29})
Peak (Ave.) power, TW (kW)	>1 (>1)
Polarization	Variable

Improved longitudinal coherence can also be obtained with self-seeding, obtained by splitting the undulator in two parts, filtering in frequency the signal from the first undulator and feeding it on the same electron beam in the second undulator [41, 42].

A comparison between seeding and self-seeding [43] options shows that in both cases the final line-width and the intensity fluctuations depend on the details of the electron bunch longitudinal distribution, in particular on the linearity of the profile of the energy distribution along the bunch. This profile is also related to the bunch compression process. In practice these effects might limit the minimum line-width obtainable to about 10^{-5}.

Example 2, the TW FEL at 8 keV, requires a very different approach. Existing hard X-ray FELs, operate in high gain SASE mode, starting from longitudinal density noise in the electron beam and reaching saturation. The saturation power is about 30-40GW.

Kroll, Rosenbluth and Morton [44] proposed to increase the energy transfer from the electron to the photon beam by adjusting the undulator magnetic field to compensate for the electron energy losses, a "tapered" undulator. Two recent papers [45, 46] have shown that it is feasible, using a tapered undulator in combination with self-seeding, to reach the 1 TW level. For such a system the higher radiation harmonics are large, for a tapered planar undulator the third harmonic at 24 keV has about 100GW.

CONCLUSIONS

X-ray FELs can be developed to reach new level of performance, generating fully coherent femto-second to atto-second pulses, or pulses with extremely small line width. With the development of high repetition rate electron guns and using CW superconducting linacs it can reach MHz level repetition rates and large average power. Using the extraordinary brightness of low-charge bunches it is possible to reduce the size and cost of the accelerator for short pulses. Near transform limited pulses can be obtained using single spike, seeding and/or self-seeding. Peak power can reach the TW level in 10 femtosecond or les, with tapered undulators.

The number of coherent photons/pulse and other characteristics can be tailored to the experiments. Systems providing only a subset of these characteristics, in particular short pulses, can be built at lower cost. Ongoing research on novel laser/plasma accelerators, high frequency RF linacs and electron guns can lead in the future to very compact FELs without sacrifice in performance.

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