START-TO-END SIMULATIONS OF THE LCLS ACCELERATOR AND FEL PERFORMANCE AT VERY LOW CHARGE*

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Abstract

The Linac Coherent Light Source (LCLS) is an x-ray Free-electron Laser (FEL) being commissioned at SLAC. Recent beam measurements have shown that, using the LCLS injector-linac-compressors, the beam emittance is very small at 20 pC. In this paper we perform start-to-end simulations of the entire accelerator including the FEL undulator and study the FEL performance versus the bunch charge. At 20 pC charge, these calculations associated with the measured beam parameters suggest the possibility of generating a longitudinally coherent single x-ray spike with 2-femtosecond (fs) duration at a wavelength of 1.5 nm. At 100 pC charge level, our simulations show an x-ray pulse with 10 femtosecond duration and up to 10^{12} photons at a wavelength of 1.5 Å. These results open exciting possibilities for ultrafast science and single shot molecular imaging.

INTRODUCTION

The LCLS accelerator has been operating since April of 2007. The injector [1] and main linac [2] have been fully commissioned and have already produced an electron beam with adequate brightness to drive the x-ray FEL. The high-brightness electron beam has been transported into the FEL undulator starting in early 2009 and achieved first lasing at 1.5 Å [3]. During the 2008 commissioning phase, the electron bunch was fully characterized at several different operating points, including a high charge mode (1 nC), a more routine setting (0.25 nC), and also a very low charge level (0.02 nC). Although the machine operates well at 0.25 nC with a transverse normalized emittance of <1 μm, there is also growing interest in a much lower bunch charge, where femtosecond pulses may be possible and injector emittance levels down to 0.14 μm have recently been observed at LCLS [4].

Although the bunch charge of $\sim$ 20 pC is much lower than the designed case of 1 nC, the final bunch length is compressed to $\sim$ 1 μm by magnetic bunch compression, resulting in an ultra-short bunch with beam brightness higher than the conventional design at 1 nC charge. Simulations suggest such a bunch is capable of generating intense x-rays in the LCLS undulator with a few femtosecond pulse duration and hence may open up new parameter regimes for the LCLS and other x-ray FEL projects under consideration. Similar low charge operating schemes have also been proposed before [5, 6], and efforts are underway at the Paul Scherrer Institute to develop an ultra-low emittance source at low bunch charge [7]. Here we report the start to end simulations for the electron beams and FELs including the experimental measurements on electrons at LCLS in a low-charge mode.

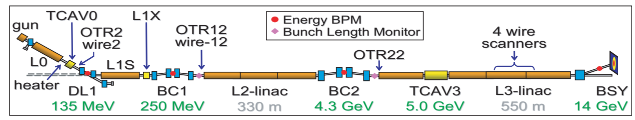

Figure 1: LCLS 1-km accelerator layout showing gun, off-axis injector, BC1 and BC2 compressors, and various linac segments. The undulator (not shown) is 400 m off scale at right.

ELECTRON BEAM MEASUREMENTS AND SIMULATIONS AT 20 PC

Figure 1 shows the layout of the LCLS accelerators. At 20 pC charge, we used a UV laser spot diameter at the cathode of 0.6 mm (0.15 mm rms), with a Gaussian temporal shape full width half maximum (fwhm) of 4 ps. The electron from the gun is accelerated to 135 MeV in the injector beam line then merged through a dogleg (DL1) to the SLAC linac, after two bunch compressors (BC1 and BC2) and linac acceleration the final energy is $\sim$14 GeV. This electron beam is then transported to the 130m undulator beam line to generate x-ray FELs. Start-to-end simulations were carried out from the photocathode to the entrance of the undulator using *IMPACT-T* [8] and *Elegant* [9] with 1 million macro-particles. Then *Genesis* 1.3 [10] is used for the FEL simulations.

The injector emittance measurements are made using an intercepting 1-μm thick aluminum screen ("OTR2" in Fig. 1) located about 14 meters downstream of the gun, where the common 'quad-scan' method is used to analyze the transverse emittance. In addition, an S-band (2856 MHz) RF deflector cavity upstream of the screen (see "TCAV0" in Fig. 1) is used to streak the beam vertically across the screen in order to time-resolve the horizontal

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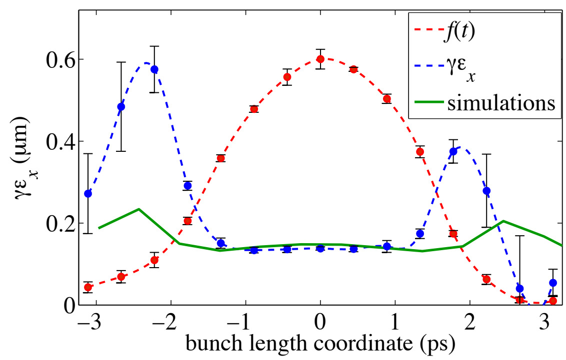

Figure 2: Measured (blue dots) and simulated (green curve) time-sliced horizontal emittance along the length of the bunch at a charge of 20 pC. Smooth curves on the measured data aid the eye and $f(t)$ is the measured bunch temporal distribution on an arbitrary scale.

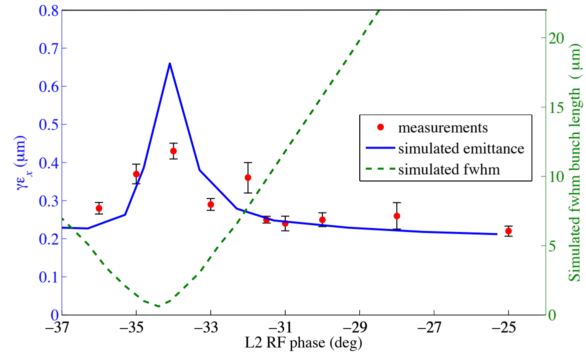

Figure 3: Measured (red circles) and simulated (blue curve) projected emittance at 10 GeV versus L2-linac RF phase with a bunch charge of 20 pC. Simulated bunch length (green dashed curve) also shown at the right axis.

emittance. The horizontal emittance is then sliced up in time and plotted versus the bunch length time coordinate in Fig. 2. *IMPACT-T* tracks the particles from the photocathode to “OTR2”, including 3D space charge force. The initial distribution is based on the measured laser shape, and a thermal emittance of 0.14 μm is used in simulations according to the measurements [4]. The simulated slice emittance at “OTR2” agrees well with the measurement as shown in Fig. 2, especially in the core part of the bunch.

The output particles from *IMPACT-T* are smoothed in the longitudinal phase space to reduce high-frequency numerical noise for subsequent *Elegant* simulations. These particles are then tracked through DL1, linacs, BC1, BC2, and the Linac-To-Undulator transport beamline to the entrance of the undulator. *Elegant* simulations include linear and nonlinear transport effects, a 1-D transient model of CSR, and longitudinal space charge effects, as well as geometric and resistive wake fields in the accelerator. We measured the emittance after BC2 at an energy of about 10 GeV in the last 200 m of the linac using four wire-scanners (see Fig. 1). The ‘time-projected’ emittance is calculated based on the four measured beam sizes using the known electron optics between scanners. The horizontal emittances from measurements and *Elegant* simulations are shown in Fig. 3, with an rf phase shift of -1.3° in simulations to fit the experimental data. This phase shift may come from rf drift during the few hour measurement session, where feedback loops are not operable at the very low charge setting. A particle truncation of 6% was applied to the bunch tails to obtain projected emittance values in simulation which are comparable to measurement methods. The simulated fwhm bunch length is also shown at the right axis. Since the compressed bunch length is not directly measurable at a 1-μm level, a photodiode with bandwidth 1.0-2.5 μm is used to collect the coherent optical transition radiation (COTR) signal of another OTR screen located just downstream of BC2 (see “OTR22” in Fig. 1). The simulated bunching form factor over the same detector wavelength range agrees pretty well with the measurements [4], indicating that the minimum bunch length may be below 1 μm for this very low charge scenario, as predicted from simulations.

FEL SIMULATIONS AT 20 PC

The macro-particles dumped from *Elegant* are used as an input for the *Genesis*1.3 FEL code to evaluate the FEL performance. The longitudinal wakefield in the undulator is negligible at this low charge and is not included in these simulations.

In order to generate very short x-ray pulses, it is advantageous to operate BC2 in the over-compression mode where the current is higher in the central part of the bunch instead of the double-horn current profile from an under-compressed bunch. This can be achieved when operating L2-linac at -35° (hereafter the phase represents the experimental phase, which is -1.3° shifted from simulations). At this phase, *Elegant* tracking shows that a fwhm bunch length of about 1 μm with a peak current above 3 kA can be expected at the undulator entrance. As shown in Fig. 4, the x-ray power at 1.5 Å saturates at about 60 m of undulator length, well within the LCLS total undulator length (132 m). The inset plot also shows a typical FEL power profile near the end of the LCLS undulator approaching 500 GW with a fwhm x-ray pulse duration of about 2 fs. The integrated photon flux is about 3×10^{11} for this 2-fs x-ray pulse with 3% statistical fluctuation. This fluctuation has its origin in shot noise startup and does not take into account machine jitters.

When the LCLS is operated at a beam energy of 4.3 GeV (turning off L3-linac), soft x-ray photons of 800 eV (1.5 nm in wavelength) will be produced. Due to this longer radiation wavelength and hence stronger slippage effect in the undulator, a single x-ray spike with full longitudinal coherence may be expected. In the over-compression mode, with the L2-linac phase setting at -35.5°, the *Genesis* simulation in Fig. 5 shows the 1.5 nm FEL may reach saturation at $z = 25$ m with a nearly single longitudinal spike of 2 fs duration. The integrated photon flux is about 2.4×10^{11} with 20% statistical fluctuation at this saturation point.

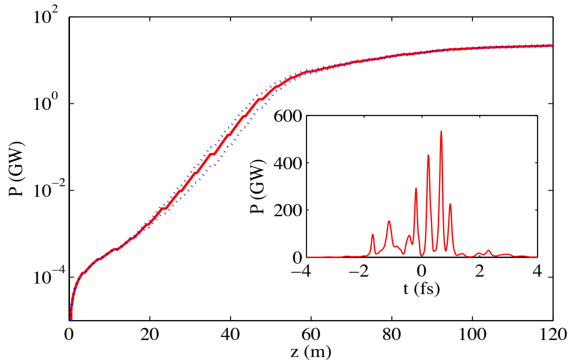

Figure 4: *Genesis* simulation at 1.5 Å. The average FEL power (solid line) and the rms fluctuation (dashed lines) along the undulator. The inset plot shows a snapshot of a typical 2-fs FEL pulse at 100 m. The RF phase of L2-linac is $-35°$ in simulations.

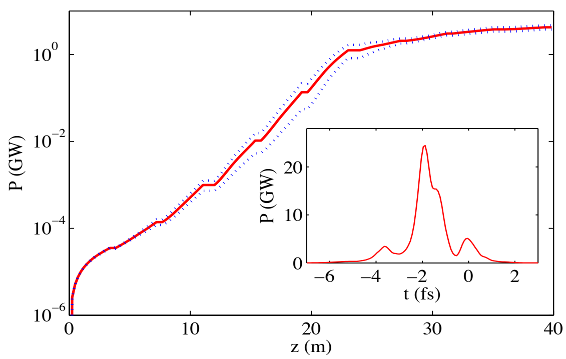

Figure 5: *Genesis* simulation at 15 Å. The average FEL power (solid line) and the rms fluctuation (dashed lines) along the undulator. The inset plot shows a snapshot of a typical 2-fs FEL pulse at 25 m (inset). The RF phase of L2-linac is $-35.5°$ and L3-linac is switched off in simulations.

We recently observed the FEL lasing at 1.5 Å with 20 pC charge, with an FEL power gain of more than 5 orders. Further experimental studies are undergoing.

CHARGE DEPENDENCE STUDIES

Simulations suggest a bunch of 20 pC is capable of generating intense x-rays with a few femtosecond pulse duration. Compared with the nominal charge of 250 pC, a shorter FEL pulse is generated with 20 pC but also with less photons. It is interesting to check the FEL performance at different charges, hence it may produce FELs for different users with a special requirement on the pulse length and photon number. We studied the FEL performance at different bunch charge of 20 pC, 50 pC, 100 pC and 250 pC based on start to end simulations. The UV laser spot size on the photo-cathode is adjusted to minimize the emittance from the thermal part and the space charge. And the laser phase is set at -15 degree for the first 3 charge cases to produce a shorter bunch length from velocity bunching in the injector region, while for the nominal charge of 250 pC a laser phase of -30 degree is used. BC1 and BC2 are fixed at the nominal setup (BC1 R_{56}=45.5mm, BC2 $R_{56} = 24.7mm$), and the L2-linac rf phase is tuned to get a reasonably good emittance and a high peak current after BC2. To get a short FEL pulse length, all the cases are operated at over-compression mode except for the 250 pC case, which is the nominal mode operating at under-compression. The resistive wake fields in the undulator vacuum chamber are included in 100 pC and 250 pC cases.

Table 1 summarizes the simulated main electron and FEL parameters at four different charges. With the charge above 100 pC, it is possible to generate the FEL pulse with 10^{12} photons at 1.5 Å wavelength. At 100 pC, the fwhm x-ray pulse is about 10 fs, which is suitable for pursuing experiments such as single shot molecular imaging.

Table 1: Simulated 1.5 Å FEL Performance at 4 Charges.

Bunch charge (pC)	**20**	**50**	**100**	**250**
UV laser diam.(mm)	0.6	0.6	1	1.2
UV laser fwhm (ps)	4	4	7	7
laser heater (KeV)	off	10	10	10
Inj. σ_z (rms)	260	370	475	690
Final I_p (kA)	$\sim$3.5	$\sim$5	$\sim$5	$\sim$3
Final slice $\gamma\varepsilon_x$ (μm)	$\sim$0.3	$\sim$0.3	$\sim$0.35	$\sim$0.6
FEL pulse fwhm(fs)	$\sim$2	$\sim$4	$\sim$10	$\sim$60
FEL photons (10^{11})	$\sim$3	$\sim$3	$\sim$10	$\sim$10

In summary, we have shown the extraordinary brightness of a low charge bunch produced by the LCLS injector and accelerator. FEL simulations indicate such a bunch may generate hundreds of GW of hard x-ray power at 1.5 Å and nearly a single longitudinal spike of 2 fs at 1.5-nm wavelength. Such high-power, ultrashort x-ray pulses may open up new applications in many areas of science. In addition, the achieved beam brightness may enable a more compact design of a future hard x-ray FEL facility.

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