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INVESTIGATION OF ATTOSECOND PULSE GENERATION SCHEMES FOR UK XFEL

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Abstract

Intra-atomic dynamics are fundamental to organic processes such as photosynthesis. X-Ray spectroscopy, using pulses of tens of femtoseconds durations generated by Free-Electron Lasers (FELs), has enabled great progress in understanding this field. Sub-femtosecond pulses would enable new discoveries in the ultrafast timescales of reactions and transitions. In this paper, attosecond pulse generation is investigated for the UK XFEL Conceptual Design project's short pulse requirements, with a focus on the XLEAP (X-Ray Laser Enhanced Attosecond Pulses) scheme from LCLS. Simulation studies using the code Genesis 1.3 (v4) are used to investigate and optimise the FEL output properties and further explore methods of enhancing the output power. Simulation results indicate that a post saturation magnetic chicane can be used to double the FEL pulse peak power.

INTRODUCTION

Attosecond pulses are essential for probing intra-molecular dynamics at subfemtosecond timescales [1]. The UK XFEL Science Case has identified key uses for pulses of this timescale. One example is understanding and improving the performance of photo-voltaic power sources and electrochemical energy storage methods [2]. Semiconductors forming the base of photovoltaics can be probed to better understand photoelectron generation and transport. In electrochemical energy storage, such as Lithium-Ion batteries, the interactions between electrons and electrolyte ions can be studied and the degradation dynamics of these materials better understood to improve their efficiency.

High Harmonic Generation (HHG), done by driving a gaseous medium with high power femtosecond lasers, was once the most common way to generate attosecond pulses [3]. However the work of A. Zholents on Enhanced SASE (eSASE) contributed to improving the synchronisation and power output of attosecond pulses generated by FELs [4]. XLEAP, developed by LCLS [5] and based on the eSASE method, was investigated in this paper as a candidate attosecond pulse generation scheme for UK XFEL.

SETUP OVERVIEWS

XLEAP schemes comprise the following components: a modulating undulator to apply a sinusoidal modulation onto the beam energy, followed by a dispersive magnetic chicane to shear the beam modulation and convert it into a current distribution consisting of sharp spikes, and finally a radiator section to generate and amplify the FEL interaction. Figure 1 illustrates the basic setup.

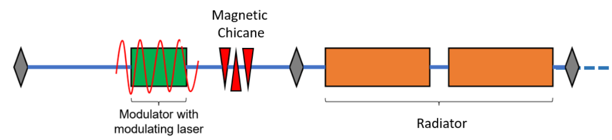

Figure 1: Illustration of Setup 1. For the simulations multiple radiator sections were included. Setup 2 adds a magnetic delay chicane and further radiator sections.

After optimising and investigating the performance of Setup 1, the possibility of elongating the electron bunch to generate a train of current spikes was investigated. It was thought that adding magnetic delay chicanes to shift the radiation spikes to the adjacent current spikes might allow higher power pulses to be produced. Setup 2 included these additions to Setup 1.

ELECTRON BEAM GENERATION

For quicker initial parameter optimisation electron beam profiles which modelled the physical effects of modulation and chicane compression were generated. These were imported directly into the radiator section in Genesis 1.3 (v4) simulations. Figure 2 shows an example—the top row (left to right) shows the initial current profile, the longitudinal phase space after modulation and the sheared phase space after the chicane. The bottom row (left to right) shows the slice analysis of energy, energy spread and current after the chicane.

The macroparticles comprising the electron bunch were initially distributed with Gaussian distributions in position s and energy E. The beam had peak current $I = 3\,\mathrm{kA}$ and charge $Q = I\sigma_t\sqrt{2\pi}$, where σ_t is the standard deviation of the profile. A sinusoidal energy modulation was constructed with modulation depth M (double the amplitude) as a percentage of E, and modulation period λ_M. This was imposed onto the initial distribution in E. Shearing of this modulated beam energy was achieved using the magnetic chicane's dispersive parameter R_{56} where

$$\Delta s = R_{56}\frac{\Delta E}{E}. \quad (1)$$

Here ΔE is the energy offset from resonance E and Δs is the shift in particle position due to the chicane. The resultant beam energy E, energy spread σ_E, and current profiles were sliced into histogram bins which were averaged and the final values were saved onto the beam profiles. The number of

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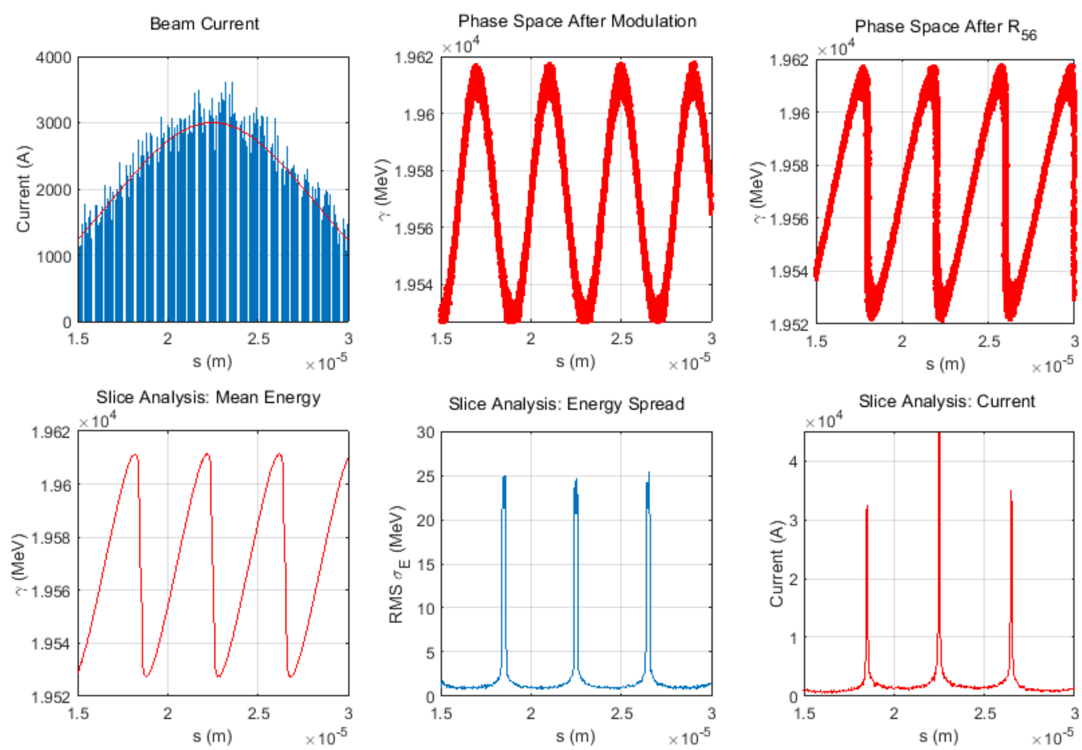

Figure 2: Overview of generated beam properties.Top row (left to right): the initial current profile, the longitudinal phase space after modulation and the sheared phase space after the chicane. Bottom row (left to right): slice analysis of energy, energy spread and current after the chicane.

macroparticles was increased until numerical convergence was achieved.

PARAMETER OPTIMISATION

Undulator and electron beam parameters were optimised by investigating values near theoretically predicted ones (where applicable) or by starting with a larger sample space and converging. The merit functions for the optimisation were minimal temporal durations of the FEL pulses and power per undulator length.

Whilst simulating Setup 1, λ_M was initially set to 800 nm. After parameter optimisation, the peak power results were significantly lower than the results reported from LCLS [5]. As a result, λ_M was increased to 4 µm, a typical value used at LCLS, which generated a shorter FEL pulse with higher peak power. Simulations were done of an equivalent SASE case to determine the FEL cooperation length l_c. This was done to compare the pulse durations achieved in the XLEAP simulations. The cooperation length was estimated in two ways—firstly by calculating the average spacing of the SASE spikes and using the fact that this spacing is $\approx 2\pi l_c$, giving a value of l_c=110 as, and secondly via the power gain length L_g using $\rho = \lambda_w/(4\pi L_g\sqrt{3})$ and $l_c = \lambda_r/(4\pi\rho)$, which gave l_c=140 as.

For Setup 2, the electron bunch length was increased to generate a longer train of current spikes. The number of chicane delays added post saturation was investigated. A single delay and additional FODO cell provided a significant increase in FEL power and is the most efficient and sustainable choice in terms of pulse power generated per metre. The position of this delay was also optimised. Table 1 outlines an overview and comparison of key parameters with reported values from the XLEAP configuration at LCLS.

RESULTS

Best results from full scale simulations of Setup 1 and Setup 2 with optimised parameter values, where the modulation and chicane stage were fully modelled in Genesis 1.3, are shown in Fig. 3. The modulating laser power was set to generate the optimal value of M on the beam. The shortest FWHM pulse durations were 122 as from Setup 1 and 136 as from Setup 2. The addition of a chicane delay, 6 metres of undulator length, and lengthening of the electron bunch to form Setup 2 produced a peak power of 2.8 TW in a train of spikes, double the maximum power of 1.4 TW from Setup 1. These values give predicted output pulse energies of 170 µJ for Setup 1 and 380 µJ for Setup 2.

CONCLUSIONS AND OUTLOOK

The schemes simulated produce pulse energies and durations comparable to those reported from the XLEAP scheme demonstrated at LCLS. Setup 2, in which a delay chicane is

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Table 1: Parameter Overview

Parameter	**Setup values**	**XLEAP values** [5]
Beam Energy E	10 GeV	3–5 GeV
Resonant photon energies	1–2 keV	570–905 eV
Normalised emittance ϵ	0.2 µm	0.4 µm
Peak current (before compression) I	3 kA	2.5–3.5 kA
Modulator period λ_{MOD}	0.385 cm	0.32 cm
Modulator parameter a_w	89.2	0–74
Radiator period λ_{RAD}	0.0435 m	0.03 m
Radiator parameter a_w	3.1412	6.90–7.02
Compression chicane R_{56}	3.2×10^{-4} m	$0-9.0 \times 10^{-4}$ m
Modulation depth M	0.43%	<1%
Electron bunch length	40 µm (Setup 2)	N/A
Post saturation delay chicane R_{56}	1.9×10^{-4} m	N/A

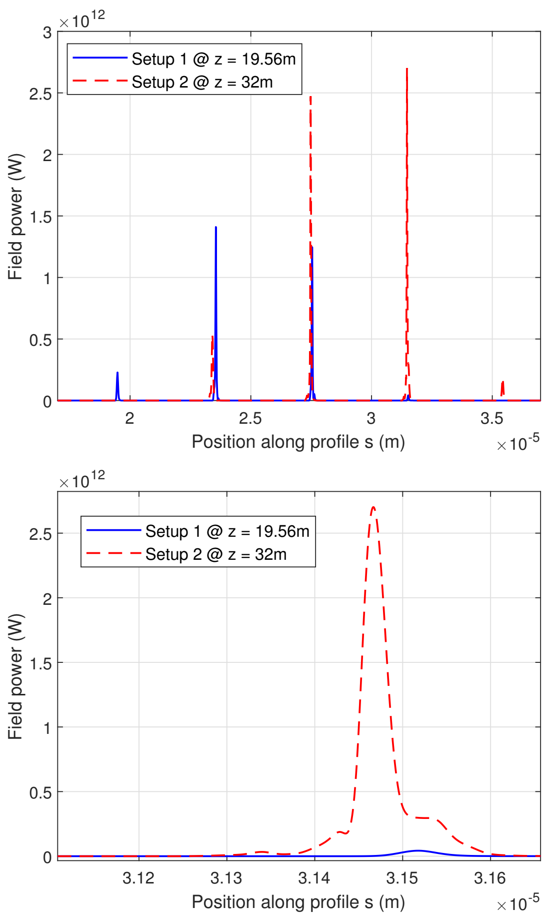

Figure 3: Pulse profiles from each setup. Top: the full pulse. Bottom: enlargement.

used to realign the FEL pulse with a current spike further along the bunch, produced double the peak power of Setup 1 with only a small increase in pulse duration. The pulse durations are close to l_c values of the radiator undulators which are lower bounds, suggesting the system is well optimised and pulses are close to Fourier-transform limited. However, predictions of performance are based on simulations only, assuming ideal electron bunches with no system errors, whereas the results from XLEAP are measured experimental values. Nevertheless, the work done so far sets the scene for further investigation of new XLEAP-based configurations for the generation of short pulses at a future UK XFEL. Future work will include the introduction of more realistic electron bunch distributions, analysis of the effect of electron beam energy spread and emittance on the FEL output, and investigation of new methods for isolating a single FEL pulse from within the train of pulses.

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