Self-seeded FEL wavelength extension with high-gain harmonic generation

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Abstract: We study a self-seeded high-gain harmonic generation (HGHG) free-electron laser (FEL) scheme to extend the wavelength of a soft X-ray FEL. This scheme uses a regular self-seeding monochromator to generate a seed laser at the wavelength of 1.52 nm, followed by a HGHG configuration to produce coherent, narrow-bandwidth harmonic radiations at the GW level. The 2nd and 3rd harmonic radiation is investigated with start-to-end simulations. Detailed studies of the FEL performance and shot-to-shot fluctuations are presented.

Keywords: FEL, self-seeding, HGHG

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1 Introduction

X-ray free electron lasers (FELs), which demonstrate an improvement in peak brightness of approximately ten orders of magnitude over third-generation light sources, have shown remarkable scientific capabilities in chemistry, biology, material science, as well as many other disciplines. There are two main schemes for single pass short wavelength FELs: self-amplified spontaneous emission (SASE) [1, 2] and high-gain harmonic generation (HGHG) [3, 4]. Until recently, most modern high-gain FELs in the short wavelength (e.g., X-ray) region, such as the LCLS and the SACLA FEL [5, 6], have been operated in SASE mode, which is characterized by excellent transverse coherence. However, SASE FELs have poor temporal coherence and large shot-to-shot fluctuations in both the time and frequency domains, since they start from shot noise [7].

HGHG FELs can generate fully coherent, high gain harmonic radiation from a seed laser. However, the harmonic number \((n)\) of a single-stage HGHG FEL is limited by the requirement that the induced energy spread be less than the Pierce parameter \((\rho)\) in the radiation undulator ( radiator) to achieve high gain. So far, the highest harmonic obtained with single-stage HGHG is the 13th harmonic at 20 nm using a 1.2 GeV electron beam at FERMI [8]. In order to reach higher harmonics, so as to obtain shorter wavelength fully coherent FEL, several schemes have been proposed in recent years. Among them, the cascaded HGHG scheme with the help of the “fresh bunch” technique was proposed in 2001 [9]. Recently, 4.3 nm radiation (60th harmonic of a 260 nm UV seed laser) has been achieved with a two-stage HGHG configuration at FERMI [10]. One other scheme, EEHG [11], was first proof-of-principle demonstrated at SLAC [12]. In 2011, researchers from Shanghai Institute of Applied Physics (SINAP) also observed the third harmonic from EEHG, which was further amplified to saturation [13]. Currently, EEHG at 160 nm (15th harmonic of a 2400 nm seed laser) has been produced at SLAC [14]. However, the cascaded HGHG and EEHG still have difficulty in generating hard X-ray FELs due to a lack of external seeds at X-ray wavelengths [15].

To solve the difficulty of external seeding at very short wavelengths, colleagues at DESY proposed an approach of self seeding in 1997 [16], and recently a simplified monochromator version for hard X-rays [17]. This self-seeded FEL starts from a SASE stage, which operates in the linear regime. A following monochromator is used to generate a purified seed from the SASE radiation, and meanwhile the electron beam after the SASE stage goes through a bypass chicane. They recombine in an amplification undulator (amplifier stage) for further interaction, where the seed radiation gets amplified to saturation, producing near Fourier transform limited X-rays. The self-seeding approach works for both soft and hard X-ray FELs and has been successfully demonstrated recently [15, 18]. It is worth noticing that two different configurations of monochromator have been used depending on the spectral range. For X-ray FELs...
with the photon energy below 2 keV, a grating-based monochromator has been used [15], while for X-ray FELs with the photon energy above 4.5 keV, a diamond-based monochromator is more popular [18]. Within the photon energy range from 2 keV to 4.5 keV, the self-seeded FEL is difficult due to a lack of monochromator materials. This motivates to study alternative schemes to cover the energy gap from 2 to 4.5 keV.

In this paper, we study a new scheme combining the self-seeding approach with HGHG to produce fully coherent X-rays. It can not only fill the above photon energy gap not easily achieved by regular self-seeded FELs, but also extend the wavelength of a soft X-ray FEL machine to the harder X-ray region. This self-seeded HGHG scheme will be described in Section 2, followed by the FEL simulation results in Sections 3 and 4.

2 Self-seeded HGHG Scheme

The proposed setup of the self-seeded HGHG scheme is shown in Fig. 1. It consists of two stages: the SASE stage and the HGHG stage. The SASE stage follows the regular self-seeding configuration, comprising a SASE undulator, an X-ray monochromator, and an electron beam bypass chicane allowing room for the monochromator. An electron beam first traverses the SASE undulator, generating SASE radiation in the linear regime. After the SASE undulator, the radiation goes through the X-ray monochromator, which transmits a narrow band of wavelengths. The transmitted radiation is then used as a seed for the following FEL amplifier. Meanwhile, the electron beam from the SASE undulator goes through a bypass chicane, being properly delayed, and recombines with the seed radiation at the entrance of the HGHG stage. The bypass chicane also helps to wash out the microbunching of the electron beam built up in the SASE undulator.

Compared to the external seed laser in the regular HGHG scheme, the seed radiation from the SASE stage has a much lower power, limited to a few hundred kilowatts because of the damage threshold of the state-of-the-art X-ray monochromator optics [15]. As a result, we need to use a long modulation undulator with two combined functions. The first function is to amplify the seed radiation from the SASE stage, which is mainly achieved with the upstream part of the modulation undulator. The second is to introduce energy modulation to the electron beam, as in a normal HGHG modulator. The energy modulated electron beam then goes through the dispersion chicane with proper $R_{56}$, getting density modulated, and radiates at the harmonic wavelength of the seed.

In this self-seeded HGHG scheme, the electron beam quality inevitably degrades when it is used to amplify the seed radiation from the SASE stage. Therefore a compromise should be made between the modulation radiation power and the induced electron energy spread growth in the HGHG modulator. In this paper, the modulation laser power is kept at hundred megawatt level to avoid a significant energy spread degradation of the electron beam in the seed amplification process.

To eliminate the impact of electron energy spread degradation in the seed amplification process, we have also proposed a self-seeded HGHG FEL setup with separated seed amplifier and modulator (see Fig. 2). In this case an electron beam with longer bunch length is used, which generates double-spike seed after the X-ray monochromator. The head spike of the seed is then aligned with the tail part of the electron bunch at the entrance of the amplifying undulator ($U_A$). Therefore only the tail part of the electron bunch is used to amplify the seed while the head part is kept undisturbed and “fresh”. After the $U_A$ undulator, the electron bunch is delayed by a small chicane ($C_{B2}$), and consequently the head part is aligned with the seed radiation in the modulation undulator ($U_{M2}$) and gets energy-modulated. After the $U_{M2}$ undulator, the electron beam undergoes the same procedure as the above setup.

In the following discussions, the first setup is referred to as the long modulator case, while the second setup is referred to as the “fresh bunch” case.

![Fig. 1. Schematic of self-seeded HGHG FEL. $U_S$ is a SASE undulator, $U_M$ is a long modulation undulator with combined functions as seed amplifier and HGHG modulator, and $U_R$ is a radiation undulator (radiator) of HGHG. $C_B$ is a bypass chicane steering the electron beam around the X-ray monochromator, while $C_D$ is a dispersion chicane of the HGHG stage.](098102-2)
3 FEL simulation of long modulator case

As a representative example, we use the soft X-ray self-seeded (SXSS) FEL at LCLS to illustrate the feasibility of this scheme. Parameters are assumed based on the SXSS FEL for time-dependent FEL simulation using GENESIS [19] code. The electron beam has a central energy of 4.3 GeV, an uncorrelated energy spread of 1.0 MeV, and a normalized transverse emittance of 0.5 mm-mrad. It has a uniform current profile with a pulse duration of 30 fs and peak current of 2.5 kA. The SASE undulator (Uₗ) is resonant at 1.52 nm. It uses 5 LCLS undulator segments and has a total length of 19.8 m (including the focusing optics in between). This is based on the consideration of keeping the SASE FEL power at the highest level while avoiding damage to the X-ray monochromator optics. The monochromator is assumed to have a Gaussian spectral response with a maximum power efficiency of 0.02 at 1.52 nm. An example of the FEL power profiles and power spectra after the SASE undulator and X-ray monochromator is shown in Fig. 3. One can see from the figure that after the monochromator the radiation peak power drops to about 220 kW while a narrow bandwidth is filtered out.

For the HGHG modulator, an optimal value for the electron energy modulation amplitude $\Delta \eta_m$ is [3, 4]

$$\Delta \eta_m \approx n\sigma_\eta,$$  \hspace{1cm} (1)

with $\sigma_\eta$ the intrinsic uncorrelated energy spread and $n$ the harmonic number. In order to obtain the optimal energy modulation, the length of Uₘ undulator needs to be optimized. Herein we study the 2nd and 3rd harmonic generation and accordingly the undulator length is chosen to be 13 m and 14 m, respectively, to meet the above criteria of optimized energy modulation amplitude.

The momentum compaction factor $R_{56}$ of the chicane C₄ is set to satisfy [11]

$$R_{56} \Delta \gamma_m / \gamma \approx \lambda / 4,$$  \hspace{1cm} (2)

where $\lambda$ is the wavelength of the seed laser. In this long modulator case, the value of $R_{56}$ are 0.56 μm and 0.46 μm for the 2nd and 3rd harmonic generation, respectively. The longitudinal phase space of electron beam after the modulation undulator (Uₘ) and dispersion chicane are shown in Fig. 4.

The main electron and radiation parameters used in this study are summarized in Table 1. With these parameters, GENESIS simulations were performed. Figure 5 illustrates the evolution of the FEL power of the 2nd and 3rd harmonic radiation along the radiation undulator. We can see from the figure that the 2nd harmonic radiation at the exit of the radiation undulator is about 3.6 GW, while the 3rd harmonic radiation is about 0.9 GW. Figure 6 shows the output power profile and spectra of the 2nd and 3rd harmonic radiation at the exit of the radiation undulator, which indicate that the normalized spectral width (FWHM) of the 2nd and 3rd harmonic are $1.8 \times 10^{-4}$ and $1.5 \times 10^{-4}$ respectively.
4 FEL simulation of “fresh bunch” case

To generate the desired seed after the X-ray monochromator, a 60 fs long electron bunch is used, which is twice that used in the long modulator case. Other electron parameters are kept unchanged, as in Table 1. The SASE undulator (U_S) and the X-ray monochromator remain the same as in the long modulator case.

An example of the FEL power profiles and power spectra after the SASE undulator and X-ray monochromator is shown in Fig. 7. As shown in the figure, the temporal profile of the seed has double spikes. The head spike of the seed is then aligned with the tail part of the electron bunch at the entrance of the amplifying undulator (U_A) by fine-tuning the bypass chicane (C_B) at μm level. The seed radiation copropagates with the electron bunch in the undulator and gets amplified. The length of U_A undulator is chosen based on the consideration that the seed laser power can be amplified as much as possible while keeping the head part of the electron bunch fresh. In this case, the U_A undulator length is 11 m.

The evolution of the seed radiation pulse and electron bunch in U_A is shown in Fig. 8. It can be seen from the figure that, while the peak power of the radiation is amplified to about 100 MW in the U_A undulator, the head electrons in the bunch do not get disturbed. It is obvious that the energy spread of the tail electrons becomes larger, however, it is also worth noting that the energy spread increase is not significant.

After the U_A undulator, the electron bunch is delayed by the C_B2 chicane, and the head part electrons are aligned with the seed radiation in the U_M2 modulation...
The length of $U_{M2}$ undulator is optimized according to Eq. (1). For the 2nd and 3rd harmonic generation, the undulator length is chosen to be 2.5 m and 3.5 m, respectively. The dispersion chicane $C_D$ in this "fresh bunch" case has an $R_{56}$ of 0.50 m and 0.42 m for the 2nd and 3rd harmonic generation, respectively, according to Eq. (2).

Figure 9 shows the evolution of the FEL power of the 2nd and 3rd harmonic radiation along the radiation undulator. The length of the radiation undulator $U_R$ is 20 m and 28 m, respectively. As shown in the figure, the 2nd harmonic radiation at the exit of the radiation undulator is about 7.8 GW, and the 3rd harmonic radiation has a power of about 1.9 GW.

The output power profile and spectra of the 2nd and 3rd harmonic radiation at the exit of the radiation undulator are shown in Fig. 10, which demonstrate that the normalized spectral width (FWHM) of the 2nd and 3rd harmonic are $1.6 \times 10^{-4}$ and $1.4 \times 10^{-4}$ respectively.

5 Conclusion

In this paper, we have proposed a self-seeded HGHG scheme, which may be an attractive way to extend regular self-seeded FELs to shorter wavelengths, especially within the photon energy range from 2 keV to 4.5 keV, which is difficult to achieve due to a lack of monochromator materials. This method is also applicable to extend hard X-ray self-seeding with crystals to even shorter wavelengths.
wavelengths. We use parameters based on the SXSS FEL at LCLS to simulate the scheme in two cases. In the long modulator case, we obtained 2nd harmonic with FEL power 2.3 GW and normalized spectral width (FWHM) $1.8 \times 10^{-4}$, and 3rd harmonic with FEL power 0.7 GW and normalized spectral width $1.5 \times 10^{-4}$. In the “fresh bunch” case, we obtained 2nd harmonic with FEL power 5.6 GW and normalized spectral width $1.6 \times 10^{-4}$, and 3rd harmonic with FEL power 1.7 GW and normalized spectral width $1.4 \times 10^{-4}$.

Note that in these demonstration examples, we chose a fundamental energy at 810 eV to calculate the second and third harmonic performance. The soft X-ray self-seeding setup can work at 1.5 keV fundamental energy with the same monochromator, so we can scale up to reach 4.5 keV at the third harmonic to cover the energy gap we discussed earlier. Also, we used a conserved energy spread of 1 MeV rms based on the present LCLS operation parameters. A lower energy spread is possible based on LCLS-II design studies, which should help the harmonic performance. This will be investigated in the future.

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