Harmonic lasing in X-ray FELs

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ABSTRACT

Contrary to nonlinear harmonic generation, harmonic lasing in a high-gain FEL can provide much more intense, stable, and narrow-band FEL beam which is easier to handle if the fundamental is suppressed. We performed thorough study of the problem within framework of 3D model taking into account all essential effects. We found that harmonic lasing is much more robust than usually thought, and can be widely used in the existing or planned X-ray FEL facilities. LCLS after a minor modification can lase at the 3rd harmonic up to the photon energy of 25-30 keV providing multi-gigawatt power level. At the European XFEL the harmonic lasing would allow to extend operating range ultimately up to 100 keV.

Keywords: Free electron laser, X-ray, harmonic lasing

1. INTRODUCTION

Harmonic lasing in single-pass high-gain FELs, i.e. the radiative instability at an odd harmonic of the planar undulator developing independently from lasing at the fundamental wavelength, might have significant advantages over nonlinear harmonic generation providing much higher power, much better stability, and smaller bandwidth.

Thorough revision of the parameter space for harmonic lasing has been performed recently within framework of 3D FEL theory and taking into account all essential effects. It has been found that harmonic lasing can be of interest in many practical cases. In fact, gain at higher harmonics can be higher than that at the fundamental for diffraction limited electron beams with small ratio of emittance to radiation wavelength. This parameter space corresponds to the operating range of soft X-ray beamlines of X-ray FEL facilities. For hard x-ray FELs are in this parameter range the properties of saturated harmonic lasing at a given wavelength are approximately the same as those of the retuned fundamental.

In this paper we consider a possible application of harmonic lasing to different X-ray FEL facilities, and conclude that they can strongly profit from this option. In particular, LCLS can significantly extend its operating range towards shorter wavelengths making use of the third harmonic lasing with the help of the intra-undulator spectral filtering and phase shifters. In the case of the European XFEL, the harmonic lasing can allow to extend the operating range, to reduce FEL bandwidth and increase brilliance. Similar improvements can be realized in other X-ray FEL facilities with gap-tunable undulators like FLASH II, SACLA, LCLS II, etc.

2. GAIN LENGTH

In the linear regime of a SASE FEL operation the fundamental frequency and harmonics grow independently with gain lengths \( L_g^{(h)} \) (here the superscript denotes harmonic number). In the case of the simultaneous lasing in the parameter range \( 2\pi\epsilon/\lambda \lesssim 1 \) the third harmonic always has the shortest gain length, i.e. it saturates first. Let us formulate the problem differently. We can produce radiation at a target wavelength \( \lambda \) by two ways. First option is tuning of FEL amplifier to the fundamental wavelength \( \lambda \). Second option is tuning of FEL amplifier to the fundamental wavelength \( \lambda/h \) and generate \( h \)-th harmonic with wavelength \( \lambda \). The question is which option provides shortest gain length.

Tuning of the FEL amplifier can be performed either by increasing electron energy, or reducing the undulator parameter \( K \) as it is implemented in x-ray facilities. For the case when we can neglect energy spread effects,
and assuming that the beta-function is tuned to the optimum value corresponding to maximum gain for each case we have:\(^\text{10}\)

\[
\frac{L_g^{(1K)}}{L_g^{(h)}} = \frac{h^{1/2}KA_{JJh}(K)}{K_{re}A_{JJ1}(K_{re})},
\]

\[
\frac{L_g^{(1\gamma)}}{L_g^{(h)}} = \frac{h^{5/6}A_{JJh}(K)}{A_{JJ1}(K)}.
\]

The superscripts \((1K)\) and \((1\gamma)\) refer to retuning of the undulator parameter and electron energy, respectively. \(A_{JJh}\) is coupling factor defined in a standard way.\(^\text{2,4,10}\) The retuned undulator parameter \(K_{re}\) is given by \(K_{re}^2 = (1 + K^2)/\hbar - 1\) (obviously, \(K\) must be larger than \(\sqrt{\hbar - 1}\)). For large \(K\) the ratio in the first line of Eq. (1) is reduced to \(hA_{JJh}/A_{JJ1}\), so that the gain length of the retuned fundamental mode is larger by a factor of 1.41 (1.65) than that of the third (fifth) harmonic. For an arbitrary \(K\) we plot in Fig. 1 the ratio of gain lengths (1). It is seen that the third harmonic always has an advantage (in case of negligible energy spread), i.e. its gain length is shorter for any value of \(K\).

In the case of boosting electron energy for lasing at three times reduced fundamental wavelength, the advantage of using the 3rd harmonic is not that obvious (since an increase of electron energy at the same wavelength leads to a decrease of the parameter \(2\pi\epsilon/\lambda\) thus improving FEL properties, in general). However, even in this case, the gain length for the third harmonic is shorter if rms value of \(K\) is larger than 1.4.

Let us present a numerical example for the European XFEL. New baseline parameters\(^\text{16–18}\) assume operation at different charges from 20 pC to 1 nC and three different electron energies: 10.5, 14, and 17.5 GeV. Let us consider operation at 1 Å with the charge 0.5 nC, peak current 5 kA, normalized emittance 0.7 \(\mu\)m, and electron energy 10.5 GeV in a planar undulator with the period 4 cm. For the rms K value of 2.3 the fundamental wavelength is 3 Å, which is suppressed by using phase shifters and/or spectral filtering.\(^\text{10}\) Then we have third harmonic lasing at 1 Å with the field gain length of 6.9 m for \(h = 3\). Now we change the rms K value to 1.05 so that lasing at the fundamental frequency occurs at 1 Å. In that case for \(h = 1\) we find that the gain length is 10.4 m, i.e. about 50 \% larger than in the case of 3rd harmonic lasing. If, instead, we increase beam energy to 17.5 GeV and lase at 1 Å with \(K = 22\), the gain length is 7.9 m, i.e. it is still visibly larger than in the case of low energy and the 3rd harmonic lasing.

3. INCREASE OF BRILLIANCE

FEL properties at saturation can be calculated with the help of a numerical simulation code (for 1-D simulations see Refs.\(^\text{3}\) and\(^\text{10}\)). Here we present a qualitative consideration for the case when the energy spread effect is a
relatively weak correction to the FEL operation, and the tuning to the same wavelength is achieved by changing parameter K. A simple estimate ("effective" parameter $\rho_3^{30}$ is reduced depending on harmonic number) suggests that in the case of harmonic lasing, both the saturation power and the bandwidth are reduced by the same factor. Degree of transverse coherence is about the same for a harmonic and for the fundamental mode since this quantity is mainly defined$^{26-28}$ by the parameter $2\pi \epsilon/\lambda$, which is the same in the considered case. Thus, the brilliance (a figure of merit for performance of X-ray FELs), depending on the ratio of peak power to bandwidth, remains about the same. In other words, use of harmonic lasing instead of lasing at the fundamental frequency is equivalent to a mild monochromatization of the X-ray beam.

Here we propose a simple method of brilliance improvement. In a gap-tunable undulator one can combine a high power and a narrow bandwidth. A possible trick is to use harmonic lasing in the exponential gain regime in the first part of the undulator, making sure that the fundamental frequency is well below saturation (two options can be considered: with and without disruption of the fundamental by phase shifters, depending on the ratio of gain lengths). In the second part of the undulator the value of K is reduced such that now the fundamental mode is resonant to the wavelength, previously amplified as the harmonic. The amplification process proceeds in the fundamental mode up to saturation (see Fig. 2. In this case the bandwidth is defined by the harmonic lasing (i.e. it is reduced by a significant factor depending on harmonic number) but the saturation power is still as high as in the reference case of lasing at the fundamental, i.e. brilliance increases. Important is that this option does not require extra undulator length.

4. PRACTICAL APPLICATIONS

4.1 LCLS

Linac Coherent Light Source (LCLS) is the first hard X-ray free electron laser.$^{11}$ Due to the limited electron energy and fixed-gap undulator, the facility can presently cover photon energy range up to 10 keV. LCLS undulator$^{31}$ consists of 33 identical 3.4-m-long segments, undulator period is 3 cm, and the peak undulator parameter is 3.5 (rms value of K is 2.5). The 16th segment is replaced with a chicane for operation of the self-seeding scheme.$^{20}$ When this scheme is operated, a crystal monochromator is inserted on-axis while the electron beam goes through the chicane thus by-passing the crystal. We notice that a simple add-on to this setup, namely an insertable filter, would allow the use of the intra-undulator spectral filtering method described in.$^{10}$ As a possible realization of the filter we propose here a silicon crystal (diamond can be considered as an option as well) that is not supposed to spoil phase front$^{15}$ of the third harmonic radiation while attenuating the fundamental harmonic by orders of magnitude. A thickness of the crystal is defined by a required attenuation factor and an expected photon energy range. As an example we consider here the thickness of 600 $\mu$m and third harmonic lasing at 25 keV. Attenuation length at 8.3 keV is $\mu^{-1} = 73 \mu$m, and at 25 keV it is $\mu^{-1} = 1.85 \text{ mm}$, so that the corresponding transmission factors are $2.7 \times 10^{-4}$ and 0.72. With a given thickness of the crystal the scheme would work well in the range 20-30 keV, and for lower photon energies of the third harmonic a thinner crystal would be needed.
In the considered parameter range the spectral filtering method alone is not sufficient, therefore we suggest to combine it with the phase shifters method. We propose to install phase shifters with the shift $4\pi/3$ (the definition of Ref. is used here) after undulator segments 1-5 and 17-22, and with the shift $2\pi/3$ after segments 6-10 and 23-28. As a possible space-saving technical solution one can consider insertable permanent-magnet phase shifters with a length of a few centimeters and a fixed phase shift. Of course, if space allows, the tunable (electromagnetic or permanent-magnet) phase shifters would be more flexible. Note also that phase shifters without spectral filtering might not be sufficient for a sure suppression of the fundamental harmonic.

Let us consider a specific parameter set for third harmonic lasing at 0.5 Å (photon energy 25 keV). The electron beam parameters are as follows: energy is 13.6 GeV (the fundamental wavelength is 1.5 Å), peak current is 3 kA, normalized slice emittance is 0.3 µm, uncorrelated energy spread is 1.4 MeV. The beta-function in the undulator is 30 m. The smallest possible delay (given by either the required beam offset or minimum $R_{56}$ for smearing of beam modulations at the fundamental wavelength) would define the shortest electron bunch that can be used for operation of this scheme. In our simulations we do not consider a specific bunch length, so that our result is the peak power of the third harmonic radiation in the part of the pulse that overlapped with the electron beam after the chicane. One should also notice that an easy control of the third harmonic pulse duration is possible by changing the delay.

We performed simulations with the code FAST, the results are presented in Fig. 3. The averaged peak power of the third harmonic radiation is 6 GW, and an intrinsic bandwidth is $3 \times 10^{-4}$ (FWHM). The power incident on the crystal is in the range of tens of megawatts, and should not be problematic from the point of view of peak and average power load. Note that the saturation of the third harmonic lasing is achieved after 28th segment, so that there is a sufficient contingency for given wavelength and beam parameters. It means, in particular, that the saturation at 30 keV could be in reach, or the saturation at 25 keV with a larger emittance is possible. We should also note that a reduction of the beta-function would increase the contingency. If one considers the scheme for operation in the range 10-20 keV, it would work with a significantly loosened requirements on the electron beam quality.

As a quick test of harmonic lasing at LCLS one can consider operation with the filter only (without phase shifters), making use of nonlinear generation of the third harmonic in the first part of the undulator if the fundamental harmonic enters nonlinear regime there. The main issues are high power load on the filter and an increase of energy spread in the beam. However, the last issue might be partially tolerated. Indeed, in a SASE FEL the radiation intensity and beam modulations in energy and density consist of random spikes that have a typical duration of FEL coherence time. Thus, energy spread after the chicane is modulated on the same time scale. One can have the situation when some of the third harmonic intensity spikes overlap after the chicane with unspoiled parts of the electron beam, and are amplified in the second part of the undulator without gain.
suppression due to a large energy spread (however, the slippage effects in the second part must be considered). In principle, these spikes can reach saturation in the second part at a high power level before they are caught up by the fundamental harmonic.

4.2 European XFEL

The gap-tunable hard X-ray undulators SASE1 and SASE2 of the European XFEL consist of 35 segments each, the length of a segment is 5 m, the undulator period is 4 cm. The phase shifters are installed between the segments, so that the number of the shifters is big. This means that, at least in some cases, the phase shifter method alone might be sufficient for suppression of the fundamental harmonic. As an example we consider the third harmonic lasing at 0.2 Å (photon energy 62 keV) by the electron beam with the energy of 17.5 GeV and the charge of 100 pC, slice parameters are the same as those given in, beta-function is 60 m, the rms undulator parameter is 1.6. Note that the considered wavelength cannot be reached by lasing at the fundamental harmonic because the undulator parameter is too small in this case. The results of numerical simulations are presented in Fig. 4. Indeed, one can disrupt the fundamental harmonic and let the third harmonic saturate. The averaged peak power is 3 GW, and the bandwidth is $2 \times 10^{-4}$ (FWHM). One can still notice that a stronger suppression of the fundamental would be desirable, so that the spectral filtering method would improve operation of the facility in such a regime. Eventually, the self-seeding scheme will be implemented at the European XFEL, then it is also worth to install a filter. Another option is a closed bump (made by movable quadrupoles between the segments). Such a bump involves two segments with an insertable filter installed between them. We should note that if we consider a 20 pC electron bunch with slice parameters from start-to-end simulations, the third harmonic lasing to saturation can be extended to photon energies up to 100 keV.

Another attractive option that one can consider in the case of the European XFEL is a reduction of the bandwidth by going to harmonic lasing instead of lasing in the fundamental mode. If one combines them as described in, this will happen without reduction of power, i.e. the brilliance will increase. Although this increase is essentially smaller than in the case of application of seeding and self-seeding schemes, the method of combined lasing does not require extra undulator length, is not restricted by a finite wavelength interval, and is completely based on a baseline design. For many experiments, however, such a mild reduction of the bandwidth (to the level of few $10^{-4}$) would be desirable. The detailed numerical simulations of combined lasing will be presented elsewhere.

In conclusion we note that relative intensities of the fundamental and the third harmonics can be easily controlled by changing phase shifters. The simultaneous lasing at the fundamental and the third harmonics with comparable intensities for jitter-free pump-probe experiments can be realized in a wide range of wavelengths and radiation intensities.
4.3 Other facilities and applications

Similar improvements can be realized at other X-ray FEL facilities like SACLA, FLASH II, LCLS II etc. In particular, FLASH II can cover the whole water window with the help of the third harmonic lasing. According to our estimates, one would need to combine phase shifters with intra-undulator spectral filtering, so that some modifications in the undulator beamline would be necessary.

We also suggest that even if fixed-gap undulators are supposed to be used in some X-ray FEL facilities, phase shifters should be incorporated into an undulator design such that the option of harmonic lasing is enabled.

We should also note that electromagnetic phase shifters can have an advantage in comparison with permanent-magnet ones. Indeed, the electromagnetic phase shifters can be switched on and off between electron pulses (or macropulses) so that one can switch between two colors and then to deliver them to different experiments.

One more application of the harmonic lasing is the operation of compact X-ray FEL facilities using relatively low energy of electron beams. In order to reach short wavelength they rely on the technology of short-period small-gap in-vacuum undulators. As an alternative one could consider a more standard and robust undulator technology by going to larger period undulators with larger gaps, and lasing at the third (or even the fifth) harmonic. We estimated, in particular, with the help of formulas of Section 2 that it could be an interesting option for the Swiss FEL.

4.4 Possible technical issues

One can identify possible issues using the fact that the harmonic lasing is more narrow-band process than lasing at the fundamental wavelength (parameter $\rho^3$ is smaller). In particular, harmonic lasing is more sensitive to the undulator phase errors, undulator wakefields etc.

However, undulators for X-ray FELs are usually designed and built with a sufficient safety margin in terms of length and quality. For example, LCLS undulator has phase shake about 1-2 deg for the fundamental wavelength, which means 3-5 deg for the third harmonic. This is still too small phase shake to have a significant impact on the third harmonic lasing.

The wakefields in the undulator can have an impact on the amplification process in X-ray FELs, a relevant parameter is a relative energy change per gain length, divided by $\rho$. However, they can be compensated by using undulator taper as it was successfully demonstrated at LCLS. The harmonic lasing is more sensitive to wakefields, however a proper optimization of the taper would allow to diminish this effect in many practical situations, especially for low charge scenarios.

We have shown in the paper that the application of harmonic lasing allows to generate FEL radiation with intrinsically narrow bandwidth. However, from practical point of view it is important that the energy chirp in the electron beam and energy fluctuations are smaller than a half of that bandwidth. For example, in the case of the European XFEL the chirp can be kept under control and the energy stability can be provided at the level of $10^{-4}$ or better. This would allow to make use of the narrow-band nature of harmonic lasing.

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