Triple modulator–chicane scheme for seeding sub-nanometer x-ray free-electron lasers

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Abstract. We propose a novel triple modulator–chicane (TMC) scheme to convert external input seed into shorter wavelengths. In this scheme, high-power seed lasers are used in the first and the third modulator, while only a very-low-power seed is used in the second modulator. By properly choosing the parameters of the lasers and chicanes, we show that ultrahigh harmonics can be generated in the TMC scheme while simultaneously keeping the energy spread growth much smaller than the beam’s initial slice energy spread. As an example, we show the feasibility of generating significant bunching at 1 nm and below from a low-power (∼100 kW) high harmonic generation seed at 20 nm assisted by two high-power (∼100 MW) UV lasers at 200 nm while keeping the energy spread growth within 40%. The supreme up-frequency conversion efficiency of the proposed TMC scheme, together with its unique advantage in maintaining beam energy spread, opens up new opportunities for generating fully coherent x-rays at sub-nanometer wavelength from external seeds.

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1. Introduction

Free-electron lasers (FELs) can provide tunable high-power coherent radiation, which has wide applications in biology, chemistry, physics, material science and so on. In the x-ray wavelength range, most of the FELs operate in the self-amplified spontaneous emission (SASE) mode [1, 2]. One FEL working in the SASE mode has been successfully operated at hard x-ray wavelengths [3], which marks the beginning of a new era of x-ray science [4–6]. Very recently, a compact SASE FEL that employs a medium-energy beam and in-vacuum undulators also lased at hard x-ray wavelength [7]. While the radiation from a SASE FEL has excellent transverse coherence, it typically has rather limited temporal coherence and relatively large statistical fluctuations, because a SASE FEL starts from electron beam shot noise. There are many applications (such as soft x-ray resonant inelastic scattering, spectroscopic studies of correlated electron materials, etc) that require, or could benefit from, improved temporal coherence. Seeding the FELs with external coherent laser pulse not only improves the temporal coherence of the radiation, but also provides an FEL signal with well-defined timing with respect to the seed laser, thus allowing pump–probe experiments to be performed with high temporal resolution.

The most direct way to seed an FEL is to use an external coherent source of radiation and the undulator tuned to the same wavelength to amplify the seed. In addition to the requirement for coherence, to achieve a fully coherent FEL output the intensity of the seed should be high enough to dominate over beam shot noise. Seeding at 160 nm [8] and 61 nm [9] from a high harmonic generation (HHG; [10]) source has been demonstrated. Direct seeding with an HHG source is also under study at SPARC [11] and FLASH [12], and seeding at ∼10 nm is being considered in several FEL projects [13–15]. Seeding with an HHG source at even shorter wavelengths (∼1 nm and below) is believed to be difficult because of the relatively low power of the HHG seed.

To circumvent the need for a high-power seed at short wavelength, several frequency up-conversion techniques [16–22] have been envisioned to convert the external seed to a shorter wavelength. These techniques typically use seeds at a UV wavelength where high-power lasers are available together with dispersive elements (i.e. chicanes) to generate density modulation at a shorter wavelength in the electron beam. The beam is then injected into a long undulator tuned to some harmonic frequency of the seed, and the bunching on that harmonic frequency generates a powerful coherent signal to dominate over beam shot noise so that a fully coherent FEL output is obtained.

Among the several frequency up-conversion schemes, the recently proposed echo-enabled harmonic generation (EEHG), which uses a double modulator–chicane system, has the highest up-conversion efficiency [19, 20]. The key advantage of the EEHG scheme is that the bunching factor of the high harmonics is a slow decaying function of the harmonic number so that relatively small energy modulation can lead to considerable bunching at very high harmonics. Recent studies showed that EEHG is capable of generating soft x-rays with a wavelength of a few nm from UV seed lasers in a single stage [20, 23, 24]. Further extension of the radiation wavelength to 1 nm and below with EEHG is possible, but will most likely involve a large chicane with strong momentum compaction that makes the preservation of the phase space correlations technically challenging. Also the final energy spread will be much larger than the initial value due to the energy modulation in the modulators.

While tremendous progress has been made in seeding the FELs, there is no clear path on how to extend the radiation wavelength to sub-nanometer wavelength. In this paper, we
propose a triple modulator–chicane (TMC) scheme, for seeding sub-nanometer x-ray FELs. We will show that the TMC scheme can make full use of the low-power HHG seed such that ultrahigh harmonics can be generated while the energy spread growth is kept much smaller than the beam’s initial slice energy spread. As an example, we show the feasibility of generating significant bunching at 1 nm and below from a low-power (∼100 kW) HHG seed at 20 nm assisted by the high-power (∼100 MW) UV laser at 200 nm while keeping the energy spread growth within 40%. The supreme up-frequency conversion efficiency of the proposed TMC scheme, together with its unique advantage in maintaining the beam energy spread may allow the generation of fully coherent x-rays in the sub-nanometer wavelength from external seeds.

2. Methods

The layout of the TMC scheme is shown schematically in figure 1. As the name indicates, the TMC scheme consists of three modulators (M1, M2 and M3) and three chicanes with dispersive strength characterized by the factors \( R_{56}^{(1)}, R_{56}^{(2)} \) and \( R_{56}^{(3)} \), respectively. Here we will limit ourselves to the scenario where the lasers in M1 and M3 have the same wavelength, but \( \pi \) phase difference, and the first and the second chicane have the opposite momentum compaction factors \( R_{56}^{(2)} = -R_{56}^{(1)} \).

Following the analysis in [19, 20], we assume that the bunch length is much larger than the wavelength of the lasers so that we can assume a longitudinally uniform beam the initial longitudinal phase space distribution of which is \( f_0(p) = N_0 (2\pi)^{-1/2} e^{-p^2/2} \), where \( N_0 \) is the number of electrons per unit length of the beam, \( p = (E - E_0)/\sigma_E \) is the dimensionless energy deviation of a particle, \( E_0 \) is the average beam energy and \( \sigma_E \) is the rms energy spread. After interaction with the laser with wave number \( k_1 \) in M1, the particle’s energy changes to\( p' = p + A_1 \sin(k_1 z) \), where \( A_1 = \Delta E_1/\sigma_E \), \( \Delta E_1 \) is the energy modulation amplitude and \( z \) is the longitudinal coordinate in the beam. The distribution function after interaction with the laser becomes \( f_1(\zeta, p) = N_0 (2\pi)^{-1/2} \exp[-(p - A_1 \sin \zeta)^2/2] \), where \( \zeta = k_1 z \). Sending the beam through the first chicane converts the longitudinal coordinate \( z \) into \( z' = z + R_{56}^{(1)} p \sigma_E/E_0 \).
and makes the distribution function \( f_2(\zeta, p) = N_0(2\pi)^{-1/2} \exp\left[-\left(p - A_1 \sin(\zeta - B_1 p)\right)^2 / 2\right] \), where \( B_1 = R_{56}^{(1)} k_1 \sigma_E / E_0 \). Note that for the chosen coordinates with bunch head at \( z > 0 \), the momentum compaction of a simple four-bend chicane is positive. Negative momentum compaction can be obtained by adding quadrupoles in the four-bend chicane.

The final distribution function at the exit from the third chicane can be easily found by applying consecutively four more transformations to \( f_2(\zeta, p) \). The first and the third of these four transformations correspond to the modulation in M2 and M3. The second and the fourth correspond to the passage through the second and the third chicane. The final distribution function under the conditions \( R_{56}^{(2)} = -R_{56}^{(1)}, k_3 = k_1 \) and \( \phi_2 = \pi \) is

\[
f_f(\zeta, p) = N_0(\sqrt{2\pi})^{-1} \exp\left[-(1/2)[p + A_3 \sin(\zeta - B_3 p) - A_2 \sin[K(\zeta - B_3 p)] + K B_1(p + A_3 \sin(\zeta - B_3 p)) + \phi_1] - A_1 \sin[(\zeta - B_3 p)] \right]
+ A_2 B_1 \sin[K(\zeta - B_3 p) + K B_1(p + A_3 \sin(\zeta - B_3 p)) + \phi_1]]^2, \tag{1}
\]

where \( A_{2,3}, k_{2,3} \) and \( \phi_{1,2} \) are the dimensionless energy modulation, the wave number and the phase of the laser in M2 and M3, \( B_3 = R_{56}^{(3)} k_1 \sigma_E / E_0 \) and \( K = k_2 / k_1 \).

Integration of equation (1) over \( p \) gives the beam density \( N \) as a function of \( \zeta \), \( N(\zeta) = \int_{-\infty}^{\infty} dp f_f(\zeta, p) \). We define the bunching factor \( b \) as \( b = \frac{1}{N_0} |\langle e^{-i\alpha \zeta} N(\zeta) \rangle| \), where \( \alpha \) is a number, and the brackets denote averaging over the coordinate \( \zeta \). Analysis shows that the bunching factor is non-zero only if \( a = n + km \), which means the presence of a modulation with the wave number \( k_T = ak_1 + nk_3 + mk_2 \), where \( n \) and \( m \) are integers. After some mathematical manipulation, we found that the bunching factor is

\[
b_{n,m} = \sum_{j=-\infty}^{\infty} e^{-1/2[(B_3(Km+n) - B_1 Km)^2 + \sin\phi_1]} J_m(A_2 B_1 j + A_2 (B_1 - B_3) (Km + n)) \times J_j(-A_2 B_3 (Km + n)) J_{n+j}(A_1 B_1 Km - A_1 B_3 (Km + n)). \tag{2}
\]

For a given harmonic number \( a \) and energy modulation \( A_1 \), analysis shows that minimal energy spread is achieved when \( A_3 = A_1 \), and in this case optimal bunching is achieved when \( B_1 \approx a/A_1 K, A_2 \approx A_1 K/a \) and \( B_3 \approx 1/A_1 \).

3. Simulation

To illustrate the physics behind the TMC scheme, the evolution of the beam longitudinal phase space is shown in figure 2. For simplicity, we assume that the lasers have the same wavelength in the three modulators and only the phase space within one wavelength region is shown. The parameters used to obtain figure 2 are as follows: \( A_1 = A_3 = 5, A_2 = 0.05, B_1 = -B_2 = 4.7 \) and \( B_3 = 0.176 \).

The beam phase space after interaction with the first laser is shown in figure 2(a). The modulation introduces a local energy chirp, defined as \( h = d p / d \zeta \), into the beam’s longitudinal phase space. Similar to the EEHG scheme, separated energy bands are generated (figure 2(b)) after the beam passes through the first chicane, which has a large momentum compaction \((B_1 = 4.7)\). For the particles around the zero-crossing of the laser \((h_1 = A_1)\), the compression factor in the first chicane is \( C_1 = 1/(1 + h_1 B_1) \approx 1/A_1 B_1 \). Because of the large \( B_1 \), the modulation is locally decompressed in the first chicane, which leads to separated energy bands in
the beam phase space with a spacing of about $2\pi\sigma_E/B_1$ and the rms energy spread for each band is roughly equal to $C_1\sigma_E \approx \sigma_E/A_1B_1$. Accordingly, the chirp is reduced to $h_2 = C_1h_1 \approx 1/B_1$.

After interaction with the second laser with $A_2 = 0.05$, the beam phase space evolves to that in figure 2(c). Because the energy modulation is much smaller than the beam’s initial energy spread, it is actually very difficult to see the difference in figures 2(b) and (c). The second chicane with $B_2 = -4.7$ compresses the beamlets with a compression factor $C_2 \approx A_1B_1$ and amplifies the modulation imprinted in M2. The resulting beam phase space is shown in figure 2(d), which is similar to that in figure 2(a). If $A_2 = 0$, the second chicane should restore the beam phase space to the same distribution as that before the first chicane. As long as $C_2A_2$ is not much larger than unity, the second chicane will transform the beam phase space to a distribution similar to that before the first chicane with the presence of energy modulation from M2 superimposed on the modulation from M1 (figure 2(d)).

The laser in M3 is chosen to give the beam the same modulation amplitude ($A_3 = 5$) as that in M1, but with a $\pi$ phase shift, so that the overall energy modulation in M1 is canceled in M3. After the cancelation, the modulation from M2 becomes dominant, as shown in figure 2(e). The wavelength of the modulation in figure 2(e) is roughly $C_2$ times smaller than that in M2. A third chicane with small momentum compaction ($B_3 = 0.176$) further converts the energy modulation into density modulation (figure 2(f)). Using the particle distribution in figure 2(f), we found that significant bunching (7%) at the harmonics around $a = 22$ is generated with a modulation in M2 that is 20 times smaller than beam slice energy spread.

Due to the effective cancelation of the energy modulation in M1 and M3, the final energy spread growth (about 15%) is mainly from the modulation in M2. Since in the TMC scheme only a very small energy modulation (typically comparable to the energy spread of each energy band) is needed in M2, the final energy spread growth can be controlled to a very low level.

Figure 2. Longitudinal phase space evolution in the TMC scheme: (a) after the first modulator; (b) after the first chicane; (c) after the second modulator; (d) after the second chicane; (e) after the third modulator; (f) after the third chicane.
4. Seeding with the triple modulator–chicane scheme at 1 nm and below

The unique advantages of the TMC scheme—namely, that only a small energy modulation is needed in M2 and the second chicane compresses the modulation imprinted in M2 to a shorter wavelength—open new opportunities for using an HHG source to seed x-ray FELs. Here we show how one can generate bunching at 1 nm and below using the TMC scheme with the low-power HHG source as the seed in M2. As an example, we assume that the HHG source has a wavelength of 20 nm and the wavelengths of the lasers in M1 and M3 are 200 nm. The electron beam parameters used in the following analysis are similar to those in the proposed high rep-rate FEL at LBNL [23], with beam energy $E = 2.4$ GeV and slice energy spread $\sigma_E = 150$ keV.

For $A_1 = A_3 = 3$, $A_2 = 0.1$, $B_1 = -B_2 = 6.46$ and $B_3 = 0.327$, the longitudinal phase space at the exit of the third chicane simulated with our 1D code is shown in figure 3(a). The total energy spread growth is about 40%. The bunching factor calculated using the particle distribution in figure 3(a) is shown in figure 3(b), where one can see that the bunching factor at 1 nm ($a = 200$) is about 5% and there is also considerable bunching (1.5%) at 0.5 nm ($a = 400$). The bunching factor may be large enough to dominate over shot noise and sending the beam through a radiator tuned to the harmonic radiation wavelength may allow the generation of fully coherent x-rays at 1 nm.

The required energy modulation (450 keV) in M1 and M3 can be achieved with 100 MW 200 nm lasers with a waist of 0.6 mm (assuming a 10-period modulator with a period length of 15 cm), as estimated with equation (14) in [20]. The small energy modulation in M2 (15 keV) can be achieved with a 100 kW HHG source at 20 nm with a waist of 0.4 mm (assuming a 35-period modulator with a period length of 6 cm), which is readily reachable with existing technologies [25]. The required momentum compaction of the first chicane is reasonably small, i.e. $R^{(1)}_{36} = 3.29$ mm. For such a small chicane, analysis shows that the energy spread growth from incoherent synchrotron radiation can be easily controlled to be much smaller than the spacing of the adjacent energy bands so that the phase space correlation can be preserved.

In the above analysis, we assumed that the energy modulation in M1 and M3 is exactly the same and the laser phase difference in M1 and M3 is exactly $\pi$. In reality, these values may fluctuate. To identify the sensitivity of the performance of the TMC scheme to these fluctuations, we simulated the bunching factor at 1 nm with four sets of two parameters ($A_1$ and $A_3$, $A_2$ and $A_3$, $B_1$ and $B_3$, and $\phi_1$ and $\phi_2$) varied while keeping other parameters at the optimal values (figure 4).
Figure 4. Bunching factor at 1 nm for various $A_1$ and $A_3$ (top left); $A_2$ and $A_3$ (top right); $B_1$ and $B_3$ (bottom left); $\phi_1$ and $\phi_2$ (bottom right).

The top left plot in figure 4 shows that the bunching is more sensitive to $A_3$ than $A_1$. To maintain a large bunching factor at 1 nm, the power fluctuation of the laser in M3 should be controlled within 4%. While the modulation in M1 only weakly affects the bunching, effective cancelation of energy modulation in M3 still requires its power to be close to that in M3.

The top right plot in figure 4 indicates that the bunching is not sensitive to the energy modulation in M2, as long as the modulation is not too small. This loosens the requirement on the stability of the HHG seed. Since the bunching frequency is roughly $k_2B_1/B_3$, the chicane strength needs to be controlled to within a few per cent to provide a large bunching at a given frequency, as can be seen in the bottom left plot of figure 4.

Finally, the bottom right plot shows that the bunching is not sensitive to the phase difference between the first laser and the HHG seed ($\phi_1$), but is sensitive to that between the first and the third laser ($\phi_2$). Large bunching is achieved when $\phi_2$ deviates from $\pi$ within $\pi/4$. From a practical point of view, the lasers in M1 and M3 should originate from the same source so that their relative phase can be accurately controlled by controlling the path length of the lasers. Also the total momentum compaction of the beam line between M1 and M3 should be zero ($B_2 = -B_1$) to maintain a constant time-of-flight of the electron beam, so that the phase difference in the modulations is determined solely by the laser phase difference. It is worth mentioning that if no efforts are made to control the laser phase difference, there is still a probability of 25% to obtain considerable bunching.

It should be pointed out that the above example is just representative. Bunching the beam at higher harmonics with $a > 200$ can be achieved either by increasing the compression factor ($A_1B_1$) in the second chicane or by reducing the wavelength of the HHG seed in M2. Note that HHG at 4.37 nm with energy $> 10$ nJ has been obtained [26], and using a HHG seed at 4 nm in the above example may lead to considerable bunching at 2 Å.
5. Summary and outlook

In summary, we have proposed a new working scheme for harmonic generation in FELs. Compared to other harmonic generation schemes, the TMC scheme has the unique advantages that only a very-low-power HHG seed and relatively small chicanes are needed, and the total energy spread growth can be controlled to a very low level. It offers a promising solution to achieve fully coherent x-rays in the sub-nanometer wavelength range from external seeds.

The wavelength of the FEL output in the TMC scheme is roughly $\lambda_2 / C_1$, so the FEL wavelength can be easily changed by varying either the seed wavelength in M2 or the decompression factor of the first chicane. Since the final energy spread of the beam is comparable to the initial energy spread, the peak power of the FEL output will be similar to the SASE case. The pulse width of the FEL output in the TMC scheme is limited by that of the seed in M2. Note that the HHG source typically has a pulse width of a few tens of fs; in principle, the TMC scheme can provide an FEL output at sub-nanometer wavelength with a bandwidth of the order of $10^{-5}$.

Similar to EEHG, the success of the TMC scheme relies on the preservation of the long-term memory of beam phase space correlations. While recent EEHG experimental results [27, 28] are encouraging, more theoretical (i.e. particle tracking with second-order effects taken into account, noise amplification in the frequency multiplication process, etc) and experimental (i.e. tuning a chicane to negative $R_{56}$ while making $R_{51}$ and $R_{52}$ zero, accurate control of the phase difference of two lasers, etc) work is needed in order to fully address the practicality of implementing the TMC scheme at nm and sub-nanometer wavelengths.

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