Harmonic Self-Seeding for the MaRIE X-ray Free-Electron Laser*

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We describe the harmonic self-seeding method that uses the nonlinear harmonic generation power near saturation in a long-period undulator (LPU) to seed the fundamental FEL interaction in a subsequent short-period undulator (SPU). Harmonic self-seeding is being explored for the Matter-Radiation Interactions in Extremes (MaRIE) X-ray FEL to produce coherent high-energy X-ray photons. In this specific example, an LPU with 3-cm periods is used to generate both the fundamental X-rays at 14 keV and the third harmonic at 42 keV. The third harmonic radiation is then used to seed the fundamental FEL interaction in an SPU with 1.86-cm periods to produce fully coherent X-rays at 42 keV. To prevent the SASE-induced energy spread from negatively affecting the FEL interaction in the SPU, we consider both the fresh-slice self-seeding and the two-bunch harmonic seeding techniques, both of which provide the "fresh electrons" for the FEL interaction in the SPU. Time-dependent simulation results with the 3D Genesis FEL simulation code are reported.

Keywords: X-ray free-electron lasers; harmonic self-seeding; MaRIE XFEL.

1. MaRIE X-ray FEL

The Matter Radiation Interactions in Extremes (MaRIE) XFEL will provide sequences of coherent, femtosecond X-ray pulses at photon energies up to 42 keV to probe mesoscale materials in extreme conditions. The baseline MaRIE XFEL design uses a low-emittance 12-GeV electron beam to drive a self-amplified spontaneous emission (SASE) FEL to produce more than 10^{10} photons per electron bunch in the energy range 5-42 keV. The MaRIE accelerator includes an RF photoinjector, a low-energy linac that accelerates electrons up to 250 MeV, followed by a two-stage bunch compressor to compress the

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electron bunches to ~30 fs and additional linac to take the beam energy up to 12 GeV [1]. The MaRIE XFEL beamline shall be located alongside the existing Los Alamos Neutron Science Center (LANSCE) proton accelerator (Fig. 1). The 12-GeV electron beam shall be switched between different undulator beamlines, and the XFEL beams at different photon energies shall be directed toward different experimental hutches. In addition to the coherent X-ray beams, MaRIE users can also access the LANSCE proton and neutron beams for proton radiography and multi-probe diagnostic experiments [2].

In order to generate X-rays at different photon energies with fixed electron beam energy, the MaRIE XFEL undulators shall have different undulator periods to provide different-energy X-ray beams to various experimental hutches. For the specific example described in this paper, we shall select two periods, 3-cm and 1.86-cm. The 3-cm period undulator, called the long-period undulator (LPU), is used to produce X-rays in the 5-20 keV photon energy range and the 1.86-cm period undulator, called the short-period undulator (SPU), is used to produce X-rays in the 20-42 keV photon energy range [3]. We shall use the 42-keV third harmonic generated as coherent nonlinear harmonic generation [4] in the LPU to seed the fundamental FEL interaction in the SPU.

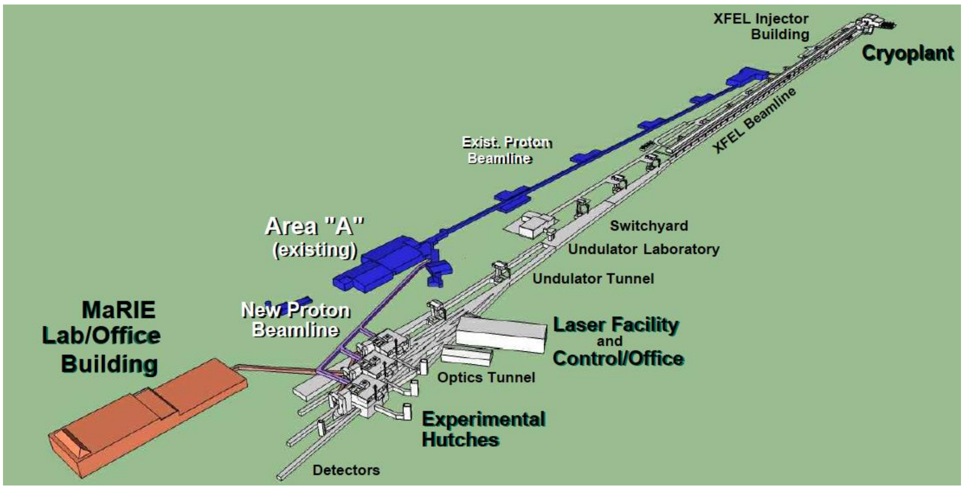

Figure 1. Layout of the MaRIE X-ray FEL beamline and experimental hutches at LANL.

The nominal electron beam parameters and the parameters of both long-period and short-period undulators, as well as the fundamental radiation parameters for the LPU at 14 keV and the SPU at 42 keV are listed in Table 1. The slice electron bunch charge and bunch length (FWHM) is one-quarter of the actual electron bunch charge (100 pC) and bunch length (28 fs), because only a small portion (slice) of the electron bunch participates in the FEL process in the fresh-slice approach [5]. An alternative is to use the dual-bunch approach where two electron bunches are generated within a few RF buckets [6]. However, the dual-bunch approach requires the third harmonic radiation generated in the first electron bunch to be delayed and overlapped temporally with the second electron bunch.

Table 1. Electron beam, undulator and radiation parameters for the MaRIE XFEL for both the long-period and short-period undulators.

Parameter	LPU Value	SPU Value
Electron beam energy	12 GeV	12 GeV
Full bunch charge	100 pC	100 pC
Fresh slice bunch charge	25 pC	25 pC
Slice bunch length (FWHM)	7 fs	7 fs
Peak current	3.6 kA	3.6 kA
Normalized emittance	0.2 μm-rad	0.2 μm-rad
Energy spread (rms)	0.02%	0.02%
Undulator period	3 cm	1.86 cm
On-axis undulator field amplitude	0.76 tesla	0.70 tesla
Undulator parameter (rms)	1.5	0.86
Fundamental wavelength	0.8857 Å	0.2952 Å
Fundamental photon energy	14 keV	42 keV
Dimensionless FEL parameter	1×10^{-3}	6×10^{-4}
Gain length, 3D	1.6 cm	2.3 cm
Undulator length	42 m	80 m
Saturated power, peak	37 GW	16 GW
X-ray pulse energy	0.25 mJ	0.11 mJ
Number of photons/pulse	1.1×10^{11}	1.7×10^{10}

2. Time-independent SASE Simulations

We performed time-independent FEL simulations with the Genesis 1.3 simulation code [7] using the SPU parameters for the MaRIE XFEL in SASE mode to calculate the number of 42-keV photons generated with a flat-top, 100-pC electron bunch as a function of the beam's relative energy spread for different values of normalized emittance (Fig. 2).

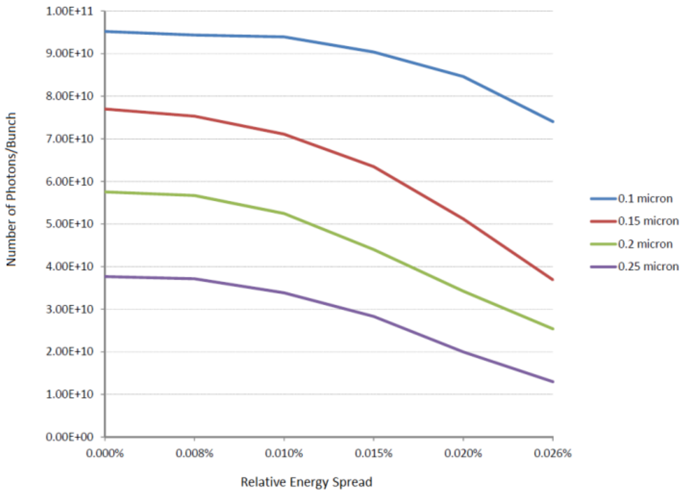

Figure 2. Time-independent Genesis simulations predicting the numbers of photons per bunch for the MaRIE XFEL operating at 42 keV at different normalized emittance versus energy spread.

3. Harmonic-seeding X-ray FEL

The harmonic seeding scheme relies the nonlinear harmonic generation (NHG) that produces harmonic radiation in the LPU as the FEL approaches saturation to provide the coherent seed at one of the odd harmonics of the FEL fundamental photon energy. In a typical plane-polarized undulator, the third harmonic power near saturation is about 1% of the fundamental power [4]. Using the parameters in Table I, we estimate the saturated fundamental power in the LPU is 37 GW, and the third harmonic power is as high as 370 MW. For the MaRIE XFEL, we select the undulator period and K parameter of the SPU such that the SPU fundamental photon energy is exactly the third harmonic of the LPU. This arrangement offers the feature of providing coherent X-rays at two different photon energies in the same X-ray beamline.

A potential showstopper for the harmonic seeding scheme is the SASE-induced energy spread in the electron beam exiting the LPU due to the strong FEL interaction at the fundamental photon energy. The SASE-induced energy spread is on the order of the FEL rho parameter for the LPU, about 0.1% and twice as high as the rho parameter for fundamental FEL interaction in the SPU (see Table I). This energy spread can severely impact the FEL gain in the SPU. For the harmonic seeded FEL to “lase” strongly, we will need to employ either the “fresh slice” technique that has been demonstrated at SLAC [5] or the “double-bunch” seeding technique [6].

Figure 3 shows the schematic of the “fresh slice” harmonic seeding method. The “fresh slice” self-seeding method, described in detail in Ref. [5], uses two different slices of the same electron bunch to separately generate and amplify the fundamental radiation in two separate undulator sections. The method has already been used at LCLS to enhance the performance of two color lasing (factor-of-10 increase in intensity) and self-seeding (factor-of-2 increase in brightness) compared to previous schemes. The “fresh slice” harmonic seeding scheme is similar to the self-seeding scheme except the harmonic radiation from the short-period undulator (SPU) is used as the coherent seed for the fundamental radiation in the long-period undulator (LPU). The “fresh slice” harmonic seeding starts with a dechirper to induce a head-tail transverse kick in the electron bunch followed by putting the orbits of the tail electrons on the LPU axis and allowing them to lase. Since the electrons in the head are not aligned and do not interact with the FEL beam in the LPU, the energy spread in the “fresh slices” at the head of the bunch remains unchanged. After the delay chicane to overlap these “fresh slices” at the bunch head with the harmonic seed, a set of orbit correctors is used to put the “fresh slices” on axis in the SPU and overlap with the harmonic seed which is now the fundamental FEL radiation in the SPU. The length of the LPU is chosen such that there is sufficient third harmonic power to overcome start-up noise in the SPU and yet the SASE-induced energy spread in the “fresh slices” remains low, which is important for efficient lasing in the SPU.

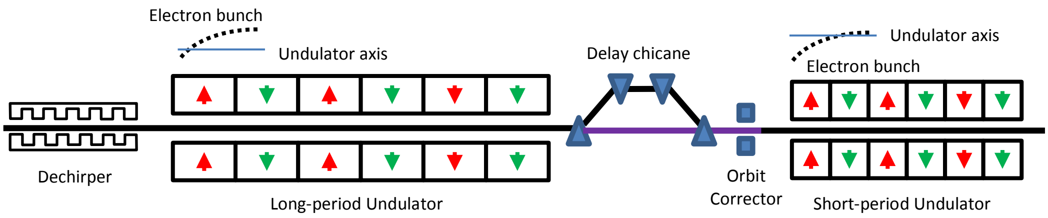

Figure 3. Schematic of the “fresh slice” harmonic seeding X-ray FEL concept.

3.1. *Time-dependent Simulations at 14 keV*

We performed time-dependent FEL simulation with the Genesis 1.3 simulation code [7] using the beam parameters for the MaRIE XFEL shown in Table I with the transverse kick similar to that at the LCLS. Due to incomplete suppression of lasing at the head of the bunch in the LPU, the SASE-induced energy in the “fresh slices” becomes noticeable after the fundamental power exceeds 10 GW. The optimum LPU length is about 42 meters, where the harmonic power is 30X more powerful than the startup noise in the SPU and the SASE-induced energy spread is low. Figure 4 plots the peak current in kA (orange), the SPU fundamental power in GW (yellow) and the third harmonic power in 100s of MW at the end of the 42-m LPU. Due to incomplete suppression of the SASE process in the “fresh slice” at the head of the bunch, both the fundamental and harmonic power are present throughout the bunch, in addition to the strong lasing at the tail of the bunch. With the LPU length set at 42 m, the SASE-induced slice energy spread remains unchanged at ~0.02% over the region of bunch coordinates between 6 and 10 microns.

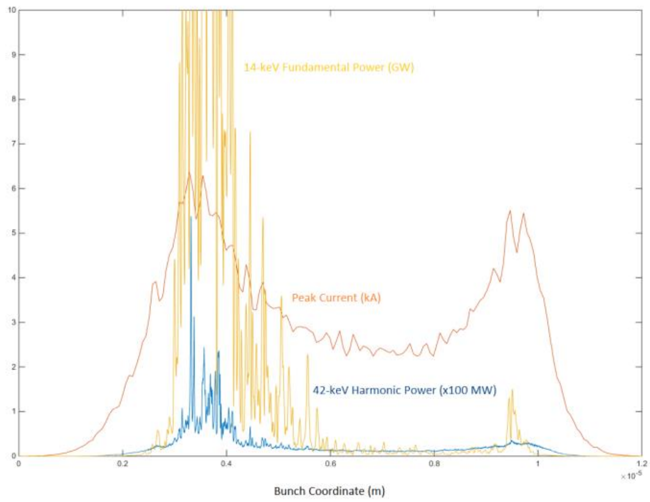

Figure 4. Plot of peak current in kA (orange), LPU fundamental power in GW (yellow), and the third harmonic power in 100s of MW (blue) versus the bunch coordinate in meter.

A more effective way of reducing the effect of SASE-induced energy spread is to use the double-bunch FEL method, where two electron bunches in different RF buckets are used, one to generate the harmonic seed and the other to amplify it, as discussed in a previous publication [6]. The "double bunch" scheme offers a particular advantage for harmonic lasing as it eliminates the trade-off between harmonic seed power and SASE-induced energy spread, which reduces the harmonic seed power due to incomplete suppression of lasing in the "fresh slices." The "double bunch" scheme, however, requires the harmonic seed radiation to be delayed by a time interval equal to that separating the two electron bunches in different RF bucket.

3.2. *Third-harmonic Seed at 42 keV*

We tried to import the third harmonic generated in the LPU directly into the SPU to seed the fundamental FEL interaction. However, due to a feature in the way the FEL wavelength is imported in the Genesis code, we had to create a new 42-keV seed radiation file with time averaging to remove the rapid phase oscillations in the NHG third harmonic. Also, instead of introducing a time delay in the electron bunch, we advanced the radiation pulse to overlap with the "fresh slices" near the head of the electron bunch as shown in Fig. 5. The peak power of the time-averaged 42-keV third harmonic seed radiation is 40 MW, substantially higher than the start-up noise at the fundamental energy of the SPU.

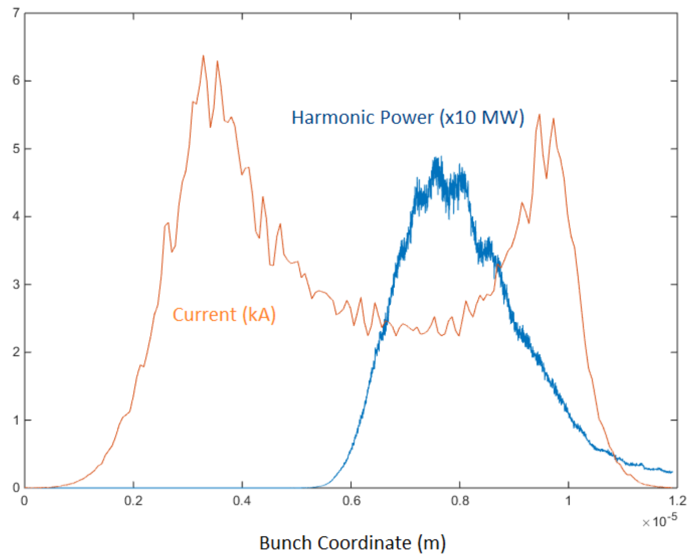

Figure 5. Plot of peak current in kA (orange) and 42-keV third harmonic seed power in 10s of MW (blue) versus the bunch coordinate in meter at the undulator entrance.

3.3. *Time-dependent Simulations at 42 keV*

Time-dependent 3D Genesis simulations of the fundamental FEL interaction in the SPU with the third harmonic seed from the LPU have been performed. Figure 6 plots the pulse energy of the 42-keV FEL radiation in hundreds of μJ as a function of position in the SPU. The rise and fall of pulse energy in each undulator segment are indicative of power modulations as the FEL radiation is first amplified and later reabsorbed by the electrons as the latter undergo synchrotron oscillation in the undulator segments. In the range of z positions up to 60 m, the FEL radiation is monochromatic with little contribution from SASE. However, as z increases past 60 m, the SASE radiation begins to appear over most the electron bunch. This SASE radiation is expected to continue and eventually reach a maximum of about 250 μJ, corresponding to 10 GW peak power at SASE saturation.

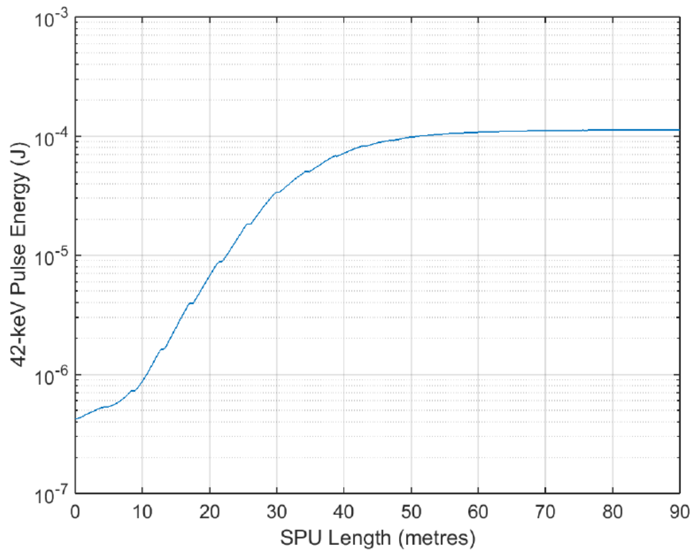

Figure 6. Semi-log plot of 42-keV pulse energy in J versus position in the SPU with the third harmonic of the LPU as the seed for the fundamental radiation of the SPU.

Fig. 7 plots the peak current in kA and the seeded 42-keV fundamental power versus the bunch coordinate at z = 60 m. The peak power of the 42-keV radiation has grown from 40 MW to more than 12 GW, a gain of 300X in peak power. The width of the peak power modulations is the coherence (slippage) length which is about 1 micron. This is significantly longer than the width of high-frequency SASE spikes as can be seen in the plot of power versus s for the unseeded case (Fig. 8). While the monochromatic 42-keV radiation appears to saturate at about 25 GW, the SASE peak power continues to grow beyond 50 GW (Fig. 8) and expand to other parts of the bunch that have not lased.

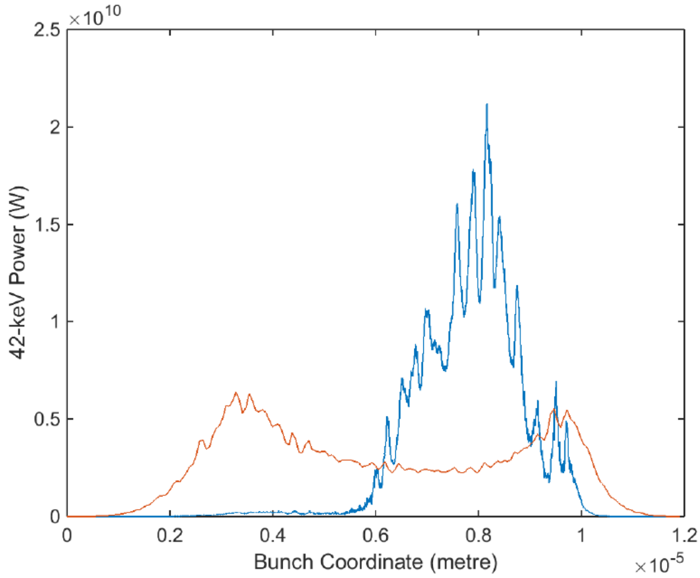

Figure 7. Electron peak current (orange) magnified by 1X6 and peak power (blue) of the monochromatic 42-keV radiation at z = 60 m in the SPU versus electron bunch coordinate.

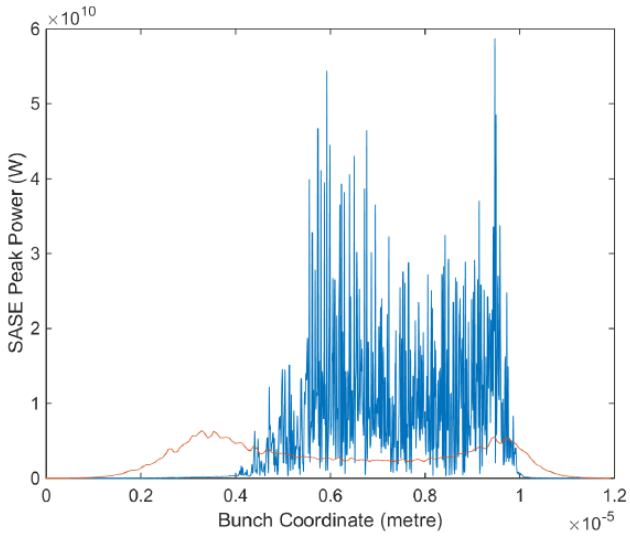

Figure 8. Electron peak current (orange) magnified by 1X6 and peak power (blue) of the unseeded SASE radiation at z = 60 m in the SPU versus electron bunch coordinate.

4. Improved Spectral Brightness

A more significant benefit of harmonic seeding is the improved spectral brightness in the harmonic seeded output (Fig. 9) versus that of the SASE output (Fig. 10). Figure 9 plots the spectral power on logarithmic scale versus wavelength at the 60-m location of the SPU. As can be seen in Figs. 9 and 10, the peak at 42 keV in the seeded case is about two orders of magnitude higher than the SASE peak, and the spectral width is narrower by approximately the same magnitude. Moreover, the contrast between the 42-keV peak and the adjacent background is greater than 10^4 in the seeded case whereas that between the SASE peak and the adjacent background is less than three orders of magnitude. It is worth noting that we had to optimize the undulator taper and the FODO lattice of the SPU to increase the peak power of the seeded FEL radiation.

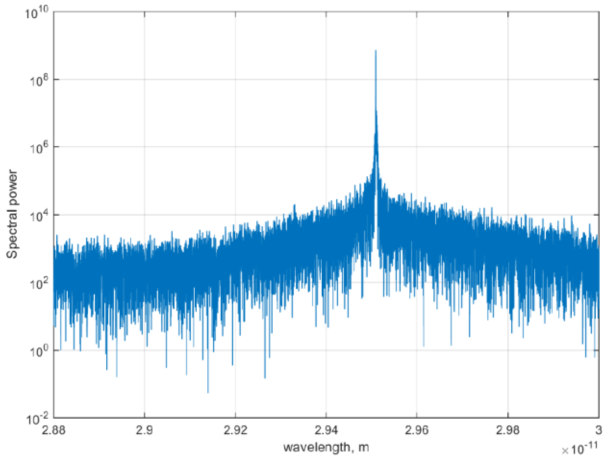

Figure 9. Semi-log plot of the seeded FEL spectral power versus wavelength

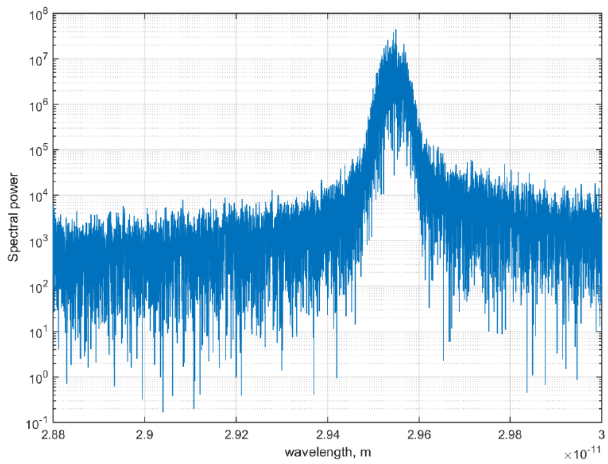

Figure 10. Semi-log plot of the SASE spectral power versus wavelength

5. Conclusions

We have performed time-dependent, 3D FEL simulations to analyze the feasibility of harmonic seeding as a new method to generate fully coherent X-rays in the energy range of 42 keV. Using the MaRIE XFEL as the test case, we show that with realizable values of electron beam and undulator parameters, we can achieve substantial power at the third harmonic of the long-period undulator to seed the fundamental FEL interaction in the short-period undulator. With harmonic seeding, the number of photons is reduced to about one-half that of SASE, but the spectral linewidth is reduced by a factor of 250, resulting in an increase in spectral power by more than two orders of magnitude. We have also demonstrated other benefits of harmonic seeding, including longer coherence length and much lower background compared to SASE. The use of harmonic seeding can potentially lead to a new class of X-ray FELs with the upper end of the photon energy tuning range extended beyond 50 keV.

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