

Broad-bandwidth x-ray free-electron lasers driven by plasma wakefield accelerators

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Broad-bandwidth x-ray free-electron lasers (FELs) are critical scientific tools across diverse disciplines such as biology and chemistry. While substantial efforts have been devoted to achieving FEL bandwidth broadening, existing methods face limitations. This paper proposes a simple yet effective scheme for spectral broadening that utilizes a plasma wakefield accelerator (PWFA) to impart a large energy chirp to an electron beam. A specifically designed transport system then selectively injects the portion of the beam meeting the lasing requirements into the undulators for FEL generation. A start-to-end simulation demonstrates that the scheme can effectively manipulate the longitudinal and transverse phase space of the PWFA electron beam that subsequently generates a high-brightness x-ray FEL exhibiting a full-width bandwidth reaching 20%.

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I. INTRODUCTION

Plasma wakefield accelerators (PWFA) driven by high-current charged particle beams [1–4] can accelerate electron beams to giga-electron volts within a few centimeters, achieving accelerating gradients orders of magnitude larger than those of conventional radio-frequency (rf) accelerators. This promises compact accelerators for future high-energy applications such as colliders and coherent light sources [5,6]. After decades of development, PWFA has reached numerous milestones. For example, on a meter-scale accelerating length, the accelerating field can double the energy of a 42 GeV electron beam [7]. In addition, beam-driven wakefields have also demonstrated high-efficiency high-energy acceleration for both electrons and positrons [8–10]. Furthermore, self-amplified spontaneous emission (SASE) and direct-seeding FELs based on beam-driven plasma wakefield acceleration have been experimentally verified [11,12], advancing the technology toward practical applications.

Soft or hard x-ray FELs, with wavelengths spanning from 0.1 to 10 nm, hold significant potential for applications such as ultrafast spectroscopy and imaging [13–15].

Among them, x-ray FEL pulses with broad bandwidth are highly desirable for studies in molecular structural dynamics and spectroscopy, including investigations of microcrystalline materials [16,17], x-ray absorption spectroscopy [18], and multiwavelength anomalous diffraction [19]. The FEL resonance wavelength λ is given by $\lambda = \lambda_u / 2\gamma^2 (1 + K^2/2)$ [20,21], where λ_u is the period length of the undulator, γ the mean Lorentz factor of the electrons, and K the field parameter of the undulators. Differentiating this resonance relation yields $|\Delta\lambda/\lambda| = 2|\Delta\gamma/\gamma|$, indicating that a larger relative energy chirp ($\Delta\gamma/\gamma$) directly produces a larger relative spectral broadening ($\Delta\lambda/\lambda$). Meanwhile, generating broad-bandwidth x-ray FELs typically requires a drive electron beam with a central energy between 1 and 10 GeV [22,23].

In conventional rf accelerators, the energy chirp introduced by overcompression is constrained at high energies, primarily due to the narrow accelerating phase range [24]. The maximum bandwidth achieved via overcompression is about 4.79% in full width (FW, measured from peak intensity to $1/e^2$) in simulations and is only 3% FW in experiments [24–26]. Beyond their role as an acceleration medium, plasma wakefields are also efficient tools for manipulating electron beam phase space. For instance, a uniform or hollow-channel plasma can be used to dechirp an electron beam, reducing a percent-level energy chirp to a slice energy spread near 0.1% [27–29]. Conversely, a plasma can also act as an energy chirper for a beam with no initial chirp, which is applicable to scenarios that require a large energy spread. A recent study demonstrated that using a hollow-channel plasma to preserve the beam's

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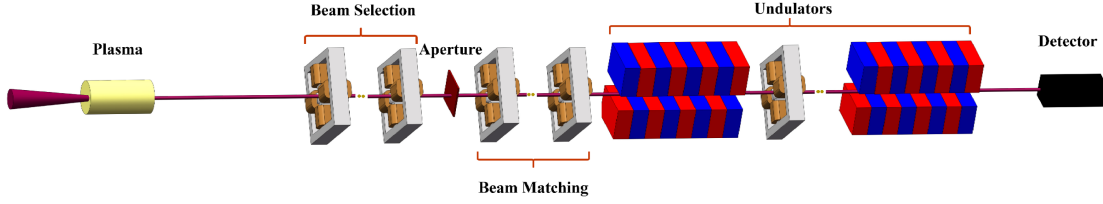


FIG. 1. Scheme of the broadband x-ray FEL driven by a beam-driven wakefield accelerator. The beam selection and the beam matching sections each comprise six quadrupoles. Two additional quadrupoles between every pair of undulators provide transverse beam confinement.

transverse phase space quality enables spectral broadening up to 24% FW [30], significantly surpassing conventional accelerator technologies. However, this approach demands precise coaxial alignment between the electron beam and the hollow channel, posing a major experimental challenge.

In this article, we demonstrate that a uniform-density plasma in PWFA can also impart a large energy chirp to the electron beam, offering greater experimental feasibility compared to the hollow-channel scheme. To achieve saturation gain in the undulators, however, a specialized beam transport line is essential. This line serves two primary functions: filtering out the heavily degraded head portion of the beam and reducing its divergence to enable lossless transmission through the undulators. Conventional approaches often use a chicane-integrated slit for this selection [31,32]. However, the coherent synchrotron radiation (CSR) induced in the chicane can potentially impair beam quality. We therefore propose here a new design that replaces the chicane with a set of quadrupoles for beam selection, thereby avoiding CSR-induced quality deterioration.

The article is organized as follows. Section II describes the PWFA process that increases both the beam energy and energy chirp over 23 cm. At the plasma exit, a beam with an initial energy of 1 GeV achieves a maximum energy gain exceeding 0.8 GeV, while the slice energy spread and emittance in the tail region remain sufficient for FEL lasing. Section III illustrates how the beam transport line is configured to select electrons from the tail portion and match them to undulators to drive broad-bandwidth x-ray FEL generation. The system layout is shown in Fig. 1. The quadrupoles before the aperture focus electrons of a specific energy to a small spot size, allowing the aperture to select central electrons and maintain a low slice energy spread. The quadrupoles after the aperture reduce the beam divergence before it enters the undulators, and quadrupoles between undulator segments confine the transverse beam envelope throughout the undulators. Section IV presents simulation results of broad-bandwidth x-ray FEL generation. Concluding remarks are provided in Sec. V.

II. BEAM-DRIVEN PLASMA WAKEFIELD ACCELERATION

To validate the concept of using a beam-driven wakefield accelerator for broad-bandwidth x-ray FELs, we performed

a start-to-end simulation encompassing the wakefield acceleration process, beam phase-space manipulation, and x-ray FELs generation. The wakefield acceleration was simulated in 3D using the QUICKPIC code, a highly efficient fully parallelized particle-in-cell code based on quasistatic approximation [33,34]. The initial electron beam parameters, listed in Table I, are similar to those of beams from rf linacs in typical x-ray FEL facilities [22,35]. A 1 GeV electron beam with 0.1% slice energy spread was injected into a 23 cm long plasma with a flat-top density profile and a peak density of $8 \times 10^{16} \text{ cm}^{-3}$. It is noted that the plasma requires an additional laser to ionize the neutral gas in advance. The initial electron beam had a charge of 400 pC, a length of 120 μm and a current of 1 kA. The initial transverse normalized emittance $\epsilon_{nx,y}$ was 1 mm mrad, and the rms beam size was 8 μm . The simulation box had a size of $56 \times 56 \times 188 \mu\text{m}$ in the dimensions x, y (transverse) and z (longitudinal) directions, respectively, with a step size for pushing the relativistic electron beam of 37.6 μm . The box moved at the speed of light, following the beam and was discretized into $512 \times 512 \times 512$ cells.

The simulation results are presented in Fig. 2. As shown in Fig. 2(a), when the beam propagates to $z = 1.7 \text{ cm}$, a highly nonlinear plasma wake in the blowout regime is excited. The ultrahigh transverse field tightly focuses the beam to an rms size of 2.8 μm . The red curve shows the lineout of the longitudinal electric field E_z along the beam's propagation axis. Obviously, the beam head loses energy to excite the wakefield, thereby accelerating the beam tail and inducing an energy chirp along the bunch's longitudinal position. Figure 2(b) shows the transverse distribution of E_z at different longitudinal positions. The transversely uniform region of E_z is much wider within the beam tail than

TABLE I. Input parameters of the initial electron beam.

Parameters	Value
Energy (GeV)	1
Energy spread (%)	0.1
Charge (pC)	400
rms beam size (μm)	8
Beam length (μm)	120
Normalized emittance (μm)	1

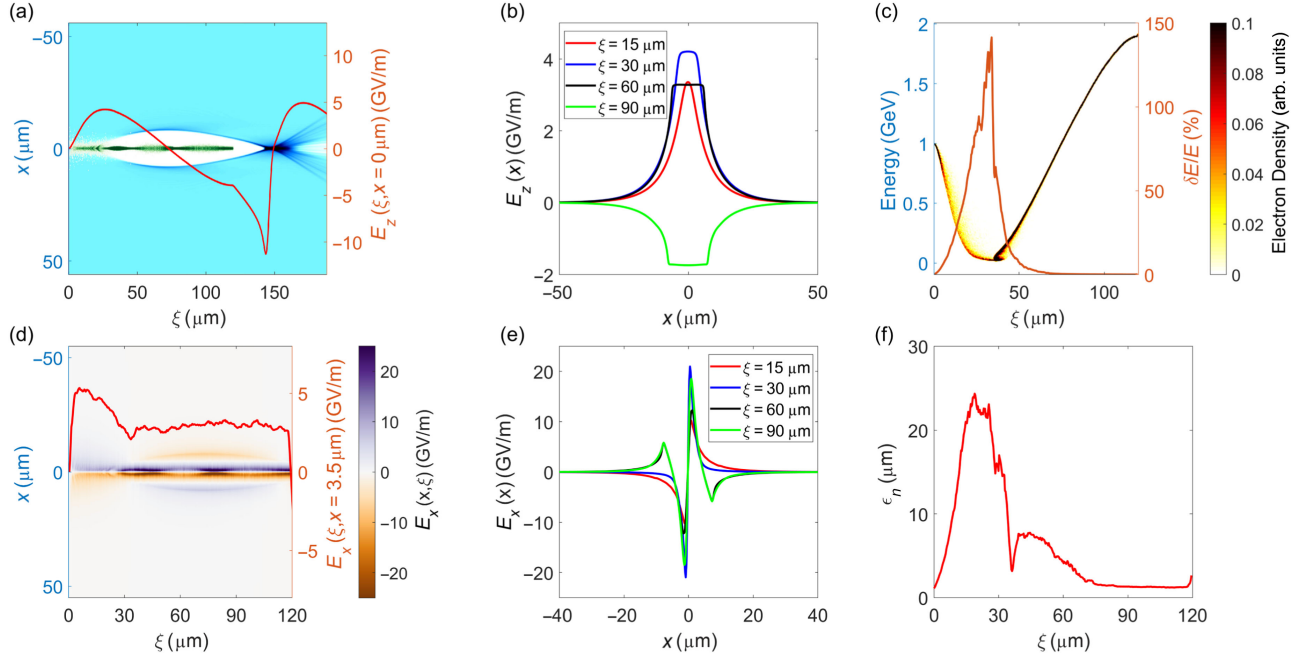


FIG. 2. 3D PIC simulation of beam-driven wakefield acceleration and electron beam qualities. (a) Density distribution of the background plasma and the electron beam in the $x - \xi$ plane at $z = 1.7$ cm. Here, $\xi = ct - z$ represents the longitudinal position relative to the beam head. The red curve is the longitudinal electric field E_z lineout along ξ at $x = 0$ μ m. (b) The longitudinal electric field E_z along x at different ξ values for $z = 1.7$ cm. (c) Electron beam longitudinal phase space and slice energy spread upon exiting the plasma. (d) The transverse electric field E_x distribution at the same position as (a). (e) The transverse electric field E_x along x at different ξ values for $z = 1.7$ cm. (f) Electron beam slice emittance after exiting the plasma.

its head, helping to maintain a low slice energy spread in the tail region. This is confirmed by the red curve in Fig. 2(c), which shows that at the beam tail ($\xi \geq 75$ μ m), the slice energy spread remains around the initial value of 0.1%. Figure 2(c) also shows the longitudinal phase space of the beam upon exiting the plasma, where one can see the beam tail achieves an energy gain of up to 840 MeV, corresponding to an accelerating gradient of over 3 GV/m. The total rms energy spread of the entire beam is approximately 71%. Fortunately, FEL lasing is primarily influenced by the energy spread within the slippage length (which is much shorter than the beam length) rather than the total energy spread. Therefore, the electron beam in the tail region still meets the slice energy spread requirement for FEL lasing.

Next, it is necessary to consider the influence of the transverse focusing PWFA field on the beam. In Fig. 2(d), the transverse electric field E_x at $z = 1.7$ cm is presented. The wakefield distribution at the beam head is complex and varies rapidly. After the beam head, a clear bubble is formed. The red curve in Fig. 2(d) represents the longitudinal lineout of E_x at $x = 3.5$ μ m, showing a field gradient correlated with the longitudinal position, especially in the beam head. This correlation severely degrades the projected emittance in the beam head region. In the blowout regime, it is known that the transverse wakefield distribution is nearly uniform along the

longitudinal direction within the bubble, which helps to minimize detrimental effects on the beam's projected emittance. Moreover, the linear variation of the focusing field E_x near the axis center at different longitudinal positions, as outlined in Fig. 2(e), ensures that most electrons of the drive beam inside the ion cavity experience a linear focusing force to preserve their emittance. Figure 2(f) plots the slice emittance of the beam after plasma exit. Consistent with the analysis above, the slice emittance in the beam head is significantly degraded, while the transverse phase space of the beam tail remains acceptable for generating a broad-bandwidth x-ray FEL.

III. TRANSPORT LINE FOR BEAM SELECTION

The plasma wakefield simulation results indicate that the beam tail acquires a significant energy chirp while maintaining acceptable slice energy spread and emittance. A well-designed beam transport line is thus required to select these electrons, and it is simulated using ELEGANT, a flexible SDDS-compliant simulation code for accelerators [36].

The designed transport line, shown in Fig. 1, consists of two sections. The first section performs beam selection using six quadrupoles that focus the nominal-energy electrons while strongly defocusing others. As shown in Figs. 3(a) and 3(c), high-energy electrons near the beam tail

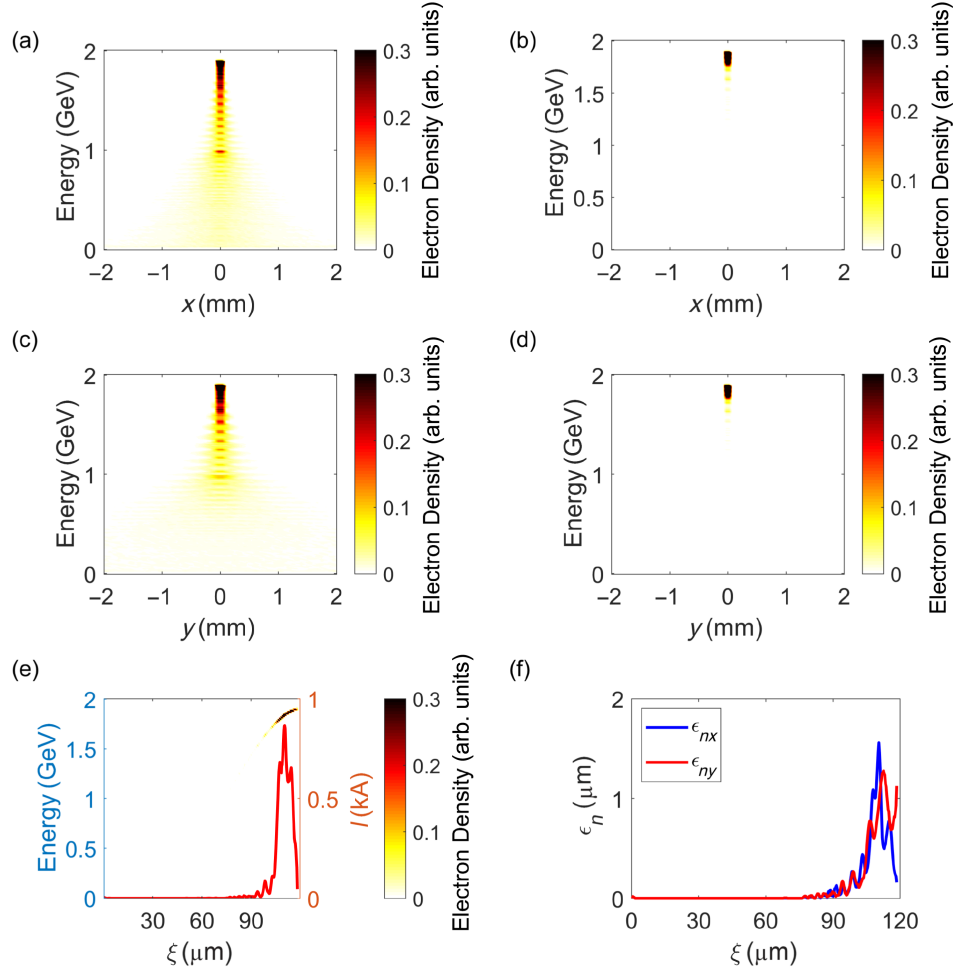


FIG. 3. Electron beam selection results. (a),(c) The electron beam $x \sim E$ and $y \sim E$ phase space before the aperture, where E denotes the beam energy. (b),(d) Phase space after the aperture. (e) Longitudinal phase space and current profile after selection. (f) Transverse slice emittance after the aperture.

are focused to a smaller spot size than lower-energy particles. A $30\ \mu\text{m}$ -diameter aperture placed after the quadrupoles then selects electrons with a transverse offset of less than $30\ \mu\text{m}$; the selected electrons are shown in Figs. 3(b) and 3(d). A small fraction of lower-energy electrons are transmitted due to transverse drift into the

central region during transport. However, as shown in Fig. 3(e), their number is much lower than that of the selected high-energy component. Besides filtering out low-energy electrons, this selection process maintains the transverse emittance [see Fig. 3(f)], keeping it within the FEL lasing requirement. After the beam selection section,

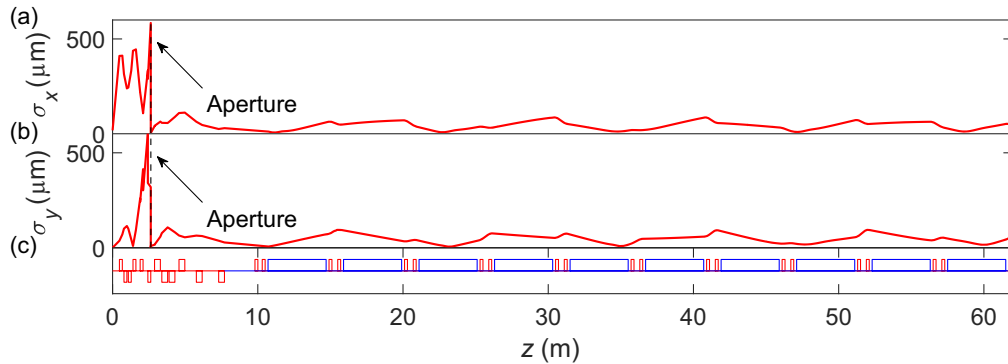


FIG. 4. Evolution of the beam size (rms) in (a) x and (b) y directions in the beamline. Lattice is shown in (c) where the red lines are quadrupoles and the blue lines are undulators.

TABLE II. Strengths of quadrupoles in the beam transport line.

Beam selection		Beam matching	
Quadrupole	Strength (T/m)	Quadrupole	Strength (T/m)
Q1	62.2	Q1	57.1
Q2	57.7	Q2	35.0
Q3	52.0	Q3	2.4
Q4	61.4	Q4	17.8
Q5	37.5	Q5	9.0
Q6	57.9	Q6	8.2

an electron beam with 33 pC charge, 850 A peak current, 1.84 GeV energy, and 1.3/1.5 μm normalized emittance is obtained to drive the broad-bandwidth FEL lasing.

Although the beam energy spread and emittance are adequate for FEL operation, its divergence must be reduced to minimize beam loss during transport through the undulators. This is addressed by the second section for beam matching, which also employs six quadrupoles to manipulate the transverse phase space. The final beam is matched to a transverse size of 30 μm and a divergence of 0.1 mrad before being injected into the undulators. Furthermore, quadrupoles placed between undulators control the transverse beam size throughout the undulator section. The evolution of the beam size along the beamline is shown in Fig. 4, demonstrating that the maximum rms beam size within the undulators is kept below 100 μm within the undulators. The strengths of all quadrupoles in the transport line are listed in Table II.

IV. BROAD-BANDWIDTH XFEL GENERATION

The FEL performance of the selected beam was investigated using the 3D time-dependent simulation code Genesis 1.3 [37]. The undulator beamline configuration mirrors that of the Shanghai soft x-ray free-electron-laser facility (SXFEL) [22,38], comprising ten 4-m-long undulators with 1.2 m matching sections between them. The undulator field parameter K was set to 1.03. The final beam parameters at the undulator entrance are listed in Table III.

For x-ray FELs based on self-amplified spontaneous emission (SASE), when the slippage length L_s is much

shorter than the beam length L_b , the beam quality within the slippage length (which is determined by both the energy chirp and the slice energy spread) plays a decisive role in the FEL gain process [39]. In our case, the slippage length ($L_s \sim N_u \lambda \sim 320$ nm) is on the order of the coherence length ($L_c \sim \lambda/4\pi\rho \sim 63$ nm) [40], where N_u is the number of periods per undulator and ρ is the Pierce parameter, which typically ranges from 10^{-3} to 10^{-4} . Given the beam parameters listed in Table III and undulator settings used in the FEL simulation, $L_s \ll L_b$ holds, and the slice energy spread increase due to the energy chirp is only 0.117%. Under these conditions, a strongly chirped beam can still drive broadband x-ray generation. Figure 5(a) shows the growth of the radiation power along the undulators. After 52 m, the peak power of the x-ray FEL pulses reaches 3 GW [see Fig. 5(b)], with a spot size of 120 μm and a divergence of 50 μrad , yielding a high brightness of 3.1×10^{31} photons/s/mm²/mrad²/0.1%BW. As shown in Fig. 5(c), the final spectrum bandwidth is 20% for full width, approximately 5 times greater than what is achievable with conventional accelerator technology.

However, this does not imply that the bandwidth can be increased indefinitely without affecting the radiation performance. As the energy chirp continues to increase (assuming the beam length remains constant), the energy spread within the slippage length—resulting from the combined contributions of the slice energy spread and the energy chirp—gradually approaches or even exceeds ρ , which can significantly suppress the radiation gain. Furthermore, the design of the beam transport line imposes two notable limitations on the increase in spectral bandwidth. First, quadrupole magnets are energy-dependent and beams with energies deviating from the design value experience poorer transverse matching as chirp increases. Second, strong focusing of the selected slice distorts the transverse phase space of the outer electrons. Increasing the energy chirp by enlarging the aperture size will include these distorted electrons, thereby degrading the beam emittance. These two effects collectively lead to a deterioration in beam matching with increasing energy chirp, ultimately resulting in a reduction in radiation power. Thus, an optimal chirp exists that balances bandwidth and emitted power.

To verify this point, we performed a parameter scan of beam chirp by varying the aperture size under the same transport line configuration. As shown in Fig. 5(d), increasing the aperture size allows more of the beam to pass through, resulting in an increase in the peak current from 0.7 to 1 kA (black line), while the beam emittance degrades from 1.1 to 3.6 μm . Additionally, the spectral bandwidth increases with energy chirp (green line), but tends to saturate when chirp exceeds 11%, while the peak power begins to decrease (red line). When the energy chirp reaches 15%, the radiation spectral bandwidth can attain 21.5%, while the radiation power drops to ~ 1 GW.

TABLE III. Final parameters of the electron beam after beam transport.

Parameters	Value
Energy (GeV)	1.84
Slice energy spread (%)	0.1
Energy chirp ($\Delta\gamma/\gamma$, %)	11
Charge (pC)	33
rms beam size (μm)	30
Beam peak current (A)	850
Normalized emittance (μm)	1.3/1.5

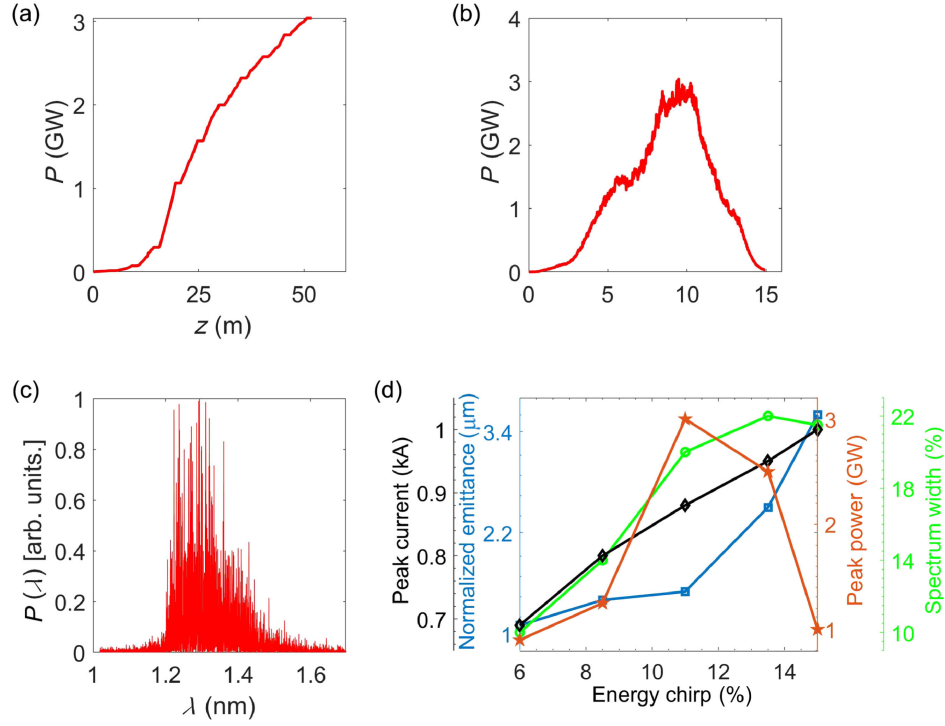


FIG. 5. Broad-bandwidth x-ray FEL generation. (a) Growth of radiation power along the undulators. (b) X-ray FEL pulse temporal profile. (c) The radiation spectrum at the undulator exit. (d) The dependence of beam's peak current, emittance, and x-ray radiation's peak power and bandwidth on the selected energy chirps via the same transport line.

Overall, under the simulation parameters considered, an energy chirp of 11% provides the best trade-off between brightness and spectral bandwidth, yielding optimal broad-bandwidth radiation.

Besides the scheme itself, we also investigated its tolerance to jitters introduced by the PWFA stage. In the scheme, an electron beam with a large energy chirp, imprinted during wakefield acceleration, undergoes beam selection via a combination of quadrupole magnets and an aperture. To ensure sufficient gain for the amplification process and thus maintain high radiation brightness, the beam trajectory must be well aligned with the transport axis at the aperture position. However, jitters from the PWFA stage may disrupt this alignment. For simplicity, we consider two primary sources of jitter: the transverse beam

offset (the deviation of the beam centroid from the axis of the transport line) and tilt angle (the angle between the beam propagation direction and the axis of the transport line).

Given the small aperture size ($\sim 30 \mu\text{m}$), a significant transverse beam offset may cause partial beam loss. Moreover, an off-axis beam experiences an additional dipole field inside the quadrupoles, leading to distortion of the phase space. To quantify this effect, we performed a parameter scan of transverse offsets from 0 to $10 \mu\text{m}$ under the same transport line design. The simulation results, shown in Fig. 6(a), indicate that for a $10 \mu\text{m}$ offset, the peak power drops from ~ 3 to ~ 0.45 GW, and the spectral bandwidth narrows from 20% to 15%. Similarly, a tilt angle at the plasma exit can cause the beam trajectory

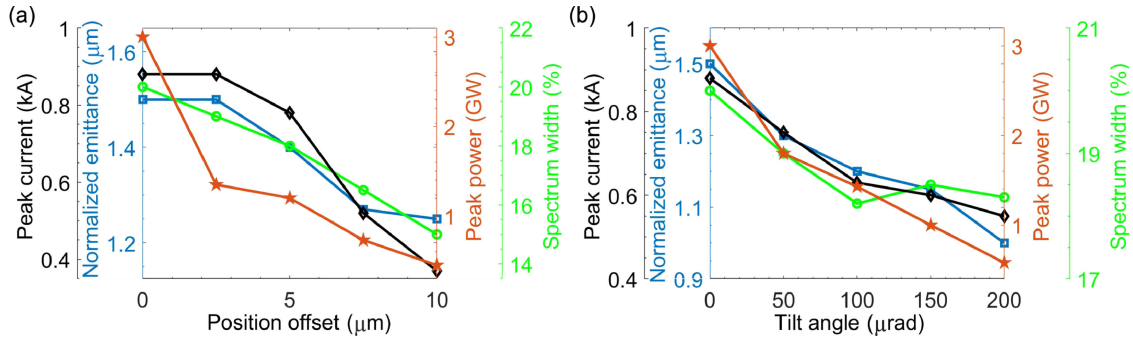


FIG. 6. Effects of transverse beam offset (a) and tilt angle (b) on the quality of selected beam and broadband x-ray radiation.

misalignment, leading to beam loss at the aperture and phase space distortion during transport. A parameter scan for tilt angles from 0 to 200 μrad is shown in Fig. 6 (b). The results show that for a tilt angle reaching 200 μrad , the FEL peak power decreases from ~ 3 to ~ 0.58 GW, and the bandwidth drops from 20% to 18%.

These results confirm that both effects can degrade radiation performance by causing beam misalignment. While the peak power is highly sensitive, the spectra bandwidth remains relatively robust, which can be considered as an encouraging result for broadband FEL applications. Fortunately, in practical accelerator operations, real-time monitoring and correction of the beam trajectory can be achieved through a combination of beam position monitors, corrector magnets, and techniques such as optimization algorithms or machine learning [41,42]. This can effectively mitigate these jitter effects.

V. CONCLUSIONS

Realizing high-brightness, broad-bandwidth x-ray FELs is a crucial scientific goal. PWFA can simultaneously boost beam energy and impart a large energy chirp, thereby broadening the FEL spectrum. This paper proposes a straightforward approach combining a PWFA module with a specialized beam transport line to generate a suitable electron beam. Start-to-end simulations with achievable parameters demonstrate the feasibility and effectiveness of this method. In the near future, we plan to test this scheme at the SXFEL facility, leveraging our recently developed advanced diagnostic tools such as femtosecond ultrarelativistic electron microscopy [43–45] for real-time probing of the PWFA and beam dynamics, and machine learning techniques for online self correction [46,47]. These tools will further optimize PWFA performance and facilitate the generation of high-brightness, broadband x-ray FELs.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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