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SIMULATION AND OPTIMIZATION FOR SOFT X-RAY SELF-SEEDING AT SXFEL USER FACILITY

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Abstract

The simulation and optimization studies for the soft x-ray self-seeding experiment at SXFEL have been presented in this paper. Some critical physical problems have been intensively studied to help us obtain a more stable output and a clearer spectrum. The monochromator is optimized considering various unideal conditions such as the reflection rate, diffraction rate and the roughness of the grating and the mirrors. An integrated self-seeding simulation is also presented. The calculation and simulation results show that the properties of the self-seeding can be significantly improved by using the optimized design of the whole system and the evaluation of grating monochromator shows that the presented design is reliable for soft x-ray self-seeding experiment at SXFEL.

INTRODUCTION

The successful achievement of SASE FEL [1-3] opens a new chapter to high-brightness photon source with tunable wavelength and it provides a reliable instrument to research scientific frontier within the material, biological and chemical sciences. However, SASE FEL suffers from shot noise, poor longitudinal coherence and poor spectral bandwidth. A harmonic lasing scheme with external seeding, such as HGHG [4-5] and EEHG [6-8], can be used to generate relative short wavelength radiation with longitudinal coherence. However, it is unable to probe photon energy beyond a few hundred of eV. To improve the longitudinal coherence of SASE FEL, self-seeding [9] is proposed at DESY in 1997, after that, soft and hard X-ray self-seeding are demonstrated at LCLS separately in 2014 [10] and 2012 [11] separately. Since then, self-seeding schemes are regarded as a reliable method to obtain high brightness, longitudinal coherence and short-wavelength FEL radiation.

The self-seeding scheme separates the long radiation undulator into two parts by inserting a monochromator and a four-dipole chicane. The first undulator works on the SASE mode, the radiation and electron bunch are extracted before saturation. After that, the radiation is passed through a monochromator to purify the spectrum and the electron bunch is passed through the chicane to eliminate the beam microbunching. After that, the monochromatic radiation and the fresh electron beam are sent to the radiation undulator. In the seed undulator, the monochromatic radiation is used as a seed to interact with the electron beam. Finally, the output will be longitudinal coherent when saturation. In the previous system design, we have given preliminary design and simulation for SXFEL user facility [12]. In this paper, some critical physical problems have been intensively studied to help us obtain a more stable output and a clearer spectrum. We give the simulation method to optimize the undulator length. The reflection and diffraction rate are calculated to get the transfer efficiency and the simulation process is more reliable considering the transfer efficiency. The monochromator is optimized considering various unideal conditions such as the roughness of the grating and the mirrors. In the previous optical simulation, we use shadow to simulate the power resolution of designed grating monochromator and the parameters of light source are not considered. In this paper, we use the calculated parameters of radiation pulse to simulate the power resolution of grating monochromator and we also give a detail simulation for designed simulation.

THE GRATING MONOCHROMATOR DESIGN

The layout of self-seeding scheme is shown in Fig. 1. The grating monochromator has five elements: a VLS toroidal grating monochromator disperses the light pulse to different transverse position as well as focuses the light pulse, a plane mirror reflects the light to horizontal direction, a slit selects out the light pulse wavelength, a spherical mirror focus the sagittal direction of pulse and another plane mirror reflects the light to the entrance of the undulator. In the previous optical system design, the layout and the parameters of optical elements have been described. Recently, some detail studies about grating monochromator have been carried out. In soft X-ray regime, the gold is generally chosen as the material of optical elemental. Based on the element material and the designed parameters, we calculate the reflection and diffraction rate of the gating monochromator. For a grating, the diffraction efficiency can be expressed as follows:

$$E_0 = \frac{R}{4}\left(1 + 2(1-P)\cos\left(\frac{4\pi\cos(\alpha)}{\lambda}\right) + (1-P)^2\right),$$

where α is the incidence angle, h is the depth of the grating groove, P can be expressed as: $P = (4h\tan\alpha)/d_0$, where d_0 is the line width of adjacent grating groove and R can be expressed as: $R = \sqrt{\alpha_G\beta_G}$, where $\alpha_G = \pi/2 - \alpha, \beta_G = \pi/2 - \beta$, α, β is the incidence and diffraction angle separately, and the diffraction angle is related with diffraction order, here we only consider the first diffraction order. Based on the designed parameters, the diffraction efficiency can be calculated as 0.039 with gold substrate. For optical elements, the reflection efficiency can be expressed as

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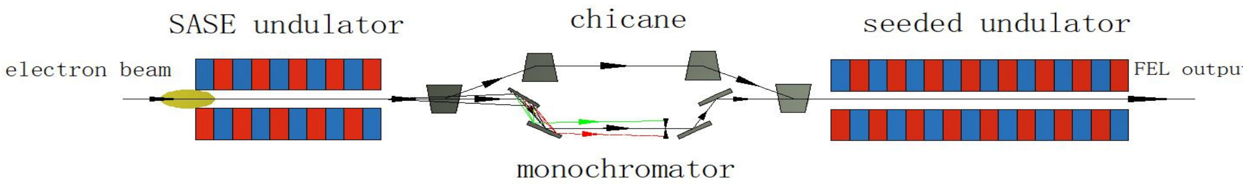

Figure 1: The layout of SXFEL user facility systems design.

$$R = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2,$$

where k_1 can be expressed as: $k_1 = (2\pi/\lambda)\, sin(\alpha)$, λ is the wavelength of diffraction pulse, k_2 can be expressed as: $k_2 = (2\pi/\lambda)\sqrt{n^2 - \cos(\alpha)^2}$, with n the atomic scattering factor, which is related to the material of optical elements. In our monochromator system design, we choose the gold as the optical elements material, the reflection efficiency can be calculated as 0.9588 for a single optical element. We consider the reflection and diffraction efficiency at the same time, the transfer efficiency of whole optical system can be calculated as 0.0329.

THE CHICANE DESIGN

In self-seeding scheme, the chicane is mainly used to eliminate the microbunching produced in SASE undulator as well as compensate the optical delay generated by the grating monochromator. The layout of designed chicane is displayed in the paper [12]. In the previous system design, the value of R_{56} of the chicane is given at the variation range from 372-446 µm, which is related to the length and the deflection angle of dipole, the relation can be expressed as: $R_{56} = L\theta^2$. Considering the actual situation, the length of dipole is chosen as 0.5 m, the variation range of deflection angle is 2.73-2.99 mrad correspondingly.

THE OPTICAL SIMULATION

In the previous optical simulation based on the shadow, we use the conventional Gaussian light and the radiation characteristic of SASE FEL is not considered. In this paper, the radiation characteristics of SASE FEL including the length, transverse size and divergence angle are considered. Based on Genesis simulations, the RMS transverse size of light pulse is 50 µm，the Rayleigh length can be calculated by:

$$Z_R = \frac{\pi\omega_0^2}{\lambda} = 6.3\,\text{m}.$$

Thus, the divergence angle of light pulse is:

$$\theta = \frac{0.2\omega_0}{Z_R} = 1.5\,\mu\text{rad}.$$

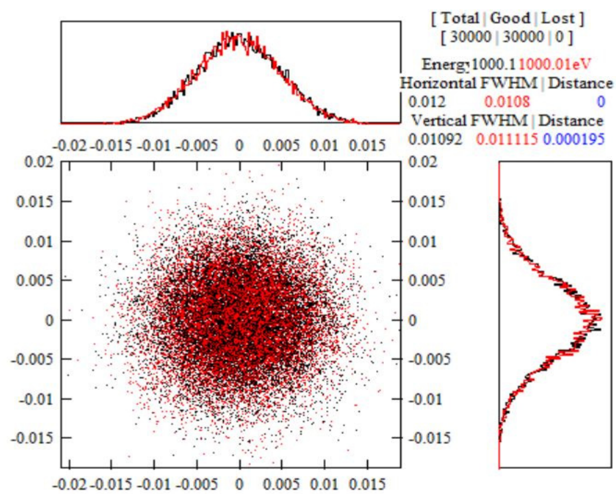

Figure 2: The transverse distribution of light source.

The RMS longitudinal depth of SXFEL user facility light pulse is 200 fs (60 µm). In the shadow simulation, the input photon energy is 1000 eV and 1000.1 eV. The transverse distribution of light source in the shadow simulation is displayed in Fig. 2. The red point is the 1000.1-eV photon and the black point is the 1000-eV photon.

In this optical system design, shadow simulation is always used to get the power resolution of monochromator. The FEL light source is passed through grating monochromator, the input parameters have been described in the paper [12]. The final transverse distribution light pulse in the shadow simulation is showed in the top figure of Fig. 3.

From Fig. 3, one can find that the photon with different photon energy is separated apparently. We can rationally point out that the resolution power is more than 1/10000. In actual situation, many unideal conditions will affect the power resolution of grating monochromator, such as the roughness of the grating surface, the variation of temperature, machining error and so on. We use the roughness of the grating surface to simulate the affection of unideal condition to grating monochromator. The final result considering the roughness is also showed on Fig. 3. One can clearly find the resolution power degree significantly comparing to the situation without roughness, it’s worth mention that some photon will also lost considering roughness.

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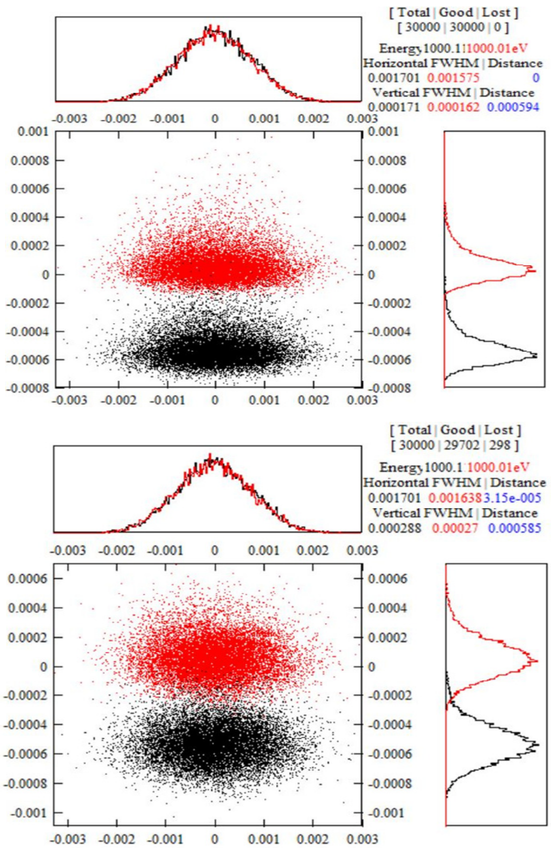

Figure 3: The transverse distribution of light pulse after the VLS toroidal grating.

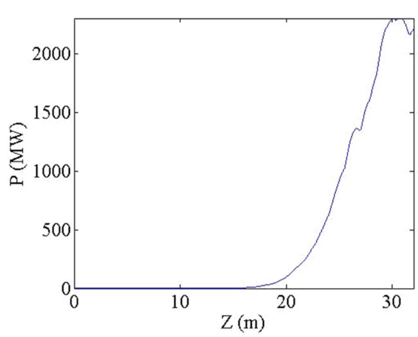

Figure 4: SASE power revolution along the undulator.

FEL SIMULATION

In the previous system design, a preliminary simulation is presented. In this paper, we present the recent simulation results based on the parameters at SXFEL user facility, the detail parameters have been displayed in the paper [12]. The SASE power revolution along the undulator, based on Genesis simulations [13], is showed in Fig. 4.

Generally, the SASE FEL radiation power in self-seeding process is two orders of magnitude lower than the saturation power, in the SASE simulation, the total SASE undulator length is chosen as 20 m. After that, the SASE radiation is purified by a monochromator. In our simulation, the transfer efficiency and power resolution of monochromator are considered. Spectrums before and after the monochromator are displayed in Fig. 5.

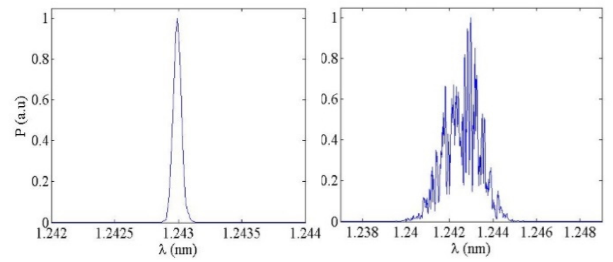

Figure 5: The spectrums before and after the monochromator.

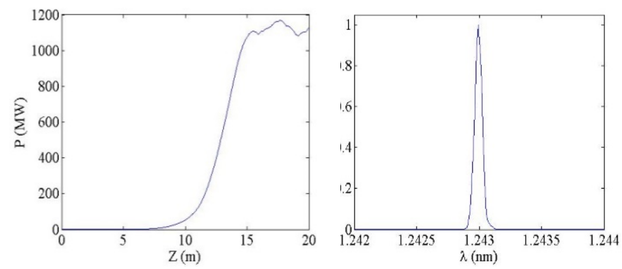

Figure 6: The power revolution along the seed undulator and the final spectrum.

Afterward, the purified spectrum is sent into the seed undulator to generate self-seeding radiation until saturation. At the end of the seed undulator, we can get the radiation with longitudinal coherence. The power revolution along the seed undulator and the final spectrum are displayed on Fig. 6. We can clearly find the final self-seeding radiation has longitudinal coherence completely and the radiation will get saturation at 15 m. To achieve self-seeding saturation output, the total undulator length is 35 m and the total length of whole scheme is about 40 m.

CONCLUSION

In this paper, the system design for SXFEL user facility is intensity studied. The diffraction and reflection efficiency of our designed optical system are calculated to obtain the transfer efficiency of monochromator. A concrete chicane design is also presented based on the previous chicane calculation. An optical simulation based on the shadow is presented; in this simulation, the characteristic of FEL radiation and the roughness of grating are considered. We demonstrated that the power resolution of grating monochromator is above 1/10000 and the power resolution will decrease when the roughness is considered. Finally, a detailed self-seeding simulation is given and one can easily find that the self-seeding scheme is efficient to generate FEL radiation with longitudinal coherence. We can also conclude our system design can achieve self-seeding saturation output within a distance of 40 m. Further effort will detail the system design, such as the mechanical system, thermal effect of grating monochromator and other characteristics.

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