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Self-seeded XFEL for Science Applications

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1. Abstract

PAL-XFEL achieved the highest spectral intensity of XFEL using the self-seeding scheme. We demonstrated that the self-seeded FEL with higher reproducibility and cleaner spectrum enables a superior multiplicity of data to the SASE FEL for the serial femtosecond crystallography. Time-resolved X-ray absorption spectroscopy using the self-seeded FEL is under study.

2. Self-Seeded XFEL

The PAL-XFEL[1] hard X-ray self-seeding successfully demonstrated a forward Bragg diffraction self-seeded XFEL with unprecedented peak brightness (3.2×10^{35} photons/(s·mm^2·mrad^2·0.1%BW) at 9.7 keV) and the bandwidth of 0.19 eV [2]. We used high-index Bragg reflections (33-3 or 115) to exploit a narrow seed bandwidth < 0.1 eV and a long wake duration ~65 fs. A calm longitudinal-phase-space with energy modulation further suppressed is required to suppress pedestal effects due to microbunching instability substantially (see Fig. 1). A very small shot-to-shot electron-energy jitter of 0.012% allows us to get > 94% of the shots having an intensity higher than the average SASE intensity [3]. Using high-index Bragg reflections (53-3), we could achieve similar self-seeding performance at a photon energy of 14.6 keV (see Table 1). The bandwidth of 14.6 keV seeded FEL is 0.32 eV limited by the energy chirp of the e-bunch, and the peak brightness is 1.3×10^{35} photons/(s·mm^2·mrad^2·0.1%BW), the highest to date. The peak brightness of 3.5 keV seeded FEL is 6.1×10^{33} photons/(s·mm^2·mrad^2·0.1%BW), the highest to date also. The pedestals from the SASE background are substantial at 3.5 keV because the SASE growth rate is high enough to compete with the amplified seed signal.

Table 1: Self-seeding parameters at 3.5 keV, 9.7 keV, and 14.6 keV.

Photon energy, keV	3.5	9.7	14.6
Crystal cut	110	100	100
Crystal thickness, µm	30	100	100
Crystal plane	1-11	33-3	53-3
FBD bandwidth, eV	0.79	0.06	0.024
Average pulse energy, mJ	0.93±0.14	0.85±0.14	0.26±0.07
Spectral bandwidth, eV	0.95	0.19	0.32
Peak spectral brightness, photons/(s·mm^2·mrad^2·0.1% BW)	6.1×10^{33}	3.2×10^{35}	1.3×10^{35}

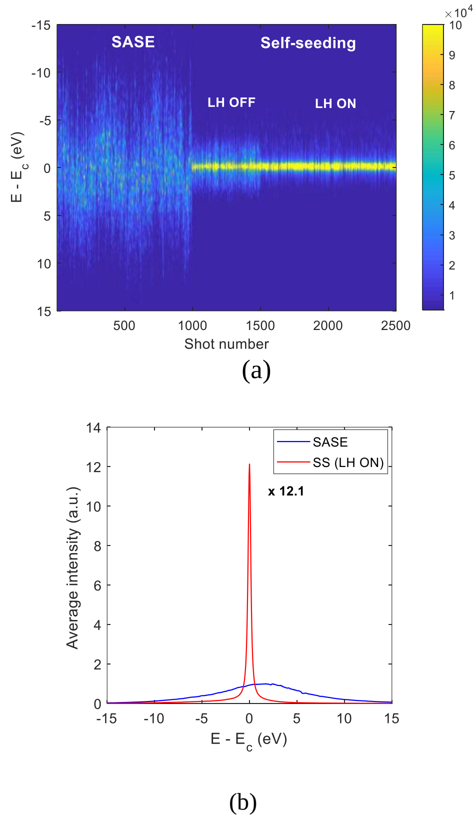

Fig. 1. The spectral intensity of self-seeded vs. SASE XFEL for 9.7 keV FEL. a) Color maps of 1,000 SASE and self-seeded FEL spectra measured by a single-shot spectrometer with laser heater (LH) On and OFF. b) SASE and self-seeded FEL spectra averaged over 1,000 shots, with the peak value of the SASE spectrum set to 1, and E_c = 9.7 keV.

3. Science applications

We revealed that the self-seeding data shows superior metrics than the SASE data at high resolutions through a demonstration experiment of serial femtosecond crystallography; the multiplicity of the self-seeded data sets is almost 1.4 times larger than that of the SASE (see Fig. 2). We have investigated the time-resolved X-ray absorption spectroscopy using the self-seeded FEL to compare it with the SASE data. And X-ray emission spectroscopy (XES) and X-ray absorption near edge structure (XANES) are being tested using the self-seeded FEL to compare with the SASE. In addition, we improved the control accuracy of the photon energy scan for the self-seeded FEL to facilitate spectroscopy analysis.

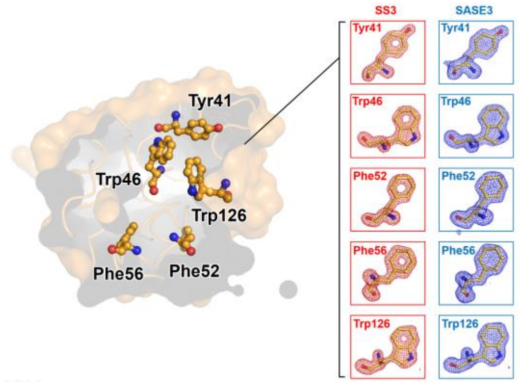

Fig. 2. Overall structures of lysozyme models (self-seeded and SASE modes) from chicken eggwhite with *mFo-DFc* electron density maps at 1.60-Å resolution.

REFERENCES

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[3] Kang, H.-S. *et al*. FEL performance achieved at PAL-XFEL using a three-chicane bunch compression scheme. *J. Synchrot. Radiat.* **26**, 1127–1138 (2019).