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OVERVIEW OF R&D ACTIVITIES IN THE PRODUCTION OF HIGH ENERGY PHOTON BEAMS FOR FUTURE USER EXPERIMENTS BEYOND 25 keV AT THE EUXFEL

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Abstract

Scientific opportunities with very hard XFEL radiation demands dedicated facility development towards FEL operation in the sub-ångström regime. Very hard X-rays provide capabilities of high Q-range coverage and high penetration, and also allow access to the K-edge spectroscopy of high-Z elements. Production of such X-rays using FELs takes advantage of general FEL characteristics such as large coherence, short pulse option, variable pump-probe delay control and higher brightness compared to conventional storage ring sources. R&D activities in the characterization and production of high energy photon beams beyond 25 keV has been launched since 2021 at the EuXFEL. Photon beams of 30 keV have been produced, characterized and delivered to experimental hutches. In this paper, we give an overview of the overall development. Obtained results will be discussed.

INTRODUCTION

The generation of femtosecond pulses of very hard X-rays (i.e., at least 12.4 keV in photon energy) at coherent light source facilities opens up unprecedented scientific opportunities in probing matters and materials at extremely fine spatial (atomic-scale) and temporal (femto- and attoseconds scale) resolutions. Great progresses have been made at existing X-ray Free-Electron Laser (FEL) facilities worldwide [1–5]. Towards even harder X-rays beyond 25 keV (i.e. 0.5 Å in photon wavelength), more physical and technical challenges must be confronted and overcome in order to push forward the frontier of delivering such X-rays to the user experiments, inspiring discoveries in the fundamental fields [6].

The European XFEL (EuXFEL) is a hard X-ray FEL based on a high-electron-energy superconducting linear accelerator [1]. It was commissioned in 2017. The first lasing was reported in May 2017. Shortly after that, the facility started its user operation. At a nominal electron beam energy of 14 GeV, stable, high-intensity SASE performance is achieved at photon energies up to 20 keV in user runs. In 2020, it was reported, for the first time, that lasing signals at 25 keV were observed [7]. The FEL performance in terms of highest achievable photon energies expected in the original technical design report has been surpassed. This has, furthermore, demonstrated a unique capability of the facility in combining a high energy linac and long flexible undulators for achieving decent lasing intensities of even harder X-rays. Interested readers are referred to [1] for more details.

MILESTONES

Proof-of-principle experiments have been performed in the past years at the EuXFEL, aiming to explore the machine performance in the sub-ångström radiation regime. In Table 1, a summary on the working progress is given. As shown, FEL lasing at 30 keV in the fundamental mode is made possible since 2021. The highest achievable photon energy so far is about 30 keV with a SASE intensity of about 340 µJ (see [8] for details). Figure 1 shows, for example, the measured SASE spectrum at about 24 keV (left) and 30 keV (right) using a Hard x-ray single-shot spectrometer [9]. The insets illustrate the FEL beam spots observed downstream on the imagers. Dedicated photon beam line studies were also carried out, through which the 30 keV FEL beams were successfully transported to the experimental hutches with reasonably high transmission rates. A first test user-experiment was conducted at the SASE1 undulator line using 24 keV FEL beams. Overall, great progress was made. During these experiments more physical and / or technical challenges have been unveiled. Two major challenges are described in the next section.

CHALLENGES

The accessible photon wavelength via the Self-Amplified Spontaneous Emission (SASE) process depends on electron beam energy, undulator parameter and undulator period. An inverse scaling of the photon wavelength with the square of the beam energy conceptually defines shorter wavelengths at given higher beam energies. The undulator parameter is proportional to the product of undulator period and the undulator magnetic field. Given a fixed undulator period, a larger undulator gap results in weaker magnetic field, which is characterized by a smaller undulator parameter, resulting in a shorter photon wavelength. Reducing the undulator period naturally shifts the emission regime towards shorter photon wavelengths. In addition, the lasing performance of an FEL depends on the achievable qualities of the electron beams in the undulators.

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Table 1: Milestones of Proof-of-Principle Experiments at the European XFEL Generating Very Hard X-Rays

X-ray Beamline	Photon energy, E_{ph}	Pulse energy, J_{ph}	Transport to exp. hutches	Exp. time
n/a	[keV]	[μJ]	n/a	Month/Year
SASE1	25	lasing signal[1]	no	Apr. 2020
SASE1	24	810	yes	Oct. 2021
SASE2	30	340	no	Oct. 2021
SASE2	30	40[2]	yes	Nov. 2022
SASE1	30	200	no	Oct. 2023
SASE2	30	120	yes	Nov. 2023

[1] Lasing signals were seen on an FEL imager downstream the undulators. No SASE tuning was carried out for increasing the obtained intensity.
[2] This was for dedicated photon beamline studies; Low requirement was made intensity-wise and thus no dedicated FEL tuning was carried out.

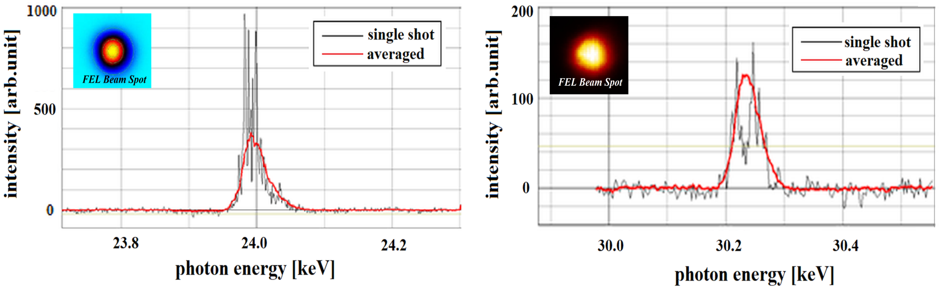

Figure 1: Measured SASE spectrum at about 24 keV (left) and 30 keV (right).

The FEL gain length increases with the increase of the transverse emittance and uncorrelated energy spread of the electron bunch, and decreases with an increase in the bunch peak current. The obtained gain length should be sufficiently small so that the SASE process at a resonant wavelength can grow within a given undulator length until saturation. An undulator length of typically 20 times the obtained gain length allows for the generation of high-power X-rays at a requested wavelength. Note that longer undulators would also add more challenges for an accurate alignment.

The main challenges for extending the operational regime of the EuXFEL towards higher photon energies in the fundamental mode mainly include: (A) further improvement in the electron bunch quality and (B) further improvement in the undulator alignment. Better bunch quality shortens the FEL gain length. Well-aligned undulators allow the SASE process to grow adequately until saturation.

Low-Emittance Electron Beams

Reducing the transverse emittance of the electron bunch can be the most efficient way to access to higher photon energies (shorter wavelengths) for an existing SASE FEL. A prerequisite requirement thus lies on the emittance optimization for the low energy beams in the photoinjector. At the EuXFEL, the emittance optimization is conducted for 250 pC electron bunches energized to 130 MeV. A typical optimization approach considers the peak cathode accelerating gradient (up to 60 MV/m), the radio-frequency (rf) gun phase and the gun solenoid strength. The cathode drive laser pulse has a temporal Gaussian distribution of 5–7 ps in full width half maximum and a transverse uniform or semi-truncated Gaussian distribution with a beam shaping aperture size of 1 mm in diameter. The emittance measurement is usually done using on-crest phasing of the first accelerating module and the third harmonics module of the injector. A detailed description can be found in [10].

Figure 2 shows long-term statistics of the measurement data during emittance optimization in the injector. A multi-quadruple scan method is used [11]. As shown, an average emittance of about 0.38 μm is usually obtained after the optimization. Specifically, for the FEL experiments as listed in Table 1, the optimized emittance was in the range from 0.31 μm to 0.34 μm. Using such low-emittance beams, it turned out the FEL had lased at 30 keV with good intensities.

Despite the obtained results with 30 keV lasing in the fundamental, there is still much room for improvement in the transverse bunch emittance. Numerical studies have been carried out to explore different working scenarios and conditions. In [12], an optimal transverse distribution of the electron bunch, namely, truncated-Gaussian (TG), is used for optimizing a charge packet of 100 pC in the injector. Such a TG distribution can efficiently linearize the space-charge fields during the photoemission and reduce the space-charge induced emittance contribution [13]. It is worth mentioning, that an optimized emittance of about 0.23 μm is obtained at 100 pC following this approach, indicating another 30% reduction compared to the presently measured emittance in the injector. Furthermore, numerical studies in [14] regarding the emittance optimization for an superconducting radio-frequency (SRF) gun based continuous-wave (CW) photoinjector, have demonstrated that the overall emittance of a 100 pC bunch can be reduced to its thermal emittance level (i.e. the fundamental limit for a smallest possible emittance), under the conditions that the bunch has a longitudinal

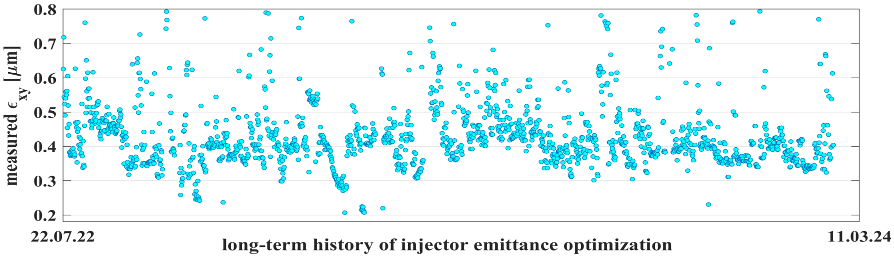

Figure 2: Long-term measurement history of transverse projected emittance of the electron bunch in the injector at 250 pC.

flat-top shape and a transverse TG shape. The required temporal and transverse shapes can be principally realized by shaping the cathode drive laser pulses. This promising approach will also be explored in the future experiments.

Undulator Alignment

The hard X-ray undulator line of the EuXFEL consists of 37 cells. Each cell is composed of a 5 m long undulator and a 1.1 m long intersection. Well-aligned undulators are of great importance to the overlap of photon and electron beams and thus for the FEL performance. This is crucial as approaching to the emission regime at 25+ keV, where the tolerances to machine uncertainties become much tighter.

Figure 3 shows the measured SASE pulse energies along the undulators. The data are extracted from the experiments in Oct. 2021 and Nov. 2023 (see Tab.1). As illustrated, the final pulse energy by the undulator cell 31 was limited to about 0.12 mJ in Experiment 2023 (red bar), and it was observed that, the last few cells downstream cell 31 did not contribute to the lasing process. Pulse-energy-wise, this result is consistent with the intensity level that was achieved at the same location in Experiment 2021 (blue bars). The difference is that the last few cells did contribute in the 2021 experiment and raised the final intensity to about 0.34 mJ by the cell 37. It is empirically known that the optimized electron bunch qualities for these two experiments were similar, as are the obtained peak currents downstream the last bunch compression stage. Assuming reasonable beam transport through the main linac until the undulator entrance, the observed discrepancy in the lasing performance between these two experiments was very likely attributed to the misalignment of the last few undulator cells. To further improve the undulator alignment accuracy, both electron-beam based alignment [15] and photon-beam based alignment [16] methods are developed and implemented. A technical goal is set to reduce the misalignment error to a level below 10 µm.

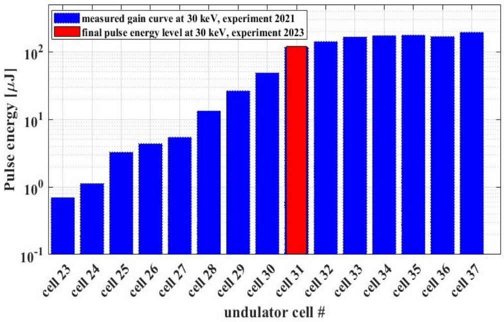

Figure 3: SASE pulse energies along the undulator cells as measured in the experiments 2021 and 2023.

USER PERSPECTIVES

Hard X-ray FEL pulses with photon energy above 25 keV from EuXFEL will open a door for various new science cases. Firstly, the high-energy XFEL will broaden the scope of diffraction experiments. Although serial femtosecond crystallography is one of the most popular experiments at current FEL facilities, the targets of these experiments have mostly been limited to macromolecular crystals. These crystals possess large unit cell parameters, resulting in a sufficient number of diffraction spots on the detector to determine crystal orientation even when selecting low photon energies (~10 keV). The very high-energy X-ray pulses from EuXFEL will expand the accessible scattering vector (Q) range and extend the capabilities of damage-free structure determination to more general samples, such as organic materials and organic-inorganic hybrid materials, both known for their high radiation-damage sensitivity. The broad Q-range accessible with high-energy FELs is also advantageous for detailed structure analysis beyond simple determination of atomic configurations. Measurement of diffraction intensity across a wide Q-range allows for imaging of density distributions of valence electrons. By combined with external pumping sources, such as femtosecond optical lasers, the visualization of valence electrons in action will be observable.

The high-energy XFEL also offers significant benefits for spectroscopic studies. The photon energies it provides can cover the K-edges of high-*Z* elements including 4d and 5d transition metals, which are essential for material science. These elements serve as the foundation for many man-made catalysis processes and strongly correlated materials that exhibit unique quantum phases. The time-resolved measurements of charge dynamics within these systems via absorption/emission spectroscopy and inelastic scattering techniques will provide a route to find out the detailed mechanisms underlying the emergence of their properties.

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REFERENCES

[1] W. Decking *et al.*, "A MHz-repetition-rate hard X-ray free-electron laser driven by a superconducting linear accelerator", *Nat. Photonics* **2020**, *14*, 391–397. `doi:10.1038/s41566-020-0607-z`

[2] E. Prat *et al.*, "A compact and cost-effective hard X-ray free-electron laser driven by a high-brightness and low-energy electron beam", *Nat. Photonics* **2020**, *14*, 748–754. `doi:10.1038/s41566-020-00712-8`

[3] P. Emma *et al.*, "First lasing and operation of an ångstrom-wavelength free-electron laser", *Nat. Photonics* **2010**, *4*, 641–647. `doi:10.1038/nphoton.2010.176`

[4] T. Ishikawa *et al.*, "A compact X-ray free-electron laser emitting in the sub-ångström region", *Nat. Photonics* **2012**, *6*, 540–544. `doi:10.1038/nphoton.2012.141`

[5] H. Kang *et al.*, "Hard X-ray free-electron laser with femtosecond-scale timing jitter", *Nat. Photonics* **2017**, *11*, 708–713. `doi:10.1038/s41566-017-0029-8`

[6] The Workshop on Scientific Opportunities with Very Hard XFEL Radiation, Jan 18—20, 2023, Hamburg, `https://indico.desy.de/event/33463/overview`

[7] European XFEL News, "European XFEL reaches world record photon energies", 8 Apr. 2020.

[8] Y. Chen *et al.*, "Virtual commissioning of the European XFEL for advanced user experiments at photon energies beyond 25 keV using low-emittance electron beams", *Journal of Physics: Conference Series* **2023**, *2420*, 012026. `doi:10.1088/1742-6596/2420/1/012026`

[9] N. Kujala *et al.*, "Hard x-ray single-shot spectrometer at the European X-ray Free-Electron Laser", *Review of Scientific Instruments* **2020**, *91*, 103101. `doi:10.1063/5.0019935`

[10] F. Brinker, "Commissioning of the European XFEL Injector", In Proceedings of the International Particle Accelerator Conference (IPAC'16), Busan, Korea, 8–13 May 2016. `doi:10.18429/JACoW-IPAC2016-TUOCA03`

[11] S. Meykopff and B.Beutner, "Emittance Measurement and Optics Matching at the European XFEL", In Proceedings of the 16th International Conference on Accelerator and Large Experimental Physics Control Systems, Barcelona, Spain, 8-13 Oct 2017. `doi:10.18429/JACoW-ICALEPCS2017-THPHA116`

[12] Y. Chen, F. Brinker, W. Decking, M. Scholz, and L. Winkelmann, "Perspectives towards Sub-Ångström Working Regime of the European X-ray Free-Electron Laser with Low-Emittance Electron Beams", *Applied Sciences* **2021**, *11*, 10768. `doi:10.3390/app112210768`

[13] Y. Chen *et al.*, "Budgeting the emittance of photoemitted electron beams in a space-charge affected emission regime for free-electron laser applications", *AIP Advances* **2020**, *10*, 035017. `doi:10.1063/1.5129532`

[14] D. Bazyl, Y. Chen, M. Dohlus, and T. Limberg, "CW Operation of the European XFEL: SC-Gun Injector Optimization, S2E Calculations and SASE Performance", arXiv:2111.01756. `doi:10.48550/arXiv.2111.01756`

[15] M. Scholz, W. Decking, and Y. Li, "Beam Based Alignment in all Undulator Beamlines at European XFEL", In Proceedings of the International Free Electron Laser Conference (FEL'19), Hamburg, Germany, August 2019. `doi:10.18429/JACoW-FEL2019-THP002`

[16] W. Freund *et al.*, "First measurements with the K-monochromator at the European XFEL", *Journal of Synchrotron Radiation* **26**, *1037* (2019). `doi:10.1107/S1600577519005307`