ISBN: 978-3-95450-227-1 ISSN: 2673-5490 doi:10.18429/JACoW-IPAC2022-TUPOPT010

VIRTUAL COMMISSIONING OF THE EUROPEAN XFEL FOR ADVANCED USER EXPERIMENTS AT PHOTON ENERGIES BEYOND 25 keV USING LOW-EMITTANCE ELECTRON BEAMS

Y. Chen*, F. Brinker, W. Decking, M. Scholz, L. Winkelmann, Z.-H. Zhu†
Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany

Abstract

Growing interests in ultra-hard X-rays are pushing forward the frontier of commissioning the European X-ray Free-Electron Laser (XFEL) for routine operation towards the sub-ångström regime, where a photon energy of 25 keV (0.5 Å) and above is desired. Such X-rays allow for larger penetration depths and enable the investigation of materials in highly absorbing environments. Delivering the requested X-rays to user experiments is of crucial importance for the XFEL development. Unique capabilities of the European XFEL are formed by combining a high energy linac and the long variable-gap undulator systems for generating intense X-rays at 25 keV and pushing the limit even further to 30 keV. However, the FEL performance relies on achievable electron bunch qualities. Low-emittance electron bunch production, and the associated start-to-end modelling of beam physics thus becomes a prerequisite to dig into the XFEL potentials. Here, we present the obtained simulation results from a virtual commissioning of the XFEL for the user experiments at 25 keV and beyond, including the optimized electron bunch qualities and corresponding FEL lasing performance. Experimental results at 30 keV from the first test run are presented.

INTRODUCTION

Linear accelerator based self-amplification spontaneous emission (SASE) free-electron lasers (FEL) produce extremely short, brilliant and coherent X-ray pulses [1–7]. This made it possible using the X-rays to probe distances at the atomic scale and explore the dynamics of atomic and molecular process on their natural length and time scale. The XFEL has greatly set forward the frontiers of resolving the structure of matters with X-rays over the last decade.

The XFELs capable of operating at short wavelengths of 0.10 nm to 0.01 nm, that is, at high photon energies of about 12.40 keV to 123.98 keV, can provide the so-called hard X-rays in the sub-ångström regime. These hard X-rays are of significant importance to temporally and spatially-resolved analysis and reconstruction of materials with various degrees of crystallinity. Harder X-rays above 12.40 keV are more beneficial to characterizing semi and noncrystalline materials, observing structural in-situ phase transitions, acquiring structural information, reconstructing material spatial distributions, etc.

At the European X-ray Free-Electron Laser (EuXFEL) [2], hard X-ray pulses have been delivered for routine user experiments since 2017. At a nominal electron beam energy of 14 GeV, stable, high-intensity SASE performance is achieved at photon energies up to 14 keV in routine user runs [8–10], while in test runs, good lasing signals towards 25 keV have been achieved with only limited tuning time. The actual lasing capability of the European XFEL in an even deeper sub-ångström emission regime is not yet demonstrated, although relevant theoretical studies have been carried out in [11, 12] under specific working modes and conditions.

SIMULATION

Here we present the obtained results from a virtual commissioning of the EuXFEL by start-to-end beam physics simulations and SASE optimization at high photon energies of 25 keV and above. Table 1 shows typical machine operation parameters which are employed correspondingly in the follow-up numerical studies. The codes OCELOT [13] and GENESIS [14] are used. The EuXFEL photoinjector [15] is optimized in the simulations taking into account the collective effects as studied in detail in [16]. The close-to cathode beam dynamics is carefully considered using the 3D approach as reported in [17].

Table 1: Machine Operation Parameters

Parameter	Value	Unit
Bunch charge	250	pC
Bunch shaping aperture [a]	1.0	mm
Cathode laser pulse shape	Gauss	n/a
Cathode laser pulse length[b]	3.0	ps
Cathode accelerating gradient	56.7	MV/m
Beam energy at BC0[c]	130	MeV
Beam energy at BC1	700	MeV
Beam energy at BC2	2400	MeV
Beam energy downstream L3[d]	16300	MeV
R56 at BC0	-50	mm
R56 at BC1	-50	mm
R56 at BC2	-30	mm
Undulator period[e]	4	cm
Undulator length	175	m

[a] in diameter
[b] root mean square value
[c] BCi stands for the i-th bunch compression stage, see Fig.1.
[d] L3 stands for the main linac, see Fig.1.
[e] for the undulators in SASE1 and SASE2 beamlines, see Fig. 1.

Figure 2 shows the slice emittance of an optimized electron bunch at the injector exit (i.e. in section I1 as shown in Fig. 1). This is done by scanning the phase of the gun

* ye.lining.chen@desy.de
† on leave from SINAP, Shanghai, China

ISBN: 978-3-95450-227-1 ISSN: 2673-5490 doi:10.18429/JACoW-IPAC2022-TUPOPT010

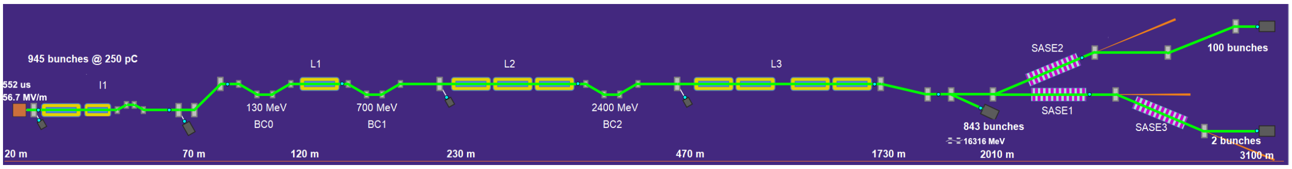

Figure 1: Schematic layout of the European X-ray Free-Electron Laser. I1: injector section; Li: the i-th linear accelerator; BCi: the i-th bunch compressor. SASEi: the i-th undulator beamlines in which SASE1 and SASE2 are hard X-ray lines while SASE3 is a soft X-ray line.

and the solenoid strength in the gun section. Thermal emittance of the photocathode is considered as the lower limit of an overall optimized bunch emittance [18]. At the European XFEL, cesium-telluride cathodes are used, the thermal emittance of which may intrinsically depend on the manufacture recipe. Here our optimization results are shown for three different thermal emittance values of the cathode, 0.85 μm/mm (blue), 0.99 μm/mm (black) and 1.11 μm/mm (red). The case with a thermal emittance of 0.99 μm/mm is selected based on previous studies (as reported in Ref. [19]) for further tracking simulations.

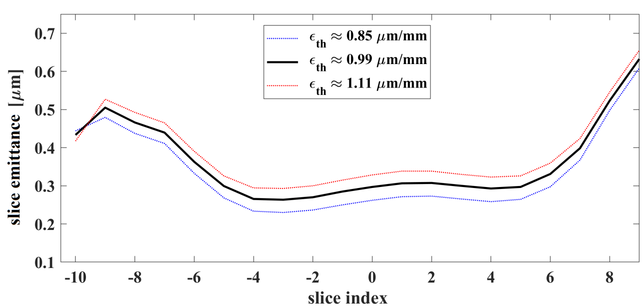

Figure 2: Optimized slice emittance at the injector exit considering different thermal emittance values of the cesium-telluride cathodes as tested at PITZ [19].

Figure 3 presents the optimized bunch qualities at the undulator beamline (i.e. SASE1 in Fig. 1) entrance via start-to-end beam physics simulations. RF parameters (amplitude and phase) of the accelerators (i.e. I1, L1, L2 in Fig. 1) are optimized compressing the bunch to 4.5 kA peak current after the second compression stage (i.e. BC2 in Fig. 1) according to the available accelerating voltages of the facility. The beam energy set-points and momentum compaction factors at individual bunch compression locations are given in Tab. 1. Collective effects through the whole accelerator beamline such as wakefields, space-charge and coherent synchrotron radiation are all included. As shown, the left plot illustrates an obtained bunch peak current of about 4.5 kA (left axis) and a slice energy spread of about 3.5 MeV (right axis). The right plot gives the bunch horizontal (green bars) and vertical (red bars) slice emittance.

Using the obtained bunch distribution as shown in Fig. 3, SASE optimization is carried out. As shown in Fig. 4, an optimized SASE intensity of about 1.8 mJ and 0.5 mJ are shown at 24.579 keV for SASE1 (left) and 30.235 keV for SASE2 (right), respectively. The corresponding fitted gain lengths are about 8 m and 10 m. The figure insets show the power distributions by the end of the undulator beamlines. In these simulations, both linear and quadratic tapers are optimized. An average beta function of 32 m is applied.

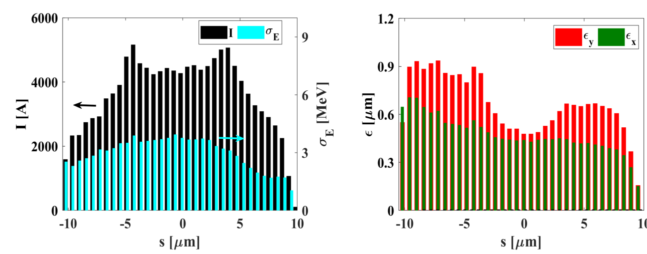

Figure 3: Bunch qualities in front of the undulator beamline SASE1. Left: peak current (left axis) and slice energy spread (right axis); Right: slice horizontal (green) and vertical (red) emittance.

FIRST TEST RUN UP TO 30 keV

First test run of the EuXFEL aiming for high photon energies above 25 keV was carried out last year on the request of the on-site users at DESY. Due to a temporary technical limit in the transport capability of the photon beam line, a target photon energy of 24 keV was preliminarily determined for SASE1 and 30 keV was requested for SASE2.

After short-term SASE tuning, in both SASE1 and SASE2 undulator lines the electron bunch lased at the aimed photon energies. The HIgh REsolution hard X-ray single-shot (HIREX) spectrometer [20] was used to verify the achieved photon wavelengths to be 24.579 keV and 30.235 keV at SASE1 and SASE2, respectively. The SASE spectrum at 30.235 keV is shown in Fig. 5. It should be noted, that for the first time, the FEL facility has ever been operated at such high photon energies. It is also worth mentioning that fairly good lasing intensities have been achieved in both beamlines at these photon wavelengths in the sub-ångström working regime.

Figure 6 shows the overall FEL performance panel corresponding to the test run in October 2021. As shown, about 0.8 mJ SASE intensity is achieved at 24.58 keV (0.5 Å) at SASE1 and about 0.3 mJ is obtained at 30.24 keV (0.4 Å) at SASE2. Additionally, the SASE3 beamline is simultaneously lasing undisturbed at 1 keV with an intensity of 10 mJ [9] during SASE tuning for the other two undulator lines.

ISBN: 978-3-95450-227-1 ISSN: 2673-5490 doi:10.18429/JACoW-IPAC2022-TUPOPT010

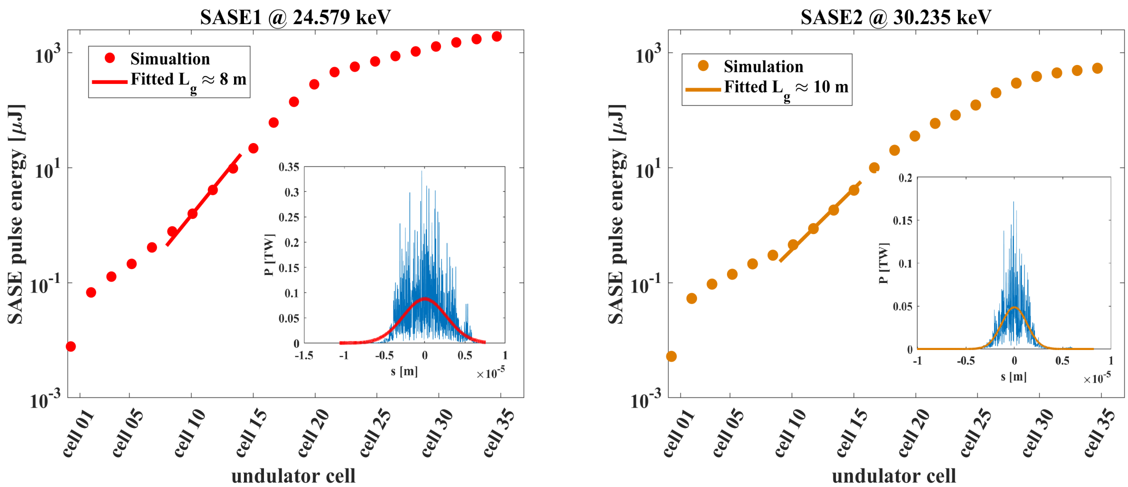

Figure 4: Simulated SASE intensities at 24.58 keV (left) and 30.24 keV (right) for beamlines SASE1 and SASE2, respectively.

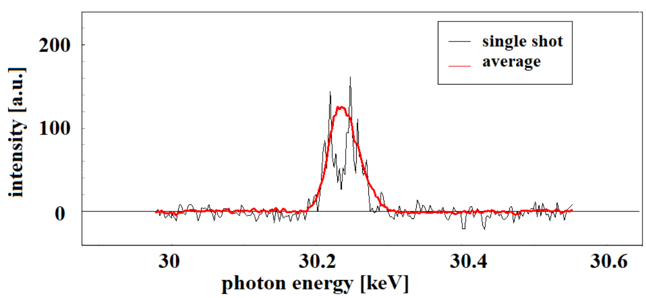

Figure 5: SASE spectrum detected by HIREX [20] for SASE2 with a central photon energy of 30.235 keV.

CONCLUSION

Virtual commissioning of the European XFEL is performed based on start-to-end electron beam physics simulations and SASE performance studies at high photon energies up to 30 keV in the sub-ångström working regime. The optimized simulation results have shown millijoule-level lasing performance. First short-term test run of the EuXFEL in October 2021 has demonstrated SASE intensities of about 0.8 mJ and 0.3 mJ at 24.58 keV and 30.24 keV, respectively, which, to the best of our knowledge, are the highest demonstrated SASE intensities at these wavelengths of the hard X-rays that are delivered to the users. More detailed characterization of the whole accelerator and undulator beam lines is planned. Comprehensive numerical and experimental studies will follow to reduce the existing discrepancies between measurement and simulation.

ACKNOWLEDGEMENTS

The authors acknowledge support from Deutsches Elektronen-Synchrotron DESY (Hamburg, Germany), a member of the Helmholtz Association HGF and European XFEL GmbH (Schenefeld, Germany). The authors thank the operation teams at DESY and the European XFEL for their experimental support.

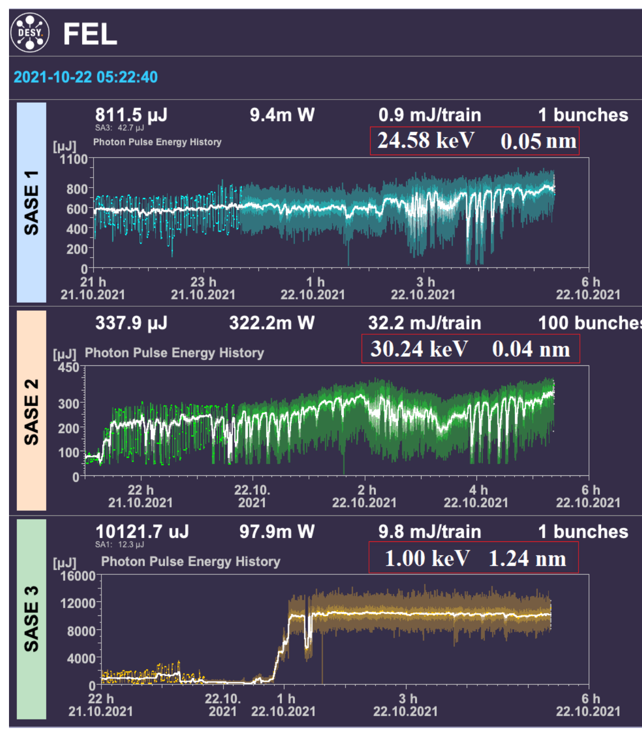

Figure 6: First test run of the EuXFEL delivering hard X-rays of about 0.8 mJ and 0.3 mJ at photon energies of 24 keV and 30 keV for SASE beamlines 1 and 2, respectively, with a simultaneous SASE pulse delivery of about 10 mJ at 1 keV for the SASE beamline 3.

REFERENCES

[1] M. Dohlus, J. Rossbach, "Synchrotron Radiation and Free-Electron Lasers". In *Landolt-Boernstein New Sewries*; Myers, S., Schopper, H., Eds.; Springer: Berlin/Heidelberg, Germany, vol. 21C, 2013. doi:10.1007/978-3-642-23053-0$_$41

[2] W. Decking *et al.*, "A MHz-repetition-rate hard X-ray free-electron laser driven by a superconducting linear accelerator",

ISBN: 978-3-95450-227-1 ISSN: 2673-5490 doi:10.18429/JACoW-IPAC2022-TUPOPT010

Nat. Photonics, vol. 14, pp. 391–397, 2020. doi:10.1038/s41566-020-0607-z

[3] 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*, vol. 14, pp. 748–754, 2020. doi:10.1038/s41566-020-00712-8

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

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

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

[7] Z. Zhu, Z. T. Zhao, D. Wang, Z. H. Yang, and L. Yin, "SCLF: An 8-GeV CW SCRF Linac-Based X-Ray FEL Facility in Shanghai", in *Proc. FEL'17*, Santa Fe, NM, USA, Aug. 2017, pp. 182–184. doi:10.18429/JACoW-FEL2017-MOP055

[8] D. Nölle, "FEL Operation at the European XFEL Facility", in *Proc. FEL'19*, Hamburg, Germany, Aug. 2019, pp. 766–771. doi:10.18429/JACoW-FEL2019-FRA01

[9] L. Fröhlich *et al.*, "Multi-Beamline Operation at the European XFEL", in *Proc. FEL'19*, Hamburg, Germany, Aug. 2019, pp. 335–338. doi:10.18429/JACoW-FEL2019-WEP008

[10] M. Scholz, "First Lasing at the SASE2 and SASE3 FELs of European XFEL", https://accelconf.web.cern.ch/fel2019/talks/moa04_talk.pdf

[11] 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*, vol. 11, p. 10768, 2021. doi:10.3390/app112210768

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

[13] OCELOT, https://github.com/ocelot-collab

[14] GENESIS, http://genesis.web.psi.ch/index.html

[15] F. Brinker, "Commissioning of the European XFEL Injector", in *Proc. IPAC'16*, Busan, Korea, May 2016, pp. 1044–1047. doi:10.18429/JACoW-IPAC2016-TUOCA03

[16] I. Zagorodnov, S. Tomin, Y. Chen, and F. Brinker, "Experimental validation of collective effects modeling at injector section of X-ray free-electron laser", *Nucl. Instrum. Methods Phys. Res., Sect. A*, vol. 995, p. 165111, 2021. doi:10.1016/j.nima.2021.165111

[17] Y. Chen, I. Zagorodnov, and M. Dohlus, "Beam dynamics of realistic bunches at the injector section of the European X-ray Free-Electron Laser", *Phys. Rev. Accel. Beams*, vol. 23, p. 044201, 2020. doi:10.1103/PhysRevAccelBeams.23.044201

[18] 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*, vol. 10, p. 035017, 2020. doi:10.1063/1.5129532

[19] P. W. Huang *et al.*, "Test of Cs2Te Thickness on Cathode Performance at PITZ", in *Proc. FEL'19*, Hamburg, Germany, Aug. 2019, pp. 473–476. doi:10.18429/JACoW-FEL2019-WEP062

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