euspen's 24th International Conference & Exhibition, Dublin, IE, June 2024
www.euspen.eu

Mechanical engineering challenges at European XFEL

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Abstract

Research facilities like European XFEL, located in Hamburg, Germany, are innovative hard X-ray photon sources that allow the exploration of previously inaccessible research areas. With the help of the 3.4 kilometre-long, underground machine, the scientists map the atomic details of viruses, decipher the molecular composition of cells, take three-dimensional images of the nanoworld, film chemical reactions, and study processes such as those occurring deep inside planets.
To deliver the X-rays to the experimental stations, the photon beam has to be manipulated by optical elements that have to preserve the unique properties of the photon beam. The optical elements are mounted in Ultra High Vacuum (<10^{-8} mbar) environment, have to be aligned and adjusted with high resolution (below 100 nm) and repeatability. The photon distribution system is 1 km long and the optical element have to drive the photons to the experimental targets with sub-micrometre accuracy. Therefore, mechanical stability and minimization of vibrations are paramount. A small part of the photon beam is absorbed by the optical elements and to avoid thermal drifts and minimize deformation of the perfect optical surface, cooling solutions based on eutectics are implemented. This contribution gives an overview of challenges and solutions for UHV compatible, high precision mechanics that support and remote control cooled optical elements for X-ray transport.

FEL, Synchrotron, SASE, Precision Mechanics, UHV, X-ray

1. Introduction

European XFEL is an X-ray Free Electron Laser research facility located in Hamburg, Germany and operational since 2017 [1,2]. The European XFEL is being realized as a joint effort by 11 European countries: Denmark, France, Germany, Hungary, Italy, Poland, Russia, Slovakia, Spain, Sweden and Switzerland. Since 2018 United Kingdom is also part of the European XFEL Convention.

The Free Electron Lasers produce coherent and intense laser-like radiation by accelerating a beam of electron bunches to relativistic speeds then passing it through a long periodic magnetic structure. As the electrons move through this magnetic field, they undergo periodic oscillations, emitting radiation in the process. Repeated interactions with the electron bunches amplify the emitted radiation, resulting in a high-powered and tuneable laser beam.

The facility is an international scientific infrastructure that generates extremely brilliant, ultrashort pulses of spatially coherent X-rays with wavelength that spans from 300 eV to 25 keV [3]. The high brilliance is enabled by the implementation of superconducting technology in the electron accelerator, while the high degree of coherence and the femtosecond pulses are the result of the self-amplified spontaneous emission (SASE) process that generates the photon beam.

Innovative and cutting-edge scientific experiments in a variety of disciplines spanning physics, chemistry, materials science and biology make use of the peculiar properties of the radiation, in particular in the investigation of ultrafast processes in atoms, ions, simple and very complex molecules, clusters or condensed matter. The high pulse energies allow the collection of meaningful data sets from single pulses, thereby enabling the study of non-reversible processes. Coherence properties are exploited in imaging techniques that aim to obtain atomic spatial resolution for weakly scattering systems. Finally, the very high X-ray pulse energies in combination with ultrashort pulses produces very high peak powers of up to several tens of GW and this enables the exploration of excited solids through non-linear X-ray scattering [4].

Besides the European XFEL in Germany, Free Electron Laser light sources able to produce hard X-rays also exist in Japan at SACLA [5], South Korea at PAL-XFEL [6], Switzerland at SwissFEL [7], and in the USA at LCLS-II [8]. In China, SHINE is under construction and is foreseen to become operational in 2025 [9]. Table 1 provides an overview and comparison of the main key parameters of the above-mentioned hard X-ray facilities.

In this contribution, following a description of the overall European XFEL facility, the main aspects, requirements, and implemented solutions for the mechanical design of photon devices are discussed. Finally, an outlook about possible future development directions and area of interest for this specific field of application is provided.

2. Layout of the European XFEL facility

The European XFEL facility consists principally of three sections: the superconducting accelerator, the electron and photon transport sections and the experimental hall. The Figure 1 provides an overview of the European XFEL facility.

The general layout of the facility is defined by three main conditions. In order to achieve high photon energy (in the order of 25 keV) and high pulse energy the electrons have to be accelerated up to 17.5 GeV. The average acceleration gradient of the implemented superconducting cavities is 20-25 MeV/m. Therefore, the total length of the acceleration section has to be in the order of 1 000 m.

Table 1 Comparison of main parameters and key figures of hard X-ray FEL facilities worldwide.

	European XFEL	LCLS-II	SACLA	SwissFEL	PAL-XFEL	SHINE
Start of commissioning	2016	2023	2011	2016	2016	2025
Accelerator technology	Super-conducting	Super-conducting	Normal-conducting	Normal-conducting	Normal-conducting	Super-conducting
Total facility length [km]	3.4	3	0.75	0.74	1.1	3.1
Maximum electron energy [GeV]	17.5	5	8.5	5.8	10	8
Maximum pulses per second	27 000	1 000 000	60	100	60	1 000 000
Minimum wavelength [nm]	0.05	0.25	0.08	0.1	0.06	0.05
Number of undulator lines	3	2	3	1	2	3
Number of experimental stations	7	10	4	3	3	10
Peak brilliance [photons/s/mm^2/mrad^2/0.1%BW]	5×10^{33}	2×10^{33}	1×10^{33}	1×10^{33}	1.3×10^{33}	1×10^{33}

The high collimated radiation produced at the end of the undulator sections, to be easily transported and manipulated by the optical systems, and stopped by the photon shutters, has to be of the size of 1 mm. The divergence of the high photon energy beam is in the order of 1 µrad and therefore the total length of the photon distribution system is about 1 000 m. The last condition is about the lateral separation of the experimental stations at the end of the tunnels that is linked to the maximum deflection angle of the electron beam. To achieve a separation of about 17 m among the beamlines, the photon transport system has to span over 1 000 m. Those conditions together with construction, installation, and possible future upgrade conditions bring the total length of the facility, from gun to experimental station, to 3.5 km.

The complete facility is constructed underground, about 25 m to 6 m below the surface. Access to tunnels for personnel and for installation and maintenance of components, is enabled by shaft buildings at the start and end of each tunnel section.

The first main element of the facility is the linear accelerator (linac) that is installed in 5.2 m diameter and about 2 000 m long tunnel. The linac accelerates the electrons to a final energy of up to 17.5 GeV by means of 96 accelerator modules operated at 2.2 K. The design of those superconducting modules was developed by an international collaboration for European XFEL based on the TESLA design [10]. Each module is 12 m long, weighs eight tons and comprises eight nine-cell Nb cavities.

The European XFEL accelerator is operated in the so-called burst mode. As depicted in figure 2, the accelerator delivers up to 2 700 electron bunches or pulses in a pulse train that lasts 600 µs. The repetition rate of the bunch trains is 10 Hz. Inside the bunch train the time distance between two consecutive pulses can be 220 ns, giving the possibility to operate at up to 4.5 MHz inside the bunch train. Electron bunches are converted in photon pulses that are going to be manipulated by the optical elements of the beam transport and then used for the experiments. This peculiar pulse structure provides very high power in the single pulse, exceeding 20 GW in the very short single pulse, but a quite mild, in the order of few watts, average power with respect to similar applications in the X-ray optic field.

At the end of the linac, after a collimation section the electrons enters in the FEL undulator sources where the electron bunches generate laser-like radiation at the X-ray wavelength [11, 12].

The electron and X-ray beam transport system is designed to accommodate up to five FEL sources. Each FEL source has a dedicated photon beam transport section to transport, guide, focus, and diagnose the X-ray beams. Distribution mirrors, installed in each FEL source, allow the delivery of the photon beam up the three experiments. the Figure 3 provides an overview of the complete electron and photon transport system.

Presently only three of the five possible FEL sources are installed and they are denoted SASE1, SASE2 and SASE3. SASE1 and SASE2 provide light in the hard X-ray regime from approximately 3 to 25 keV, while SASE3 is the soft X-ray source that spans from 250 eV to 3 keV. The entire electron and photon transport section is about 1 400 m long and the undulators are installed in a tunnel with diameter of 5.3 m while the photon transport tunnels have smaller diameter (4.6 m) because before those sections the electron beam is already separated from the photon beam and stopped on electron dumps. The undulator line consist of a sequence of 5 m long magnetic structures (NdFeB permanent magnet). Undulators are mechanical devices that can change the distance between the magnetic arrays in order to change the intensity of the magnetic field that is seen by the traveling electron beam and therefore tune the wavelength of the produced radiation. SASE1 and SASE2 are equipped with 35 undulators for a total length of 205 m, while SASE3 has 21 segments and a total length of 121 m.

The X-ray photon beam transport system is 1 000 m long and consists of optical systems to steer, slit, focus, attenuate, and monochromatize the photon beam, of diagnostic devices to characterize the photon beam properties and of shutters that can stop the photon beam to allow access in the downstream tunnel sections or experiments [15-17].

The last section is the experiment hall in which the scientific instruments are located and where the research program is run. The experiment hall has a size of 50 m along the beam direction and 90 m across to install five beam line areas.

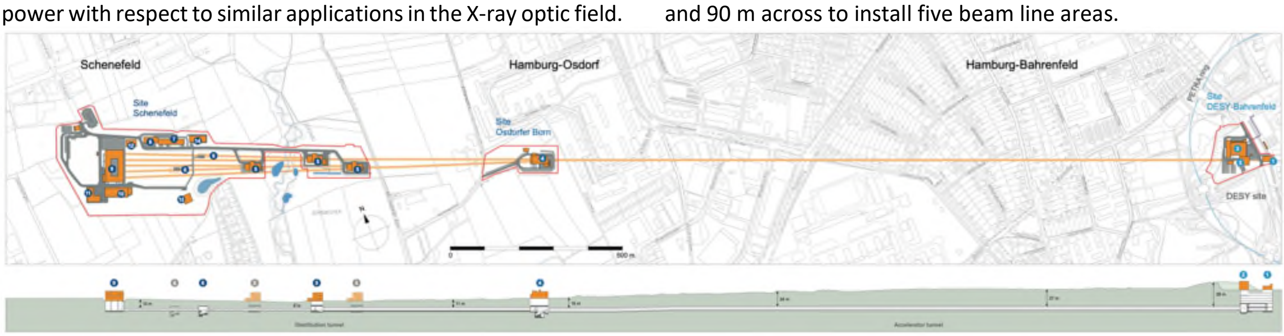

Figure 1. European XFEL facility layout [13].

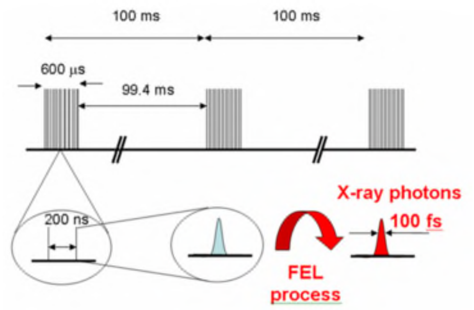

Figure 2. Time structure of the European XFEL accelerator [14].

Presently seven instruments are installed and operational: SPB/SFX and FXE at the end of SASE1, MID and HED at the end of SASE2 and SQS, SCS and SXP in the SASE3 beamline. A new instrument, HXS, located at the end of the SASE2 beamline is currently under design.

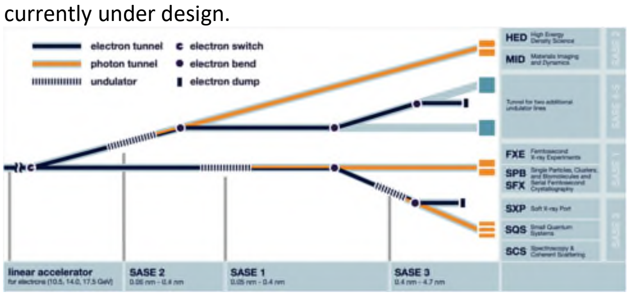

Figure 3. Electron and photon transport layout [13].

3. Challenges in the mechanical design of photon devices

The mechanical devices dedicated to supporting and adjusting the optical elements that manipulate the photon beam present challenging requirement. The complexity of the design comes from the requirement of high ultimate mechanical performance and from the boundary conditions given by the environment where those devices are installed and operated. Finite element analyses are widely used to support the design activity.

3.1. Mechanical requirements

To preserve the outstanding quality of the photon beam, the mirrors that guide and focus the X-rays have a reflecting surface with a maximum error of up to just 2 nm peak-to-valley. The mechanical interfaces have to be carefully designed to preserve the original shape at the nm level. Mirrors are made of single crystal silicon, have the shape of a rectangular parallelepiped and length up to 1 m for a total weight of about 6 kg. Mirror supports are designed as perfectly isostatic supports with three contact points from bottom located at the mirror Bessel points. In the horizontal plane there are three fixed points preloaded by custom designed pushers mounted exactly opposite [18]. In the contact area, the supporting points present spherical shape and are made of soft materials (CuSn6) in order to reduce the Hertzian contact stress. The low roughness (Ra = 0.01), spherical part of the supporting tip minimizes the friction between mirror and support. In this way two goals are achieved: the mirror is free to thermally expand minimizing the possible deformation and also the residual stress due to the mounting is minimized, making the optical metrology and the assembling process reproducible [19]. Special clamping system to transfer moment from motor actuated leaf springs to the mirror itself are designed in the case the mirror has to be bent in order to allow photon beam focusing. The design takes into account the anisotropic properties of the single crystal silicon slab and 17 MPa is considered the safe value for the ultimate tensile strength [20, 21].

The long beamlines and the small beam dimension at the experimental station set the angular stability of the reflective elements to values that are in the order of 0.1 µrad. The need to operate in a quite wide energy range requires adjustments of the optical elements in the 10 mm and 10 mrad range. A lot of effort goes in minimizing the degrees of freedom to the strict operational need and to achieve excellent and predictable mechanical behaviour. The mechanisms need to be, among other things, exactly constrained, free of backlash, extremely stiff and lightweight. Parallel kinematic systems based on flexures can be a viable option to comply to the tight specifications.

Part of the beam energy is absorbed by the optical elements and this generate thermal deformation that has to be minimized. The integrated power to be removed is rather small, in the order of 10 W, with respect to similar application but it is enough to create a thermal bump that spoils the quality of the optical elements. In vacuum and at almost room temperature conditions, the heat transfer is dominated by conduction effects: the mirror has to be connected to a heat sink that consists of a water pipe or an in-air dissipator. Critical is the connection of the cooling system with mirror because any clamping with good thermal conduction deforms the optics. Indium-Gallium eutectic, that is liquid metal at room temperature, is used as medium between mirror and cooling elements: nickel coated copper bars, connected to the heat sink with thermal braids, are immersed in grooves on the mirror that are filled with the eutectic bath.

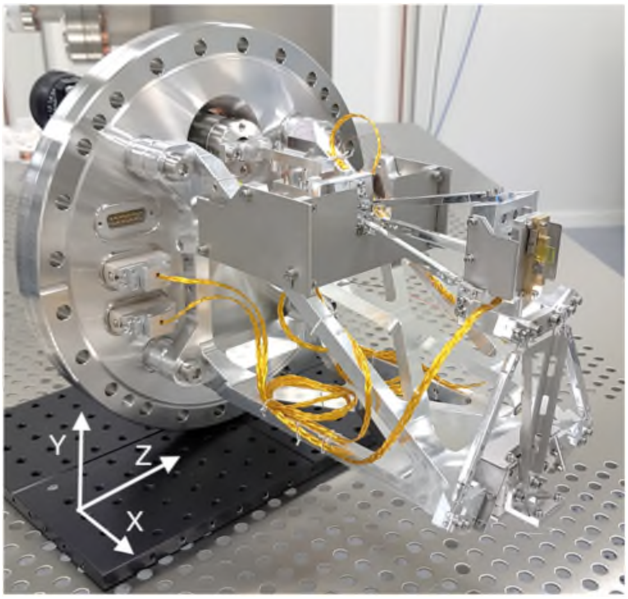

Figure 4. Example of parallel kinematic system for UHV environment.

Figure 4 displays an example of newly developed high-precision mechanics. This system is integral to the XFEL-Oscillator project, which endeavours to establish for the first time ever a laser cavity operating in the hard X-ray regime. The mechanics function to manipulate an HPHT-IIa diamond, used as crystal optics to form the cavity. Table 2 offers a summary of the degrees of freedom and their nominal performance. The motion is driven by piezoelectric positioning stages from SmarAct (SLC-1720 and SLC-2430 models), and the lever arms consist of Ti sheets that have been laser-cut and bent. The design is based on the parallel kinematics concept, realized with flexures made from metallic cables. Short metallic cables were chosen for their favourable ratio between high axial stiffness and limited bending force [22]. Laboratory testing has yielded reliable results to the micrometre level, constrained by environmental limitations. To verify performance at the nanometre level, commissioning with a photon beam is necessary. This commissioning process is scheduled to commence in spring 2024.

Table 2 Degrees of freedom and nominal performance of the crystal alignment mechanics. Figure 4 shows the cartesian axis convention.

Degree of freedom	Nominal resolution	Travel range
Translation X	1 nm	-8 mm +2 mm
Translation Y	1 nm	± 5 mm
Rotation X	8.3 nrad	± 33.3 mrad
Rotation Y	7.7 nrad	± 30.8 mrad

3.2. Installation and operation environment

The mechanical design has to take into account not only the ultimate performance but also the boundary conditions defined by the environment where the devices operate. The photon tunnels during operation cannot be accessed due to the high level of radiation generated by the traveling X-rays. The devices can be maintained and serviced only every six months. This imposes certain requirements about reliability, durability and remote control of the installed systems. The X-rays travel in an Ultra High Vacuum environment (UHV, $< 10^{-8}$ mbar) and therefore all the elements that interact with the beam have to be compliant to the UHV requirements [23]. The UHV requirements that impact the mechanical design the most are the careful choice of materials and the need to avoid lubricants for motors or linear guides. The design process has to take into account the benefit and the consequences of locating motors and position sensors inside or outside vacuum. To minimize possible optic contamination the cleaning, assembling and installation has to be done in an ISO class 5 or 6, depending of the installation area, particle free environment and this poses additional constraints to the material choices and make the handling and the life cycle of the device more complex. In the case the components are installed in the proximity of the electron beam the additional requirement of low magnetic permeability has to be accomplished [24]. Within 300 mm from the electron beam all the components should have relative magnetic permeability below 1.01 and this requirement restricts further the list of usable material and limits the use of welded solution. The high radiation level environment forces also careful considerations about the implementation of electronic elements in proximity of the electron beam. The main aspects that have to be taken into account are the possible coupling of noise in the reading and the reduced life of components.

3.3. Implementation of numerical computational techniques

Computational techniques, such as finite element analysis (FEA) and computational fluid dynamics (CFD), are widely implemented in various scientific and engineering fields. The main application areas are steady-state and transient thermomechanical simulations of optical elements under photon beam heat load, vibrational analyses, damage simulation due to heat load on solid stopper or gas-based attenuators, optimization of fluid cooling system and characterization of liquid sheet jets for sample delivery system. ANSYS and COMSOL are the commercial software that are used to perform such studies. In the case of thermal simulations that cover a wide temperature range like cryogenic elements or beam stoppers, the thermal properties of materials as function of temperature are a very relevant aspect and they are not easily available in the scientific literature. The material that are subject to the studies are mainly ceramic materials like Boron Carbide (B_4C), diamond, copper, silicon and high quality, low magnetic permeability stainless steels like AISI316LN. The transient analyses are often used to capture the behaviour of the optics under the peculiar time structure (see figure 2) of the heat load. The complexity of those simulations is given by the different dimensional scale of the elements involved: the timescale of the phenomena is in the in few hundreds of nanoseconds and therefore to satisfy the CFL condition the mesh has to be very small with respect to the beam profile and the area of interest in the optical elements that is in the millimetre scale [25]. Damage simulations allow to predict the damage limit of elements exposed to the beam taking into account a wide number of variables like photon beam size, pulse energy, number of pulses and photon energy that defines the penetration of the beam in the material. Recent developments in damage studies focus on the multiphysics problem of material ablation in the beam stopper [26].

An important topic is the reliability of the simulations and the effort that goes in setting up a systematic verification, validation and uncertainty quantification (VVUQ) process.

4. Outlook and future development direction

There is constant need of further development and innovation in the research facilities in order to enable new experiments. New FEL facilities target beamlines that offer high repletion rate and high pulse energy in a broad photon energy range. The high repletion rate and high pulse energy require more advanced cooling solutions and more careful considerations about the optics and stopper damage. Cryocooling of mirrors is an interesting solution for the thermal issues and it has already been implemented in few installations but for relatively short mirrors. The current understanding of the phenomena involved in the laser cutting technology can help in addressing part of the issues related to the optics damage and therefore a close collaboration with those institutes can be beneficial.

Quality of optics has dramatically improved in the last years and the length of the beamlines is also increased raising the mechanical stability requirements. Active controls together with precision mechanics offer a good prospective to cope with this kind of challenging requirements.

In the field of numerical simulations, the application of artificial intelligence tools and digital twins can improve the understanding of phenomena, reduce significantly the simulation time and support the mechanical design.

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