FemtoMAX

MAX IV beamline review report

The FemtoMAX beamline team

2024-06-25

This report is compiled to facilitate the 2024 external review of the FemtoMAX beamline at the MAX IV Laboratory. The report contains a description of the beamline as a unit including beamline technical specification, performance, staffing, user support, and future strategy. This document provides the review committee with sufficient details and information for the beamline performance evaluation.

Contents

1 General introduction

FemtoMAX is a time resolved X-ray scattering beamline supporting a broad user community since 2021. Time resolved X-ray studies with a temporal resolution below 140 fs, can be performed on solids and liquids in multiple sample environments including sample heating and cryo cooling. The beamline offers two-week support per user group, which is needed due to the low (10 Hz) repetition rate of the X-ray source. The two week allocations allows users to plan their experiments with less stressful time constraints compared to FEL and storage ring beamlines. To have high experimental success, a fast access route is promoted for sample screening for first-time FemtoMAX users. In-house research at the FemtoMAX beamline is driven by beamline staff which is focused on advanced sample environments and novel methods for improving beamline performance and user control system friendliness. The beamline vision and planned future instrumentation upgrades, including higher beamline operational repetition rate, will keep the FemtoMAX beamline attractive and competitive for time resolved X-ray studies.

2 Technical beamline description

2.1 Beamline design

FemtoMAX is one of the first phase beamlines at MAX IV and is dedicated to ultrafast X-ray studies in solids and liquids using multiple sample environments including local sample heating and cryo cooling. The beamline entered regular user operation year in 2021 with lower performance specifications than it was originally designed for. Ongoing beamline developments are aimed at attracting a broad user community and broadening the in-house ultrafast X-ray science program.

The FemtoMAX beamline can capture the structural dynamics of materials which enables the understanding of ultrafast processes in solids and liquids, like light driven phase transitions, chemical reactions, and relaxation processes. FemtoMAX is the only beamline at MAX IV that utilizes the MAX IV linear accelerator as an electron source to produce photon bursts <100 fs long. FemtoMAX thus combines the stability of a storage ring with the temporal resolution of a FEL.

The design of the FemtoMAX beamline is matched to the properties of the linear accelerator including the beamline repetition rate, the X-ray beam size and the X-ray beam stability. Thus, the uniqueness of the beamline has called for the development of novel timing tools. The beamline entered user operation with 2 endstations: an in-vacuum Grazing Incident X-ray Scattering (GIXS) chamber and an in-air goniometer stack (the Stack). In 2022, the G-chamber (station 3) and in 2023, the SAXS set-up (station 2) were commissioned and offered to the users. When fully developed, the beamline will consist of 3 endstations inside the beamline and additional 3 experimental set-ups with a possibility to use up to 5 available 2D detectors. The endstations at the beamline are shown in figure 1.

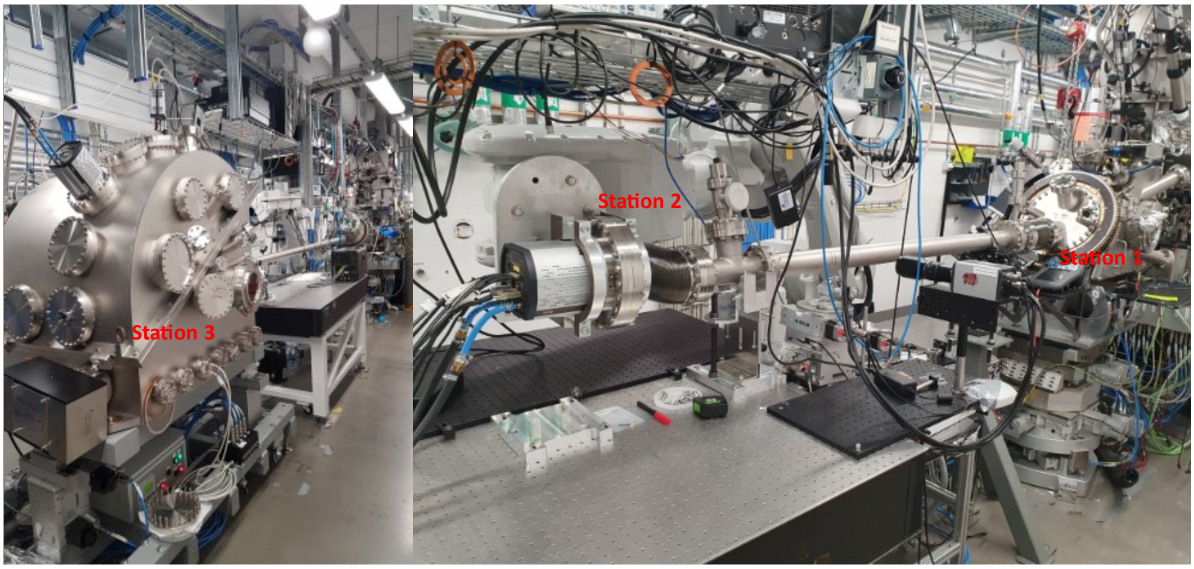

Figure 1. Endstation positions inside the FemtoMAX experimental X-ray hutch. Station 1 – GIXS, fluorescence, station 2 – SAXS, spectroscopy, station 3 – G-chamber, SAXS.

2.1.1 Undulators and front-end

The FemtoMAX beamline is equipped with two 5 m long in-vacuum undulators with a phase shifter in between. The undulators have been delivered by Hitachi/Neomax and are installed in the straight section in the Short Pulse Facility (SPF). A total 666-period short period undulator with 10 m active length was designed to cover the energy range 1.8 – 20 keV with a continuous tuning range. A schematic overview of the beamline components is shown in figure 2.

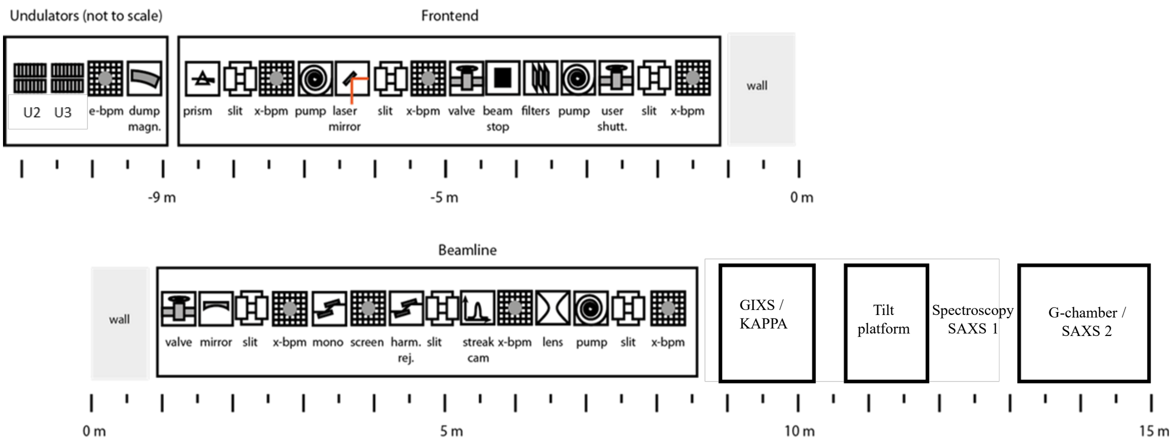

Figure 2. Schematic overview of the FemtoMAX beamline.

When the short electron pulses are sent through the undulators they emit femtosecond X-ray pulses. The generated X-ray pulses lead to a high peak power for a very short period of time, so the heat load on the X-ray optics can be neglected due to the low average power. The first element of the front-end is a dipole magnet (the dump magnet) that separates the generated X-ray light and bends the electrons onto an electron dump. The X-ray beam is defined by an adjustable slit positioned 10 m after the exit of the undulator. The position and flux of the beam can be measured using an X-ray beam-position monitor (X-BPM) based on a thin Ce:YAG screen and an absolute calibrated Si diode. The front-end also contains a user shutter, which can reduce the pulse-repetition rate of the X-rays, safety shutters, calibration and attenuation X-ray filters. The beamline performance has been measured recently and the up-to-date beamline properties are listed in table 1.

Table 1. FemtoMAX beamline properties.

Performance of the FemtoMAX beamline 2024	
Energy range	1.8 – 15 keV, 15 – 22 keV is optional with lower flux.
Photon source	2 in-vacuum undulators U15
Monochromator	Double Crystal Monochromator with InSb (111) crystal. Multi-layer Monochromator
Photons per pulse on sample 1% BW	> $7 \cdot 10^6$ at 8 keV
Repetition rate	10 Hz
Harmonic content	1:1000
Bandwidth	InSb $\Delta E/E \approx 4 \cdot 10^{-4}$ (1.8 – 15 keV) ML $\Delta E/E = 0.01$ (1.8 – 15 keV)
Monochomator throughput @ 5 keV	> 70% crystal > 50% ML
Optics	Unfocused / Rhodium coated Si-mirror, Be-lenses, Harmonic rejection mirror
Polarization	Linear
Pulse duration	< 100 fs
Synchronisation	< 1 ps (may achieve jitter compensation < 140 fs temporal resolution)
Spot size on sample	60 µm x 60 µm (FWHM, GIXS) 120 µm x 300 µm (FWHM, G-chamber)
Equipment	Ultrafast laser at sample (6 mJ @ 800 nm, 1.2 mJ @ 1200 nm), THz excitation Tilt platform, kappa goniometer, robot detector holder, Nanocell (scattering from small (< 1 µL) volume liquids) Vacuum GIXS, in-vacuum goniometer, capillary system for liquids.

2.1.2 Beamline optics

Two sets of focusing X-ray optics are available. The first one is a toroidal mirror in the beamline hutch which images the source with a magnification of 0.4 at the GIXS and Kappa endstations and the second is a set of cylindrical Be lenses which can be used to vertically obtain a magnification of 0.1 at the same endstations. The toroidal Rh-coated Si mirror, with an incidence angle of 0.14 – 0.18°, has been designed to focus the full X-ray energy range at FemtoMAX. The focusing mirror parameters can be seen in table 2. The in-vacuum undulator source point is 15 m before the mirror, and the focus can be positioned at all endstation locations. The measured X-ray focal spot from the X-ray undulator is shown in figure 3. The beam profile was recorded in air inside the first endstation 5 m away from the focusing X-ray mirror.

Table 2. Focusing mirror parameters.

Size	400 x 25 mm^2
Sagittal (horizontal) bending radius R_{min}	31.5 mm
Meridional (vertical) bending radius R_{maj}	3122 – 5644 m
Coating material	Rhodium
Incidence angle	0.14 – 0.18° or 2.363 – 3.177 mrad

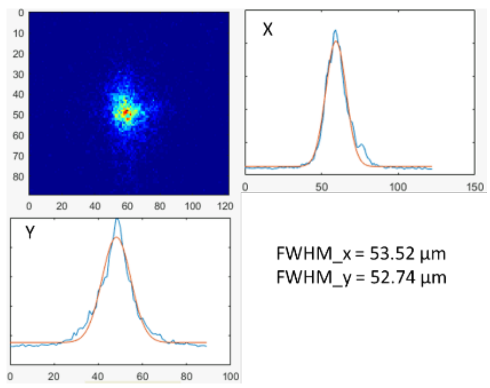

Figure 3. X-ray focal spot at a sample position inside GIXS endstation.

For many experiments a smaller spot than that achievable with the mirror system is needed, hence the use of Be lenses, at the expense of the transmitted intensity. For this set-up, the bender for the toroidal mirror is set to flat, so that the mirror only provides horizontal focusing. The distance from the end of the undulator to the sample holder in the goniometer is variable from 25 to 30 m. The focusing lens stack is placed 2.2 m before the first sample holder in the first endstation. Thus, the source is demagnified resulting X-ray spot on the sample will have a FWHM diameter of < 15 µm. The range over which X-ray beam intensity throughput is larger than 50 % can be achieved is 4.5 – 15 keV.

For X-ray monochromatization, several alternatives are available. The double-crystal monochromator (DCM) houses two sets of crystals (InSb (111), Si (111)) which can be interchanged by a translation stage. InSb (111) extends to softer X-rays and provides a wider bandwidth compared to Si (111). A multi-layer monochromator (MLM) is required to obtain the highest possible flux for wide-angle X-ray scattering (WAXS) experiments on liquids while at the same time suppressing the low-energy tail in the undulator spectrum. Three different multi-layer mirror pairs have been coated onto the same substrates together with the harmonic rejection stripe to conveniently optimize the performance for different wavelength ranges.

The X-ray beam spectral flux available at the FemtoMAX beamline has been measured first in 2020 and confirmed recently by measuring the X-ray beam intensity using an AXUV100 Si diode. The result of these measurements whilst changing the gap of a single undulator and scanning the InSb double crystal monochromator is presented in the figure 4. The beamline has a peak flux between 3 – 5 keV and can achieve energies down to 1.8 keV with the fundamental harmonic; higher energies by selecting higher harmonics albeit with decreasing brilliance. The in-coming X-ray radiation is monochromatized using double crystal monochromator (DCM) or the multilayer mirror (MLM). Switching between X-ray optics results in vertical X-ray beam height difference, which is around 4 mm while the horizontal beam position is kept constant.

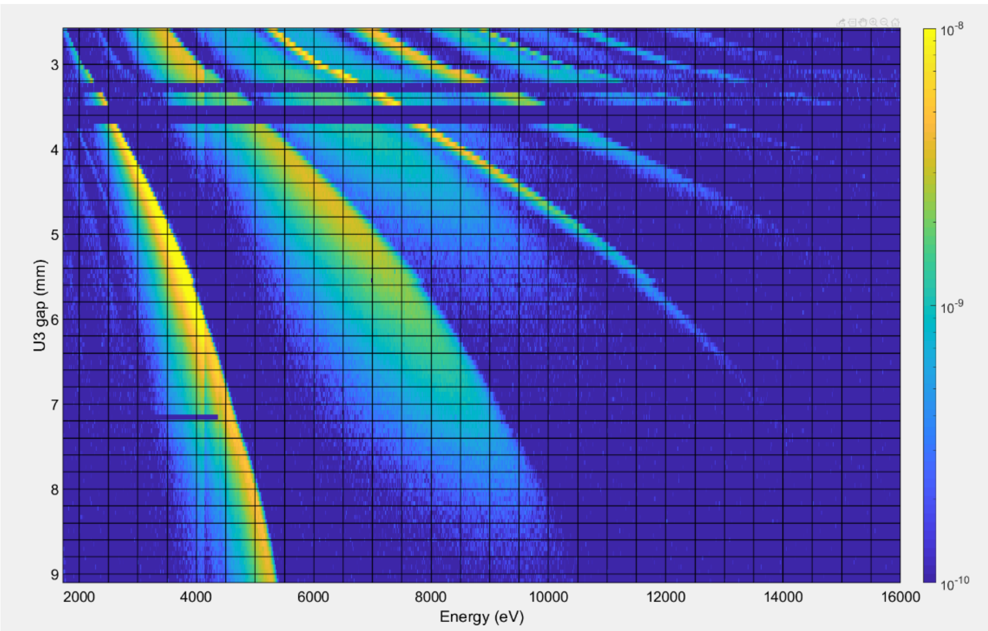

Figure 4. X-ray energies available at the FemtoMAX beamline. The figure shows the intensities of the odd and even harmonics measured upon changing the undulator gap and scanning the monochromator energy.

Due to the low photon flux at FemtoMAX, it is not possible to use conventional Si-based photodiodes for beam intensity monitoring during experiments due to the poor transmission of the X-ray beam through these devices. Instead, the incident X-ray beam intensity is measured using an in-house developed intensity monitor based on a large surface area CVD polycrystalline diamond. Tests comparing the performance of the CVD diamond unit and a Si AXUV100 photodiode, figure 5, reveal that both monitors show the same intensity response for an X-ray beam size of 300 x 300 μm^2 beam size, although the Si detector measures a stronger signal owing to a complete charge collection of the incoming X-ray beam.

Importantly, the CVD diamond unit allows about 60 % transmission of the incoming X-ray beam.

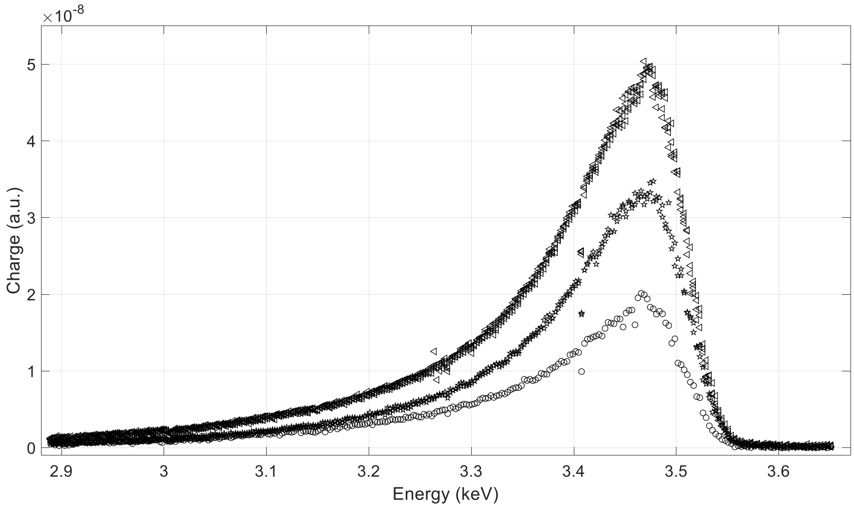

Figure 5. Response of the in-house built CVD diamond intensity monitor and the AXUV 100 photodiode for the first harmonic peak of the FemtoMAX undulator. The intensities were amplified using a Femto current amplifier DHPCA-100 and read on different channels of a Rohde & Schwarz RTO 1024 scope. The curves show the response of the Si photodiode (triangles), the CVD unit (circles) and the Si photodiode mounted in series after the CVD unit (stars).

2.1.3 Laser system

The FemtoMAX laser lab is located on the floor above the beamline X-ray hutch. It is equipped with a commercially available Ti:Sapphire based laser system from KM Labs (KML) which was originally installed in 2013. The laser chain is seeded by a 77 MHz Ti:Sapphire KML laser oscillator with a prism pair as a dispersion compensating element. The pulses are amplified in two amplifier stages, both cryo-cooled to avoid thermal lensing in the crystals, to an energy of 13 mJ, at a rate of maximum 1 kHz, and compressed to a duration of < 50 fs. The central wavelength of the output is 785 nm. The amplifiers are pumped by two Q-switched frequency doubled Nd:YAG DPSS lasers (Patara, Northup Grumman), each with a maximum power of 50 W. These pump lasers replaced the original pump lasers in 2018, which reduced the maximum repetition rate to 100 Hz.

10% of the pulse energy from the main laser system is split off and transported in a vacuum tube down to the timing diagnostic tools mounted on an optical table in the beamline hutch (see below). The remaining 90% is either directly transported to the sample environment, via a separate vacuum laser transport system, to be used in an experiment, or is used to pump an OPA (HE-TOPAS Light Conversion). The OPA system outputs 1 – 2 mJ pulses in the wavelength range of 1100 – 2600 nm. With further frequency mixing the output from the system is extended to a range of 0.2 – 10 µm. At the extreme edges of the tuning range the pulse energy drops to 10 – 20 µJ. The laser beam from the OPA is transported in the same vacuum transport system as the main beam. In order to transport very wide range of wavelengths along the same path, the vacuum transport is equipped with a set of interchangeable mirrors with different coatings.

In order to perform laser pump X-ray probe experiments, the electron pulse generating the X-ray pulse and the laser pulse has to be synchronized to a very high degree.

The FemtoMAX laser oscillator is synchronized to the LINAC 3 GHz master oscillator that is used to generate the high-power RF that accelerates the electrons. The laser oscillator is equipped with a fast 12 GHz diode that picks up the 77 MHz pulse train. This signal is then filtered at 3 GHz which corresponds to the 39^{th} harmonic of the fundamental. The resulting 3 GHz signal is fed to an electronic mixer together with the reference signal. In a negative feedback loop, the output voltage from the mixer is amplified and used to control the position of one of the intra cavity mirrors in the laser oscillator that is attached to a piezoelectric stack. This feedback keeps the repetition rate and phase of the laser oscillator locked to the reference signal. By stepwise shifting the phase of the reference signal using a voltage controlled commercially available RF phase shifter, the phase of the laser oscillator pulse train can be tuned within a 13 ns window.

Timing jitter and drifts makes it necessary to monitor the arrival time between laser and X-ray pulses on the sample. On FemtoMAX we have two operational timing diagnostics tools, with different timing ranges and accuracies that can be used for post-sorting of the data, in order to dramatically increase the time resolution of the experiment.

2.1.4 RF cavity-based timing monitor

The timing monitor based on RF cavities utilizes two fast signals derived from the laser pulse and electron pulse respectively. The electron pulse signal is picked up from one of two button antennas located next to the vacuum tube downstream from the FemtoMAX undulator pair. In the X-ray hutch this signal is combined with a signal from a fast photo diode (12 GHz), which picks up the laser pulse, in a broadband RF splitter/combiner. The combined signals then excite a 6 GHz RF cavity band pass filter that rings for a couple of ns. The ringing signals are amplified and sampled at 80 Gs/s by a 36 GHz bandwidth oscilloscope. Figure 6 shows a schematic of the setup.

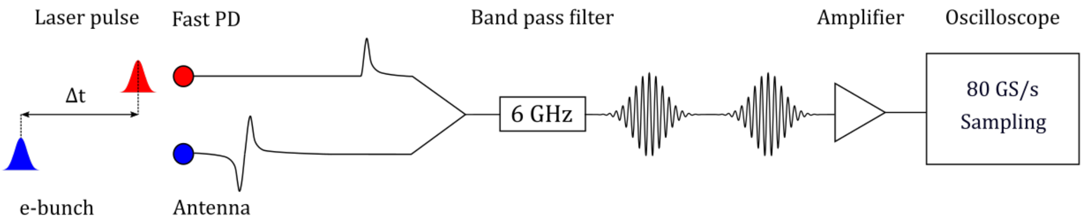

Figure 6. Schematics of the RF cavity based timing monitor at FemtoMAX.

An in-house developed algorithm is used to extract the relative time between the two signals exciting the RF cavity. It utilizes manipulations in Fourier space to calculate the Hilbert transform of the cross-correlation of the two oscillatory signals.

In order to reduce the measurement error two of these devices are run in parallel and averaged to provide a laser/X-ray time stamp for each individual shot. The accuracy of the timing measurement has been proven to be 200 fs (FWHM) at the experiment.

2.1.5 Cross correlator

This device utilizes visible light radiated in the dipole magnet which directs the electron beam to the LINAC beam dump. The beam extracted from the magnet is collimated using a single 1.3 m focal length lens sitting in front of the extraction window and is guided into the X-ray hutch where it is focused, using a cylindrical lens, to a line on a 0.3 mm thick BBO crystal. A small fraction of the main pump laser beam is also focused, using another cylindrical lens, on the same spot on the crystal. The beams cross at an angle of 11° in air but, as they are refracted in the crystal surface, the true crossing angle is 7°. At the position in the BBO crystal where both pulses overlap, a parametric sum frequency generation process will take place. The crystal is cut and oriented such that the 785 nm photons from the laser and the 650 nm photons from the bending magnet light are phase matched and generate 355 nm photons. Due to the difference in propagation angle between the two pulses, the overlap position will depend on the arrival time of the pulses and thus the sum frequency beam position will shift if the arrival time of either pulse varies.

The exit position of the summed frequency beam is registered by a simple imaging system. Behind a wavelength filter a single lens images the back of the crystal surface onto an MCP of an image intensifier from HAMAMATSU. The phosphor screen of the image intensifier is then imaged by a dedicated camera lens onto the image sensor of an Andor Zyla camera. An illustration of the set-up is found in figure 7.

The temporal resolution that is achieved with this device has not yet been characterized, however, it is expected to be as good as 20 fs or even better.

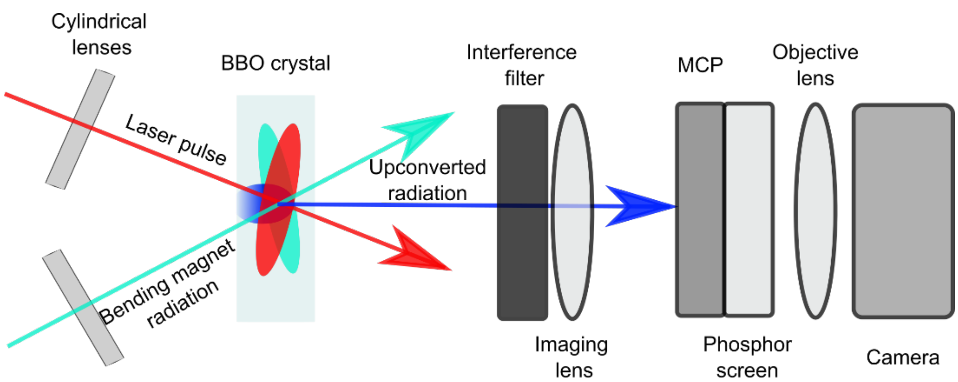

Figure 7. An illustration of the working principals of the cross correlator timing tool. The crossing angel of the beams is exaggerated for visibility.

2.1.6 THz pump

In addition to ultrashort laser excitation, FemtoMAX also provides THz pulses generated in crystals by the femtosecond laser system. These THz pulses have wavelengths in the sub-mm region and give, for example, a direct way to excite phonons in matter at THz frequencies, without any further deposition of heat or damage to the sample. User experiments with THz excitation have been performed both in air and in the GIXS chamber using samples of protein crystals and semiconductors. An average absorption coefficient of $\alpha_{eff} = 2.4\,m^{-1}$ in air between 30 – 40 % humidity has been measured in-house from THz pulses generated in a 4 -N, N-dimethylamino-4′-N′-methyl-stilbazolium tosylate (DAST) crystal. Thus, it is an advantage to build setups in vacuum due to this high absorption of THz radiation in water.

The origin of the pulsed THz radiation comes from the pulsed laser-induced second order nonlinear polarization density P_{NL} at the difference frequencies of an intense laser pulse in a crystal, given by: $P_{NL}(\omega_{-}) = 2d_{NL}{E_0}^2$. It is desirable to use a crystal with a high nonlinear coefficient d_{NL} and an intense laser pulse with high electric field E_0 to maximize the generation efficiency. To match the phase conditions of the optical laser pulse and the generated THz pulse in the crystal the most efficient pump wavelength needs to be selected.

The FemtoMAX beamline offers different types of crystals for THz generation, depending on the experiment. The currently available crystals with a high conversion efficiency (~1%) are organic crystals such as DAST, BNA and DSTMS. The generation setups can be made portable on simple breadboards due to simple collinear phase matching conditions. An example of a portable THz setup in air is shown in figure 8.

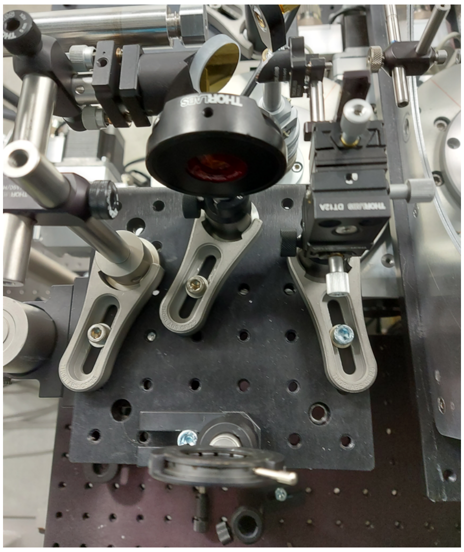

Figure 8. THz set-up at the FemtoMAX beamline.

The most commonly used crystal for the THz generation at FemtoMAX is DAST, which in addition to a broad THz spectrum also produces the most energetic THz pulses at the beamline. This crystal has best efficiency at a pump wavelength of 1500 nm, which is generated in an optical parametric amplifier (OPA) in the FemtoMAX laser lab. Currently we have measured

THz pulse energies up to 12 uJ from a DAST crystal at the sample position. Using focusing systems based on off-axis parabolic mirrors, FemtoMAX can offer intense focused THz pulses with a size down to ~ 200 µm (FWHM) with peak electric fields exceeding 3 MV/cm, see figure 9.

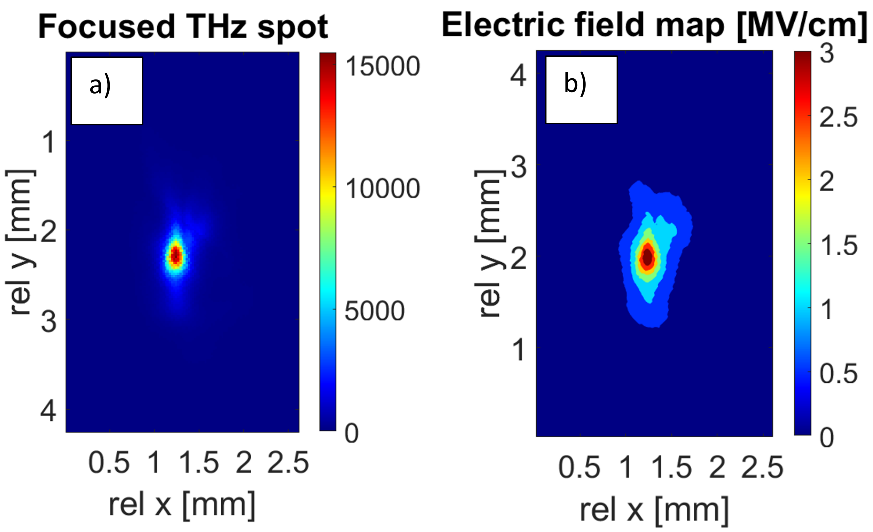

Figure 9. THz beam profile at the FemtoMAX beamline. a) measured beam profile on THz detector, b) recalculated THz beam electric field amplitude.

2.2 Endstations and sample environments

2.2.1 Overview

FemtoMAX has developed a series of endstations and sample environments for user experiments. Key in their design has been the need for versatility in order to serve a very broad set of requirements from the users' experiments. In addition, users can bring their own experimental setup for incorporation into the beamline.

For scattering experiments, there are two endstations: the in-vacuum station, well-suited for solid samples, such as semiconductors, thin films, and bulk materials, while the in-air station can be used for both liquid and solid samples. Liquid samples can be stored in a static quartz cell or in a circulating cell, the Nanocell, developed in-house and suitable for GIXS studies for samples in solutions. We also support free flow jet in-air or in a gas filled chamber. For the in-air station, the sample can be cooled by liquid nitrogen stream down to 150 K. Each endstation is equipped with a 6-axis Huber goniometer for translation, tilt, and rotation of the samples (x, y, z, pitch, yaw, and roll).

2.2.2 Support labs

FemtoMAX users are welcome to use MAX IV support laboratories. The labs are available for the users and provide access to fume hoods, pipettes, balances, hot plates, ultrasonic baths, ovens, cold storage (4°C, -20°C, -80°C, -152°C), chemical cabinets, ultra pure water, waste disposal. Access to those labs is granted via main user proposal process.

Additionally, the FemtoMAX beamline is equipped with a separate sample preparation room within which are two optical microscopes: a long range microscope and a high magnification microscope equipped with a CCD camera (figure 10). Users will also find standard equipment such as hot plate, syringe pump, ultrasonic bath, dry air supply, solvents and tools for sample cleaning and weighing. Users can keep samples in a vacuum box or dry air environment.

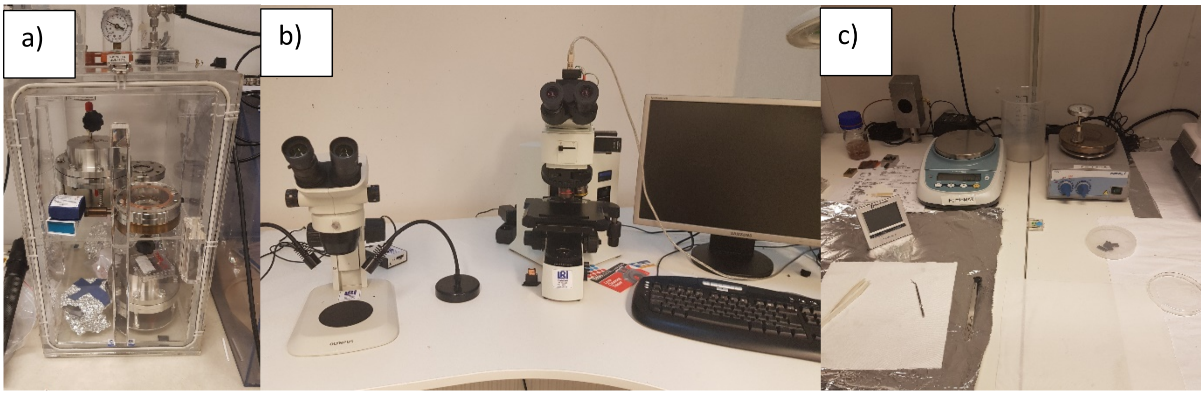

Figure 10. Available equipment for the users at the FemtoMAX prep room. a) vacuum sample storage box, b) microscopes, c) balance, hot plate and sample mixer.

If requested, atomic force microscopy (AFM), scanning electron microscopy (SEM) and 3D printing can be arranged. The beamline can provide solid sample (crystal) cut locally and thin FIB lamella preparations via Lund Nano Lab.

2.2.3 Detectors

There are five 2D detectors dedicated for user experiments at the FemtoMAX beamline, see table 3. The Dectris Pilatus, Andor Zyla and Andor Balor are operational and implemented in the FemtoMAX control system, the Andor iKon is awaiting deployment.

Table 3. List of available detectors at the FemtoMAX beamline.

Detector	Energy range (keV)	Pixel size (µm)	Sensor size (mm)	Image bit depth	Design full frame readout speed (Hz)	Achieved redout speed (Hz)
Dectris Pilatus 1.2 M	2 – 20	172	253 x 142	20	500/100*	10
Andor Zyla 4.2 M	2 – 7	6.5	16 x 14	16	49/716**	10

Andor Balor 16.9 M	2 – 7	12	49 x 49	16	34/840**	10
Andor iKon L 4.2 M	2 – 20	13.5	27 x 27	16	1/5**	Not ready yet
Lecroy wavemaster oscilloscope	NAN	NAN	NAN		36 GHz 80 Gs/s	Ready

* - lower maximum frame rate due to time over threshold calibration,

** - higher frame rates can be achieved by reading smaller sensor area only (128 x 128 pixels),

The detectors stream data to the DAQ cluster in Kubernetes and the data files are referenced in the scan Master file. During the scans the detectors are orchestrated through sardana controllers defined for each device. The sardana controller is responsible for configuring the detectors parameters according to the experiment and the current scan. In this case, it should also set the output data file directory according to the experiment configuration and configures the timing and triggering configurations of the detector. The overall software stack structure is defined as:

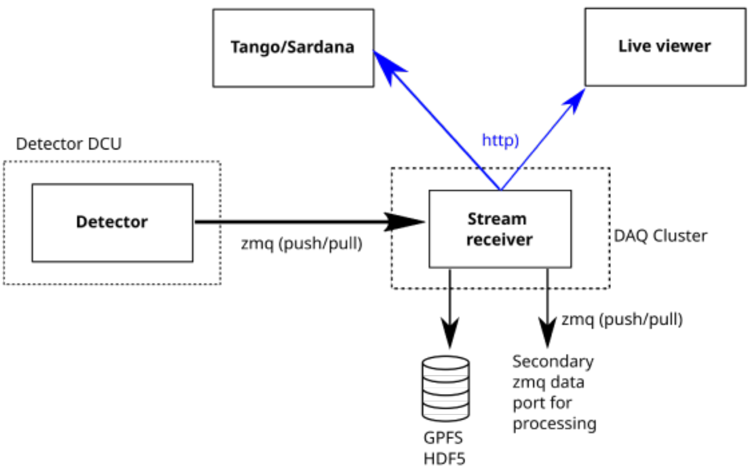

Figure 11. Graphical representation of the data stream at the FemtoMAX beamline.

2.2.4 Dectris Piltus3 1.2M (ToT)

The Pilatus3 1.2M detector from Dectris is, in its standard design, a Si-based large area photon counting detector. The 254 x 142 mm^2 detector area contain approximately 1.2 million pixels, each of 172 x 172 μm^2 in size, divided on 12 modules.

In contrast to charge integrating devices, such as for example the sCMOS image sensors, in photon counting detectors each pixel is provided with threshold comparator and a digital counter. When the pixel voltage exceeds the threshold the counter value is increased. This way of operating makes the device virtually free from thermal and readout noise. The disadvantage is however that it is very sensitive to pile-up effects, i.e. if several photons deposits in the same pixel within a timeframe that does not allow the signal voltage to return below the threshold, all but the first hit is missed. To remedy this effect the Pilatus3 ASICS was provided with a so called instant retrigger circuit which allows the counter to be retriggered after a pre-set time. This makes the detector less prone to miss counts at high count rates. Given that the retrigger time is set short the same scheme can also be used to measure the time the signal from an individual pixel stays above the comparator threshold. The retrigger circuit is thus then used as a clock. Via a pixel by pixel calibration procedure the energy deposited in each pixel can be inferred from the time the signal stays above threshold. This mode of operation is referred to as Time over Threshold (ToT) and can be said to turn the photon counting detector into a charge integrating device while maintaining the benefit of extremely low noise.

ToT operation is a good match for FemtoMAX since the detected radiation arrive in short pulses at a low repetition rate. After readout of the raw data, i.e. the 20 bit counter values, it is streamed to the MAX IV computing cluster in order to be converted into deposited energy via a pixel by pixel lookup table. This converted data is then written to file and/or presented to the user in a ”live view” application. At an early test at the FemtoMAX beamline it was shown that the detector could register up to 2.5 MeV in a single pixel with an error of less than 10% in ToT mode.

A second customization that makes the FemtoMAX Pilatus3 detector different from the original design is that it modified for handling in vacuum operation. The detector head is separated from the control electronics and mounted on a ConFlat vacuum flange. The set of cables transferring the signals between the two units are sufficiently long to allow for flexible positioning of the detector head.

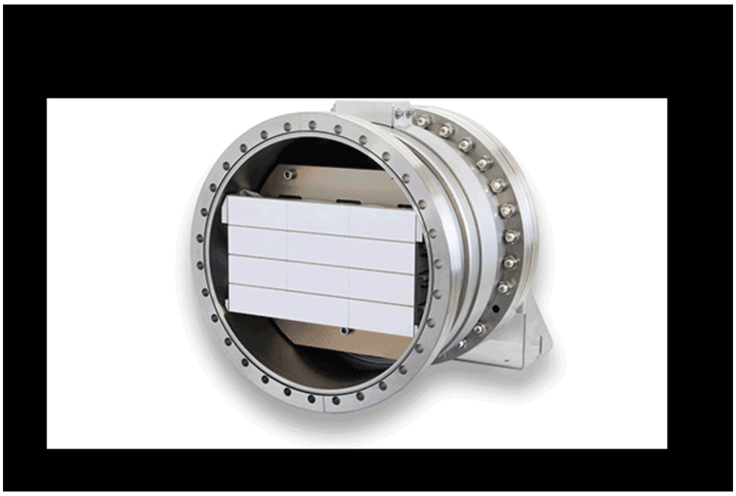

Figure 12. The FemtoMAX customized Pilatus3 1.2 M detector head

2.3 In-vacuum scattering endstation (GIXS) #1

The in-vacuum station features a large Grazing incident X-ray scattering (GIXS) chamber, mounted on a Huber goniometer, capable of holding up to 600 kg, see figure 13. The chamber has multiple entrance windows that allow the excitation laser to enter the chamber at angles of 45, 17, and 5 degrees. The X-ray incident angle can be adjusted continuously through the selection of different wedged-shaped sample holders, with inclinations from 2 to 30 degrees relative to the horizontal plane, and tuning the pitch angle. The sample yaw angle can be adjusted via the rotation stage underneath the chamber. The chamber is equipped with a cryostat system with a temperature range from 10 – 500 K.

The GIXS chamber is designed to accommodate various X-ray detectors. The most frequently used is the Pilatus3 1.2M detector, which is attached to the chamber such that its sensor plane is at 60 degrees relative to the horizontal plane, allowing capture of a large scattering vector. The detector can be rotated along the axis perpendicular to its sensor plane to adjust the position of the scattering signal on the sensor. Two rotation stages stacked off-center from each other can be used to position smaller scattering detectors, such as the Andor zyla, Andor Ikon or Andor Balor, in a variety of locations behind the sample. The large interior space of the chamber allows for the installation of various optical setups depending on the experimental needs. The laser excitation wavelength ranges from 400 nm to 1.6 μm and THz wavelengths.

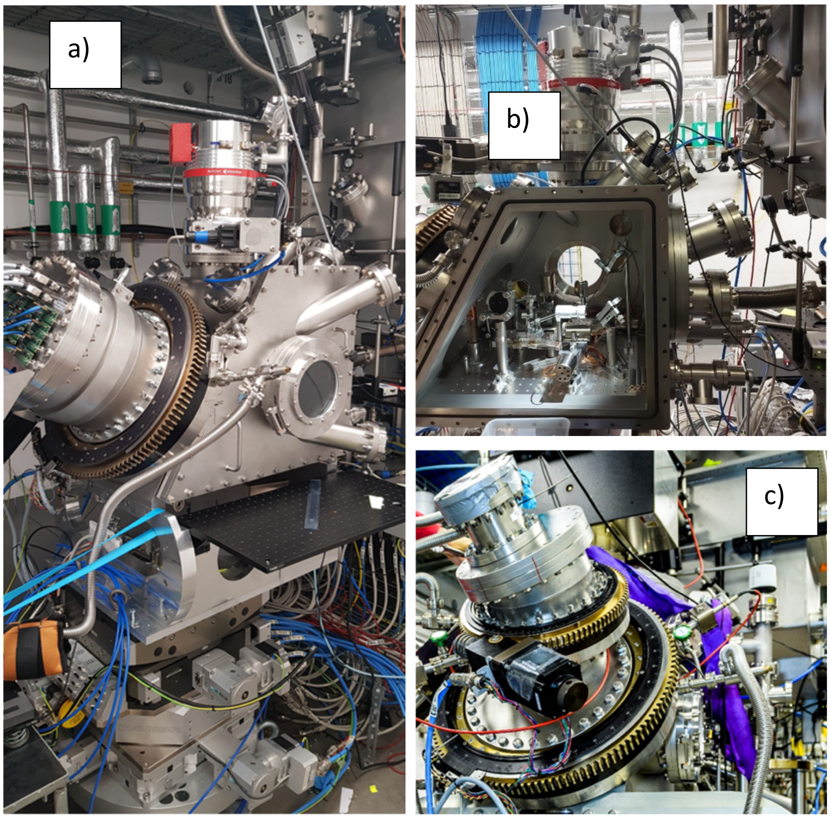

Figure 13. In-vacuum endstation. a) GIXS chamber on the 6-axis Huber goniometer with the Pilatus 3 1.2M X-ray detector mounted, b) an optical setup inside the GIXS chamber, c) an alternative detector positioner on the GIXS chamber suitable for mounting Andor Zyla detector.

2.4 In-air scattering endstation #2

The in-air scattering endstation at the FemtoMAX beamline, figure 14, allows for the easy manipulation of the laser and the X-ray incident angles on the sample, without the constraints of a vacuum chamber. The endstation's design allows for scattered X-ray signals to be detected at almost any angle and at a tuneable distance from the sample, which supports both small and wide-angle X-ray scattering experiments. However, this type of experiment is limited to high X-ray energy scattering, starting from 8 keV, as lower energy X-rays are more greatly absorbed by the long air path. For X-ray energies above 10 keV, studies[1] have shown that the FemtoMAX beamline provides data of sufficient signal to noise and resolution for analysis. The in-air scattering endstation also features a Kappa diffractometer that can rotate the sample with an increased angular range with respect to the incident X-rays.

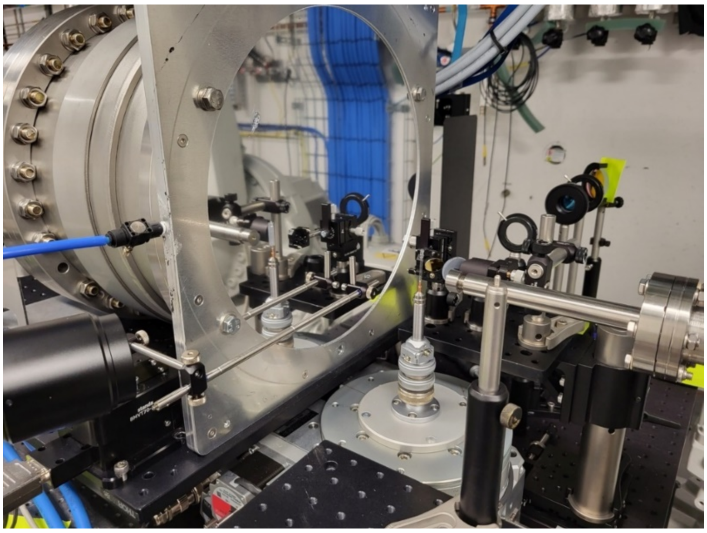

Figure 14. In-air X-ray scattering endstation showing the Pilatus detector behind protein crystal mounted on the stack sample holder.

Since 2023 May kappa goniometer has been prepared and is offered to users for all in-air experiments. Kappa and GIXS shares same position while tilt platform has a dedicated space in the beamline as can be seen in figure 2. Kappa goniometer has been requested for users that work in challenging geometries where scattering angles are $2\theta > 80$ degrees. The functionality of the tilt platform is covered by kappa goniometer therefore tilt platform will be removed from the beamline set-up in the nearest future.

2.5 X-ray fluorescence endstation #3

An endstation, figure 15, for the study of ultrafast luminescence processes upon X-ray excitation has been built within the FemtoMAX beamline by Prof. Marco Kirm and co-workers[2]. The endstation was designed to efficiently detect low intensity luminescence emissions without compromising time resolution.

[1] Maja Jensen et al. J. Synchrotron Rad. (2021). 28, 64–70.

[2] Irina Kamenskikh et al. Symmetry 2020, 12, 914.

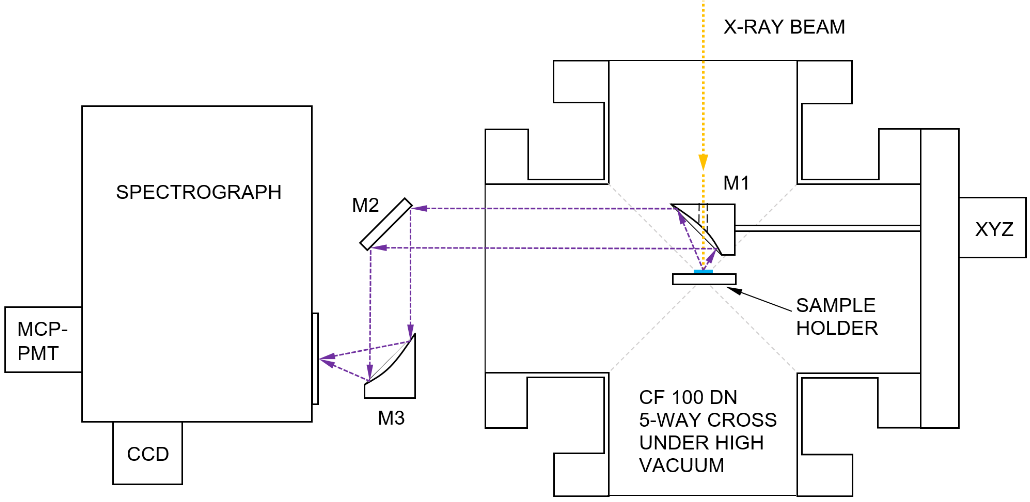

Figure 15 Schematic of the X-ray fluorescence endstation for luminescence experiments at the FemtoMAX beamline. The experimental chamber is a DN 100 CF 5-way cross mounted on a custom levelling plate. M1 and M3 are off-axis parabolic mirrors and M2 is a plane mirror. XYZ indicates a XYZ manipulator controlling the position of mirror M1. The sample holder is attached to the cold finger of the LNT cryostat (sample holder).

A Janis VPF-800 liquid nitrogen cryostat with a sample holder is mounted on the top port of a DN 100 CF 5-way cross, to achieve temperatures of 78 – 500 K under high vacuum conditions (< 10e-6 mbar). A port at the back of the experimental chamber has a CF100 glass window and is used for monitoring and alignment purposes. This port is covered during experiments to reduce any light pollution from outside the chamber, which could disturb measurements. A one inch (25.4 mm) focal distance off-axis parabolic mirror M1 (Thorlabs, Inc.) is mounted on an XYZ manipulator in front of the sample holder. The mirror has a circular hole (Ø 4.1 mm) perpendicular to the focal plane and the sample holder to allow propagation of the X-ray beam (~120 x 120 um^2) from the entry port onto the sample. The mirror collects luminescence light from the sample and directs it as a parallel beam (at 90° relative to the incident exciting X-ray beam) towards a side port of the experimental chamber fitted with a CF35 fused silica optical window. The luminescent light outside the experimental chamber is directed onto a second off-axis parabolic mirror M3 (focal distance 76.2 mm) using a plane mirror M2 (if needed). The second parabolic mirror M3 focuses the incoming parallel beam either directly onto a photocathode of a detector or onto an input slit of a spectrometer. The fluorescence spectrometer is an Andor Shamrock SR-303i (from FinEstBeAMS) equipped with a Hamamatsu R3809U-50 MCP-PMT (also used at the single bunch experiments at FinEstBeAMS). The signal from the MCP-PMT is amplified by a SHF 100 APP broadband preamplifier (12 GHz, 19 dB) and digitized by a LeCroy LabMaster 10-36Zi oscilloscope (36 GHz, 80 Gs/s). The separation of non-overlapping luminescence photons per single excitation pulse is achieved by an advanced multi-photon counting technique (in-house LabView program). Excellent time resolution of 32 ps (FWHM of IRF Gaussian fit) is achieved and is limited by the time resolution of the MCP-PMT.

2.6 G-chamber #4

In 2022, FemtoMAX commissioned a new in-vacuum end-station dedicated for studies in extreme sample geometries using multiple detectors, the G-chamber (figure 16). It is equipped with in-vacuum Huber goniometer together with fine sample manipulator from Symetrie. This set-up allows X-ray scattering geometries with scattering angles up to 2θ = 120 deg. The G-chamber has been commissioned during user beamtime in November 2022 in an experiment dedicated to study phonons in semiconductor nanowires. This first commissioning provided valuable information for future improvements. In figure 16 c), an experimental result from a time scan is shown. Here, acoustic phonons in an InSb bulk crystal are measured as a test experiment to make sure that temporal and spatial overlap is set correctly. The oscillatory pattern starts just after time = 0 ps, indicating that the spatial and temporal overlap is good. The oscillatory pattern corresponds to slow acoustic phonon modes that are produced by tuning off from the X-ray diffraction resonance condition. Achieving this signal is a must before proposed nanowire experiment could start.

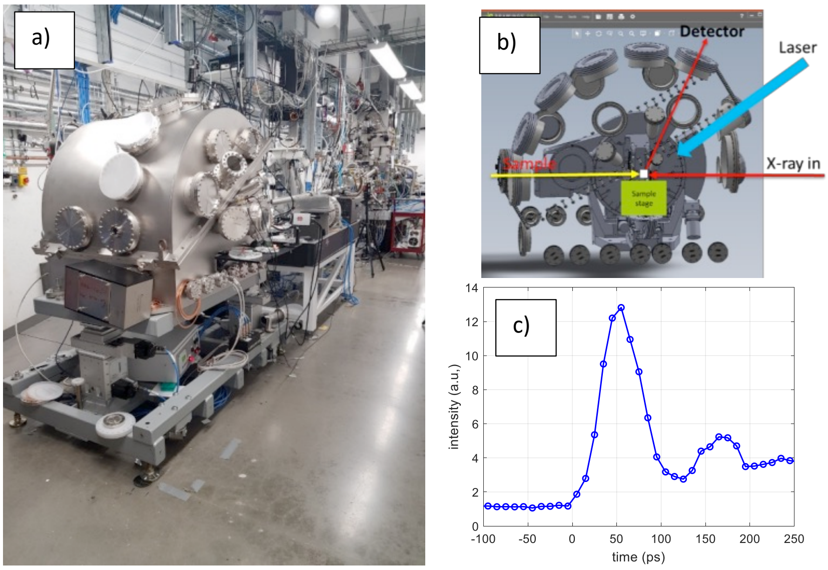

Figure 16. a) location of the endstation 3 at the FemtoMAX beamline, b) design of the G-chamber c) experimental result from the first commissioning experiment in the G-chamber recorded on the Andor Zyla camera, at the maximum diffraction geometry 2θ = 120 deg and a sample-detector distance of 120 cm.

G-chamber allows to extend sample detector distance in TR-SAXS experiments. Here large area 2D detector is mounted on the last flange seen in figure 16 a) (flange which is just above rectangular ion pump) thus increasing sample detector distance from 2.5 m to 6 m and allowing to record SAXS and WAXS patterns at the same time.

2.7 SAXS endstation #5

Experiments using time resolved SAXS at FemtoMAX was not included in the original beamline portfolio and was introduced in 2023. The SAXS set-up is flexible allowing solid and liquid samples, using either of two large area detectors (Balor and Pilatus) and a sample detector distance ranging from 1 to 6 m. A schematic of the set-up is shown in figure 17. The experiment does not rely on any new equipment or rearrangement of the beamline configuration and was therefore rapidly commissioned. The first experiment has been performed in high vacuum environment (< $5e^{-7}$ mbar) using 25 nm diameter Au particles. The sample was located inside a quartz capillary with wall thickness of 10 µm. A high spatial resolution detector Andor Balor was chosen (see table 4), and X-ray energy was set to 11 keV using multilayer mirror with sample to detector distance of 2.43 m, giving a q-range of 0.18 $Å^{-1}$.

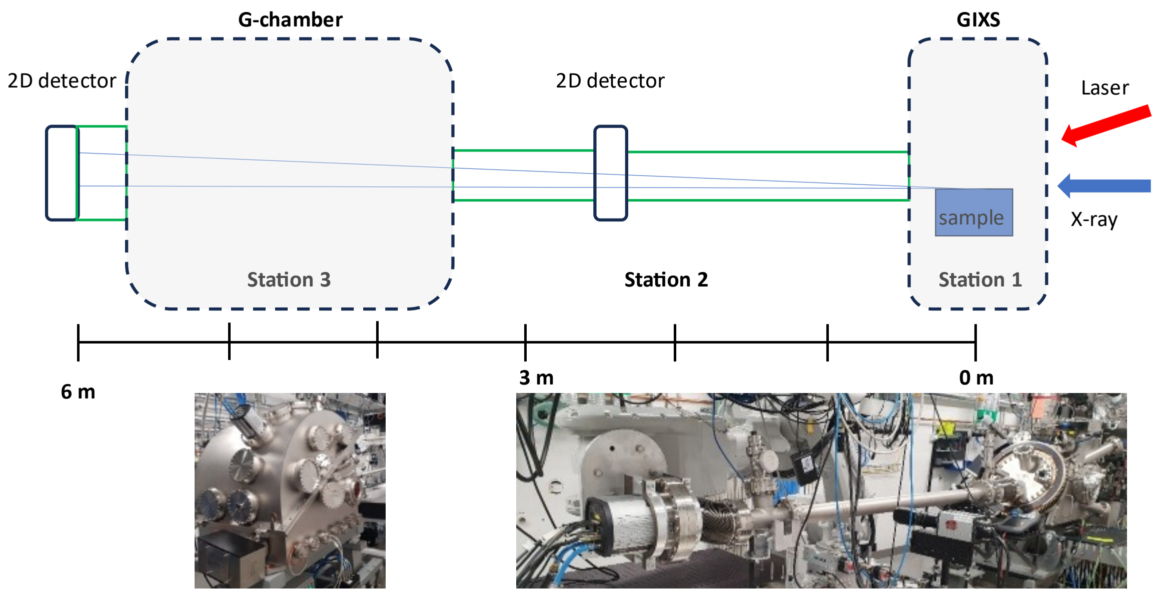

Figure 17. SAXS set-up the FemtoMAX beamline.

The SAXS signal from Au nanospheres can be observed in a single shot, however, to achieve a good S/N ratio at least 5000 images are needed. The summed 2D SAXS pattern from Au nanospheres is shown in figure 18 a). The intensity vs scattering vector Q curves at different laser irradiation is shown in figure 18 b).

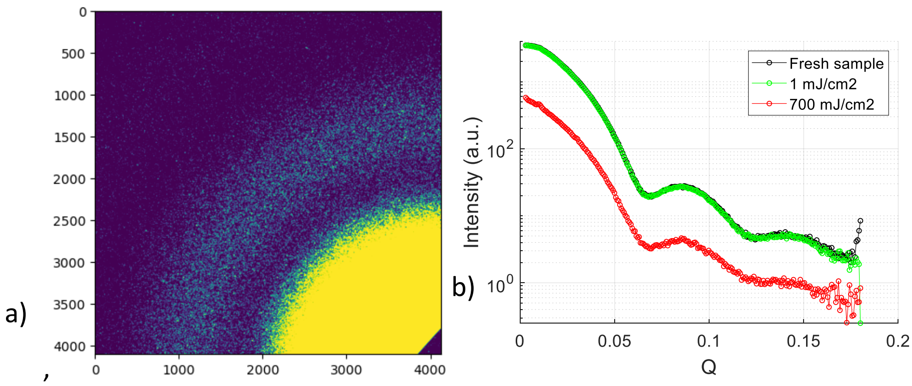

Figure 18 a) SAXS pattern from 25 nm Au particles recorded on Andor Balor detector, shown image corresponds to 10000 single summed images, b) radial lineout of the SAXS pattern before and after laser irradiation.

Future TR-SAXS experiments will be offered on heated or cryo-cooled samples since the cryo system inside the GIXS experimental chamber can be employed.

2.8 Spectroscopy endstation #6 (in commissioning)

The energy range in which the beamline can provide sufficient x-ray flux for XAS measurements is 2 to 10 keV. This energy range encompasses K-edge absorption of all the 3d transition metal elements, some of vital elements in organic molecules such as P, S, Cl, and the L and M absorption edges from alkali metal to halogenic elements. This enable studies of ultrafast chemical reaction including light induced catalysis reactions in artificial photosynthesis process, where charge transfer and molecular structural change can be observed through time-resolved XAS (TrXAS).

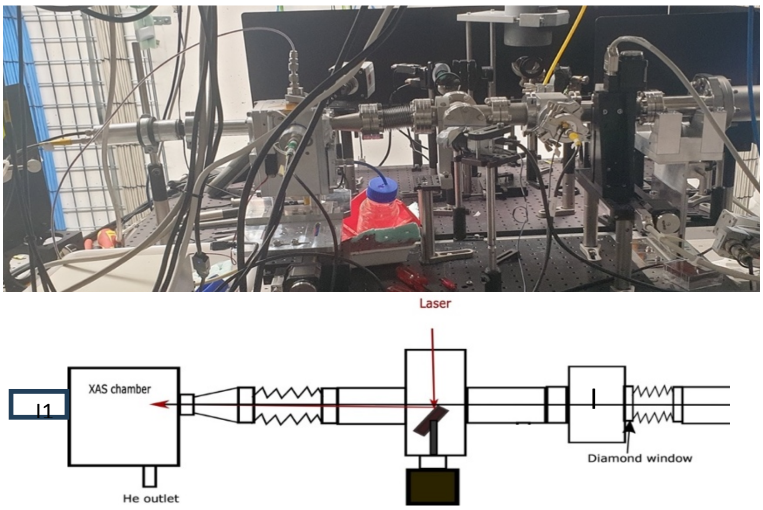

Figure 19: experimental setup for TR-XAS, the upper image shows the photo of the setup, the lower shows its scheme.

The time-resolved XAS endstation was commissioned in 2023 with two pilot experiment for two different energies at Ru L3-edge 2.8 keV and Fe K-edge 7.1 keV. The setup for Fe K-edge measurement is illustrated in figure 19. This is a portable endstation with all the components mounted on a breadboard of 0.6 x 0.45m. X-rays from the vacuum pipe enters the setup via a vacuum window which separates the vacuum and the helium environment. Thus, the x-ray flux loss due to air absorption is minimized. The incident x-ray flux is measured by a so called I0 detector located just before the EXAFS chamber. The I0 detector gives a signal proportional to the X-ray flux incident on the sample. It is composed of a Mn-coated foil whose plane creates 45 degree and very close to the sensor plane of a large area APD for a maximum solid angle. X-ray goes through the foil generating x-ray fluorescence and scattering that are then detected by the APD. The signal height from the detector represents the incident x-ray intensity (I0).

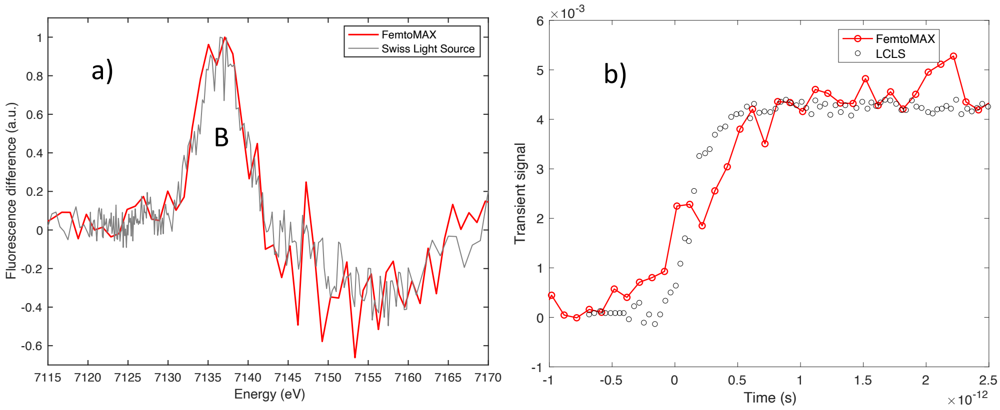

Figure 20: a) Comparison of transient signal at Fe K-edge measured in total fluorescence mode, grey trace: measured at Swiss Light Source at 100 ps delay, red trace: measured at FemtoMAX at 200 ps delay. b) dynamics measured at B feature, black circle: measured at LCLS free electron laser source (the data was rescaled for comparison), red circle trace: measured at FemtoMAX.

A one-inch mirror inside a 4-ways cross is used to couple the pump laser with x-ray into the EXAFS chamber. The angle between laser and x-ray is about 3 degrees. A gear pump is used to circulate the liquid sample that forms a flat jet with thickness of 100 um at the nozzle output. The jet is tilted 45 degree with respect to the x-ray to reduce elastic scattering. X-ray fluorescence is detected by an APD positioned at 6 mm from the sample. Another APD in the back, outside of the chamber is used to detect x-ray transmission after the sample. All APDs detectors are laser shielded to avoid the pump laser contamination to the x-ray signal.

A test sample, iron tris bipyridine, [Fe(bpy)3]2+/H2O is optically excited at 400 nm which is belong to the metal-to-ligand-charge transfer absorption band.

X-ray fluorescence is detected by APD (Perkin Elmer) and amplified by a transimpedance amplifier with gain of 104. The analog output from the amplifier is digitalzed by a Waverunner Lecroy oscilloscope. The ground loop and electronic noise is minimized by grounding the amplifier and shorten the electrical cable connecting the amplifier to the oscilloscope. The waveform from the oscilloscope is acquired during the scanning of X-ray energy or laser/X-ray time delay. The X-ray intensity is calculated by integrating the peak region before subtracting the waveform background.

We have successfully captured transient absorption of [Fe(bpy)3]2+/H2O. Figure 20 shows the energy dependent and time dependent of transient absorption measured in fluorescence mode.

The results are overlayed with previously published data. As can be seen, FemtoMAX data are in line with the literature which confirms that the endstation works as designed. In Fig. 18a, the energy dependent transient has similar signal-to-noise ratio for a similar accumulated flux compared to the data taken at the Swiss Light Source (SLS). However, the rise time of our kinetics curve (650 fs) (Fig. 20b) is slower than that of data measured at LCLS free electron laser (350 fs). The time resolution will be significantly improved when the new timing tool, cross correlator, will be used.

To evaluate the noise level of the system we compare our signal-to-noise level for a given accumulated flux with the published data that follows the Poisson statistics. The measurement accumulated 700 shots to get SN of 4, thus we accumulated about 2.8e7 photons rather than 1.3e7 photons as expected from published data. This indicates there are some electrical noises apart from the photon shot noise in the signal.

Before accepting regular users, we need to improve a number of points for this endstation, including: i) improving time resolution with a better timing tool ii) reducing electrical noise iii) improving the stability and mode of the pumping laser.

One of the most important factors for a successful ultrafast XAS measurement is X-ray flux. FemtoMAX exhibits sufficient X-ray flux for ultrafast XAS measurements, which is evident from the data. XAS at FemtoMAX would strongly benefit from a higher LINAC repetition rate.

2.9 Solution scattering using low volumes (in development)

A Si chip-based sample environment for the delivery of liquid samples has been developed for time resolved X-ray scattering experiments in grazing incidence geometry. This was needed due to the low repetition rate at FemtoMAX which means that liquid jet schemes will use too large a sample volume during these relatively lengthy experiments on weakly scattering systems, like protein solutions. A Si chip containing a small channel with a volume of 0.5 µL can be used for laser pump X-ray probe experiments, as shown in figure 21; flow rates as high as 6 mL/min can be achieved even for solutions of viscosity ηD = 5 Ns/m^2 $*10^{-3}$. The microfluidic cell has been experimentally tested at FemtoMAX with 100 % sample hit rate, the first results are shown in figure 22. The protein solution is pumped in a channel formed inside the Si substrate which is covered by a 50 nm thick Si_3N_4 window. Si_3N_4 is chosen due to its high transmission for the optical as well X-ray light. The X-ray incidence angle is kept under 2^o , while the laser excitation angle can be freely chosen. The incidence angle of the laser defines the temporal resolution of the experiment. A large area detector which can be positioned at various sample-detector distances collects scattered X-ray light and stores the data together with a time delay between X-ray light and the excitation laser pulse.
System has been stress tested using laser and X-ray radiation and is stable up to laser fluences of 20 mJ/cm^2.

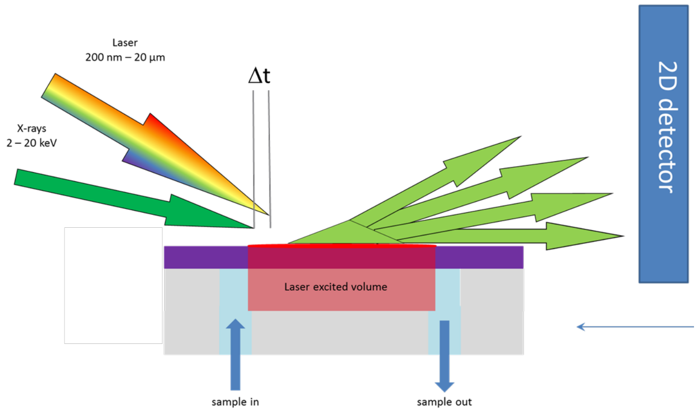

Figure 21. Conceptual design of a grazing incidence flow cell.

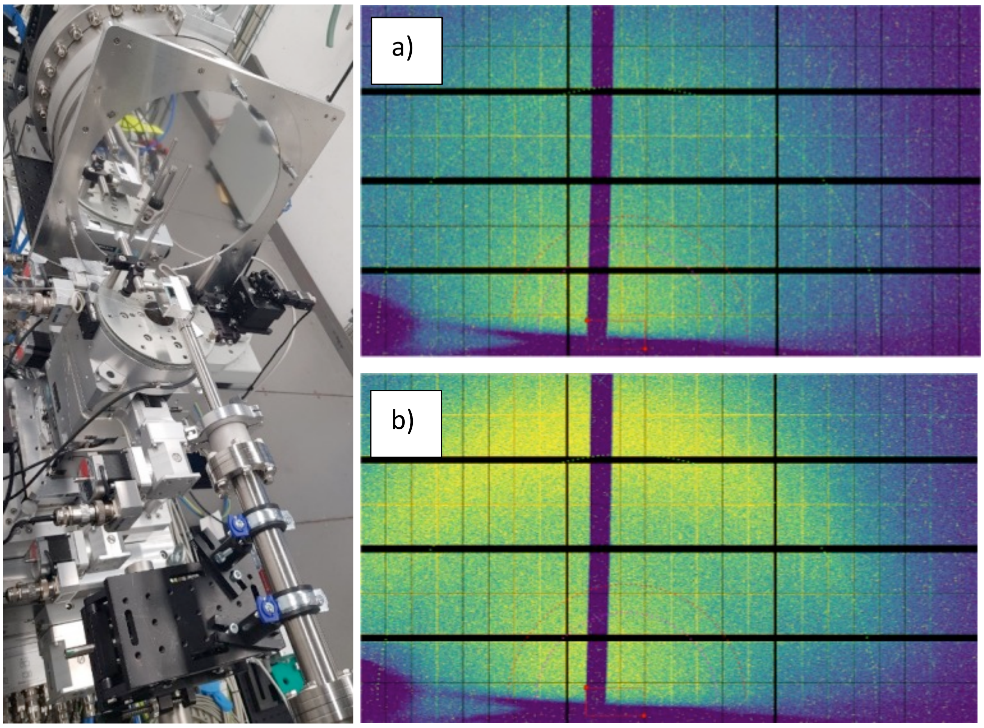

Figure 22. Results from tests of X-ray scattering from H_2O using the Nanocell at the FemtoMAX beamline. a) no sample in the Nanocell, b) sample in the Nanocell.

3 Beamline operation

3.1 Modes of operation and statistics overview

The beamline goal is to be in line with the most attractive laboratories to perform ultrafast X-ray diffraction and spectroscopy experiments in listed areas:

1. *Time resolved X-ray scattering from solids including cryo experiments down to 15 K.*
   The available monochromatic X-ray flux (1e6 ph/shot in 60 µm x 60 µm) is more than enough to study crystalline samples and collect quality data. Beamline equipment allows to perform experiments in extreme geometries with 2θ = 50 deg and sample detector distance up to 1.5 m in UHV environment.

2. *Time resolved X-ray scattering from nanostructures, thin films, and protein crystals.*
   The X-ray beam quality and stability at FemtoMAX allow to perform challenging experiments using nanostructures, thin films, and protein crystals. Ultrashort X-ray pulses at low repetition rate keep samples below the damage threshold limit which is key to preserving and performing experiments on difficult to make or rare/expensive samples.

3. *Time resolved visible fluorescence, luminescence experiments down to 15 K.*
   The nature of the X-ray pulse length at the FemtoMAX beamline is perfect to measure decay and efficiency of ultrafast-scintillating materials.

4. *Time resolved X-ray absorption experiments.*
   In the femtosecond resolution XAS, an advantage of FemtoMAX is that it has ability to scan a long range of energy and to cover a broad energy from 2 keV to 10 keV. The current X-ray flux is sufficient to study easy samples such as iron and ruthenium metal-organic compounds etc...

5. *Time resolved SAXS & WAXS from solids and liquids.*
   The flexibility of the FemtoMAX beamline allows adaptation to many user requirements concerning sample excitation, using optical or THz radiation, as well as the available time scales, ranging from tens of fs to µs. This makes the beamline suitable for a wide range of time resolved SAXS & WAXS experiments, effectively bridging the fs time scales accessed at FELs and the ps dynamics achieved by synchrotron beamlines.

3.1.1 FemtoMAX benchmarking to other beamlines

In a benchmarking exercise, FemtoMAX is compared to SwissFEL, LCLS and ID09 as they are the leading FEL and synchrotron storage ring beamlines offering broadly similar time resolution and experimental techniques, table 4. These beamlines deliver much higher photon flux on the sample at higher repetition rates compared to the operating conditions of FemtoMAX today. The lower flux at FemtoMAX may be an advantage for some experiments, allowing the possibility to extend the data collection time for radiation sensitive samples, like protein crystals, and to revisit the same sample by avoiding the destruction threshold of FELs. FELs typically operate at higher X-ray energies whereas FemtoMAX can reach softer energies down to 1.8 keV (to be exploited for Spectroscopy studies) and up to 22 keV. In addition, FemtoMAX offers the possibility to tune the X-ray energy during the beamtime, a functionality not routinely possible at FELs. The position and energy stability of the X-ray beam enables FemtoMAX to achieve data qualities comparable to the other X-ray sources. In addition, FemtoMAX offer adaptability for many experiments with the help of multiple endstations and sample excitation schemes.

Table 4. FemtoMAX comparison to key time resolved beamlines.

	FemtoMAX (MAX IV)	**Bernina (SwissFEL)**	**XPP (LCLS)**	**ID09 (ESRF)**
Operation started	2021	2020	2011	1999
Number of publications	10	18	197	192
Flux [ph/pulse]	DCM 1.5×10^{5}	DCM 1×10^{10}	1×10^{10}	DCM 5×10^{5}
Repetition rate in Hz	10	100	120	1000
Offered time resolution	< 100 fs	< 100 fs	< 100 fs	> 100 ps
Beam size [µm]	60 x 60 100 x 200	2 x 2 (up to 1000)	3 x 3 (up to 500)	25 x 25 100 x 100
Energy range [keV]	1.8 – 15	2 – 13	4 – 25	8 – 24
Techniques offered	GIXS, WAXS, SAXS, spectroscopy	Time resolved resonant and non-resonant diffraction techniques	WAXS, SAXS, spectroscopy	GIXS, Laue diffraction SSX, WAXS, SAXS, XES
Beamline staff	6*(5) (2023)	8 (2023)	11 (2023)	6 (2023)

*See section 4.2 for details

As a one of a kind beamline, FemtoMAX face challenges too, especially as the LINAC at MAX IV is a shared resource feeding two additional storage rings. This results in slightly prolonged set-up and data collection times.

3.1.2 Proposal statistics

FemtoMAX carefully considers all proposals, many of which are state of the art. This uniqueness and adjustability of the FemtoMAX technical base is not available at FELs and ring beamlines. More than 80% of all performed experiments up to 2023 at the FemtoMAX beamline are unique and complex, see details in figure 23. An outcome from this situation is that the routines and lessons learned from the previous runs cannot be applied directly and often require further modifications. Indeed, such varied, complex experiments can technical issues that are usually unforeseen in the proposal phase. This results in many quick fixes during 2-week beamtime so that users collect good data but insufficient for a publication.

FemtoMAX allocates 80 % of all available beamtime to the user community which results in up to six 2-week long beamtimes per each user cycle. A negative aspect of such long beamtimes is that not all user groups can or have resources to perform experiments for such a long period. The typical time for publication after a successful beamtime is between 12 and 36 months. The long lead time is due to complex data analysis, that appropriate theory may not exist and needs to be developed and furthermore that interpretation may be difficult as the experiments are not standardized. In figure 23 the number of proposals received and accepted is shown. If beamtime provides enough data for publication and data is being published it is counted as a successful experiment. FemtoMAX successful experiment is somehow similar to FXE beamline at XFEL[3].

	2021 fall	**2022 spring**	**2022 fall**	**2023 spring**	**2023 fall**	**2024 spring**	**2024 fall**
Total available beamtime slots (in-house included)	6	8	6	8	8	5	6
Total submitted proposals	5	3	7	6	5 (4*)	6	7
Allocated	4	3	6	5	3 (4*)	3	5
Total unique experimental configurations	4	2	5	3	0	2	2
Successful experiment	2	2	3	2	2	5, ?	?

Figure 23. Overview of the available and dedicated beamtime at the FemtoMAX beamline, * stands for commissioning experiment, ? stands for unknown outcome of the planned experiments.

In the figure 24 calendar from the FemtoMAX Digital User Office (DUO) is shown, here one can see all beamline activities.

[3] Serguei Molodtsov, European XFEL , Facility Update & Information about 11th Call for Proposals

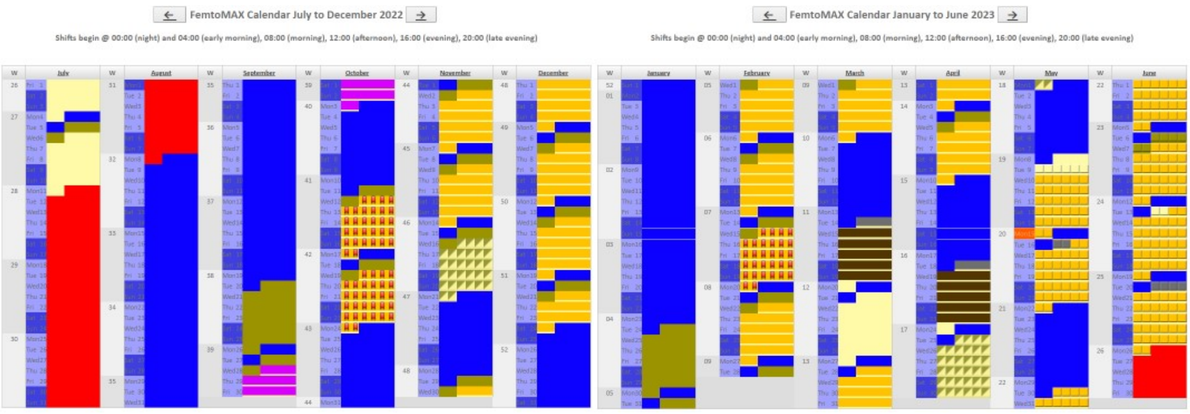

Figure 24. Here colours must be understood as follows: blue – LINAC development, purple – in-house research, yellow – planned user operations, brown – in-house commissioning, crossed light yellow – reduced X-ray beam delivery to the beamline.

3.1.3 User feedback

The user experience for experiments at FemtoMAX is summarised, for the last year, in figure 25, and is based on input into the DUO system by the users following their beamtime. Overall, the response is positive, the beamline is functioning well according to the users. The beamline instrumentation, routines and beamline staff duties are well synchronized with the user experiments. The main wishes are beamline controls becoming more user friendly and efficient data collection rates, however, some complaints need to be clarified. First the beamline control software needs support from KITS to solve issues. With the aim of providing more robust IT control software, KITS are not supporting temporary solutions; flexibility is often needed to serve all the user needs. This means that the beamline doesn't have the ability to offer temporary solutions to problems and is often unable to debug errors, reset servers, etc. without KITS support, resulting in lost beamtime. A second issue is IT infrastructure and available data analysis pipelines, collected data access and compression. This part is being solved by supporting and training users with beamline staff developed analysis scripts and analysis routines to make analysis as smooth as possible. Collected data files are large, therefore analysis or data transfer times to local user storage are very long. The possibility to compress or save ROI of the detector is missing. Additionally, old Linux machines are rarely updated. Users are missing facility input in this field. Finally the aging beamline equipment requires constant intervention, repair and maintenance which takes some time each beamtime. The most critical is the laser system that needs periodic beamline laser responsible service. A detailed user feedback can be found in Appendix B.

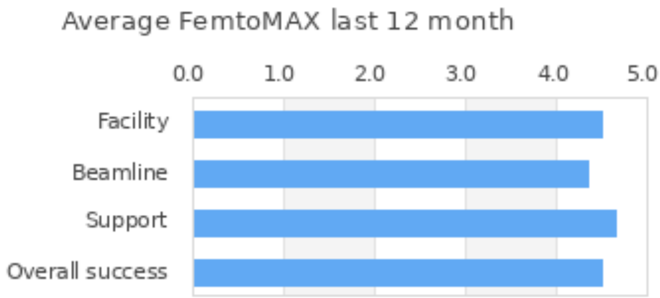

Figure 25. User feedback for experiments at the FemtoMAX beamline.

3.1.4 Publications

Currently, there are 10 published articles in peer reviewed journals. It is expected that every user call will result in at least 5 publications. There are 3 pending publications from the beamline detailing in-house developed methods, tools/sample environments and the control system. Below is a list of publications from the FemtoMAX beamline:

1. M. Burza et al. *Dispersion and monochromatization of X-rays using a beryllium prism.* Optics Express Vol. 23, Issue 2, pp. 620-627, Jan 2015.
2. A. Jarnac et. al. *Demonstration of a 20 ps X-ray switch based on a photoacoustic transducer*. Structural Dynamics, v 4, n 5, p 051102 (8 pp.), Sept. 2017.
3. H. Enquist et. al. *FemtoMAX - an X-ray beamline for structural dynamics at the short-pulse facility of MAX IV*. Synchrotron Radiation, v 25, n 2, p 570-9, 1 March 2018.
4. R. M. Turtos et. al. *On the use of CdSe scintillating nanoplatelets as time taggers for high-energy gamma detection*. 2D Materials and Applications, v 3, n 1, p 37 (10 pp.), Dec. 2019.
5. Xiaocui Wang et. al. *Role of Thermal Equilibrium Dynamics in Atomic Motion during Nonthermal Laser-Induced Melting*. Physical Review Letters, v 124, n 10, p 105701 (6 pp.), 13 March 2020.
6. J. Saaring et. al. *Ultrafast radiative relaxation processes in multi-cation cross-luminescence materials*. IEEE Transactions on Nuclear Science, v 67, n 6, pt.1, p 1009-13, June 2020.
7. I. Kamenskikh et al. *Decay Kinetics of CeF3 under VUV and X-ray Synchrotron Radiation.* Symmetry, v 12, n 6, p 914 (12 pp.), June 2020.
8. A.U.J Bengtsson et. al. *Repetitive non-thermal melting as a timing monitor for femtosecond pump/probe X-ray experiments*. Structural Dynamics, v 7, n 5, p 054303 (6 pp.), Sept. 2020.
9. M. Jensen et. al. *High-resolution macromolecular crystallography at the FemtoMAX beamline with time-over-threshold photon detection.* Journal of Synchrotron Radiation, v 28, n 1, p 64-70, 2021.
10. D. Sri Gyan et. al. *Low-temperature nanoscale heat transport in a gadolinium iron garnet heterostructure probed by ultrafast X-ray diffraction*. Structural Dynamics, v 9, n 4, p 045101 (10 pp.), 2022.

3.2 Staffing

FemtoMAX beamline team consists of 6 staff members. Andrius Jurgilaitis, David Kroon, Thai Pham, Byungnam Ahn,Carl Ekström and Jörgen Larsson,. Jörgen Larsson and Andrius Jurgilaitis joined FemtoMAX project from the planning phase. Detailed responsibilities listed below.

Prof. Jörgen Larsson, founder of the FemtoMAX project. After successfully running time resolved X-ray beamline D611 at MAXII storage ring initiated FemtoMAX project at MAXIV Laboratory. Works part time (20%) as the FemtoMAX beamline staff with a focus for scientific development, collaborations, and education outreach.

Andrius Jurgilaitis, researcher at the FemtoMAX beamline holds beamline manager responsibility. Joined FemtoMAX project as research engineer from the planning phase since 2012. Designed X-ray beam diagnostics, endstations, and experimental set-ups. Build most of the beamline and commissioned it together with present and former group members. Permanent employment, full time at the FemtoMAX beamline. Main focus is beamline technical development including new tools, methods and sample environments. Personal research focus is energy harvesting using semiconductor nanomaterials.

David Kroon, Laser scientist at the FemtoMAX beamline. Joined group 2017, responsible for beamline timing tools and laser operations/development. Permanent employment, works 80%. Focus on developing timing tools for ultrafast science. Aiming to push the temporal resolution available at the beamline as far as possible with good synchronization and data post sorting.

Thai Pham beamline scientist at the FemtoMAX beamline. Joined group 2016, responsible for ultrafast spectroscopy development at FemtoMAX. Permanent employment, full time at the FemtoMAX beamline. Personal goal is to use the time-resolved XAS setup at FemtoMAX to study photochemical processes for solar energy applications. At the same time will further improve the sensitivity and time resolution of the setup.

Byungnam Ahn, research engineer at the FemtoMAX beamline. Joined group in 2022 as partly shared resource at MAXIV Laboratory. Permanent employment, 50% time works at the FemtoMAX beamline since 2023. Responsible for laser maintenance and user support. Aims to provide beam transportation system of the ultrafast high-power laser efficiently which will help to drive the advanced research. Light interaction with nanostructures and high-resolution strain mapping of nanostructure devices is main research interest.

Carl Ekström, postdoctoral researcher. Joined group 2020, responsible for laser maintenance, user support and THz set-up at the FemtoMAX. Temporary employment, full time at the FemtoMAX beamline. Scientific interest of ultrafast pump/x-ray probe studies in condensed matter using x-ray diffraction, and development of laser-based THz setups.

Additionally, the beamline is supported via shared lab resources: ITC, scientific software, vacuum, design and floor coordinators for past office hours/weekdays.

3.3 Beamline transition to user operation

FemtoMAX construction began in 2013, with general user operation starting a decade later in 2021. All beamlines at MAX IV have been delayed in achieving baseline operation but FemtoMAX suffered many additional delays. FemtoMAX is the only beamline located at the Short Pulse Facility (SPF) and the fundamental difference from every beamline located at the MAX IV storage rings has added to the complexity of delivering FemtoMAX within the prioritization set by MAX IV for the many consecutive projects at MAX IV. Delays within the FemtoMAX project have arisen from insufficient resources between shared beamline projects for construction, commissioning/operation, and control systems. This complex situation was exasperated since resources could not be released to help complete remaining projects, as commissioning/operating beamlines have also required significant support.
In addition, a major impedance to achieving higher flux measurements at FemtoMAX has been the injection rate from the LINAC. The LINAC and FemtoMAX beamline were only permitted to operate at 2 Hz injection repetition rate by the Swedish radiation safety authority (SSM); to operate with higher repetition rates, a new permit was needed requiring extensive computer simulations and measurements. However, operational permits were needed for other beamlines first. The simulations showed that some actions were needed due to radiation shielding concern, to allow operation of the LINAC at 10 Hz, thus delaying this mode of operating MAX IV. Worldwide Covid-19 situation also contributed additional delays for FemtoMAX. A detailed path towards user operation is shown in figure 26.

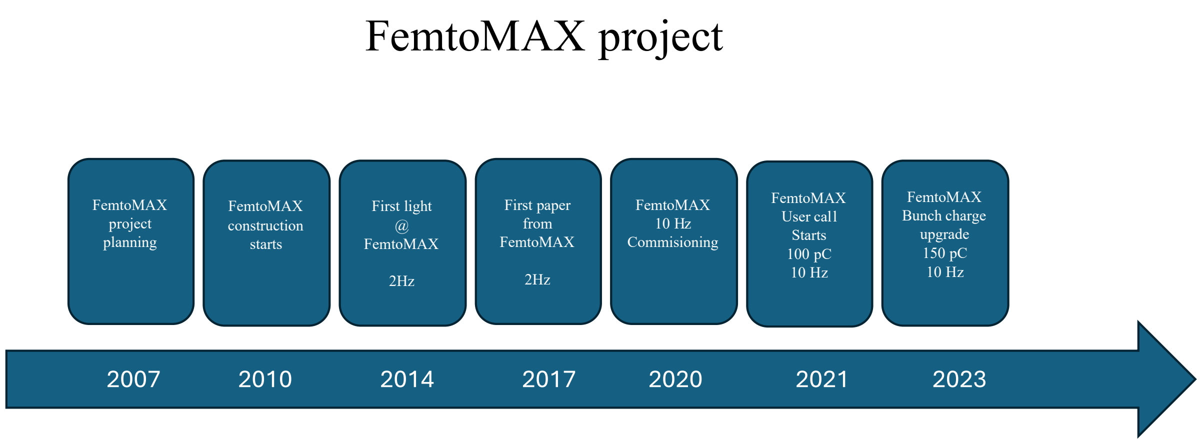

Figure 26. Time history of the FemtoMAX project.

At the present time, FemtoMAX is continuing with the LINAC injection rate of 10 Hz, which is bound to a radiation safety permit however, the design specification is for 100 Hz operation. At present there is no timeline for when higher repetition rates can be achieved due to extensive work required to update radiation safety permit, FemtoMAX time estimate when this could happen is presented in table 7. Building a vibrant user community is not easy, when the beamline has the lowest repetition rate, as presented in table 4. Additionally, the delays in getting to user operation is concerning for the beamline and within the user community, especially the negative impact of disappointing many users who built their science programs expecting delivery of new capabilities. SXL project (Soft X-ray Laser) and future klystron gallery at MAX IV, which is planned outside the FemtoMAX beamline, brings some concerns on the future of the beamline. FemtoMAX is concerned that 100 Hz might not be reached in the next 5 years and MAX IV's focus will be redirected towards the SXL project (as yet unfunded).

To mitigate the low repetition rate and shared accelerator, users receive two weeks of beamtime (66 shifts) for scattering experiments and one week (33 shifts) for the X-ray fluorescence set-up. User beamtime is scheduled from Wednesday to Monday mornings, although the beamline will use the Monday and Tuesday, before the start of a user experiment, to check the beamline performance and start building up the experimental set-up and operating conditions. This model works well with current beamline staffing, where at least 2 FemtoMAX staff are dedicated for normal user operation and on-site with user support from 08:00 – 20:00, Wednesdays to Fridays. At present there is no on-call support offered at FemtoMAX, instead the effort is spent on direct contact with the users at the beamline.

The user proposal call is twice a year. The feasibility of each submitted proposal is confirmed by the beamline staff and each proposal's scientific merit ranked by Programme Advisory Committee (PAC). A breakdown of the available time for users, in-house development, and commissioning, since beginning user operation, is shown in figure 25.

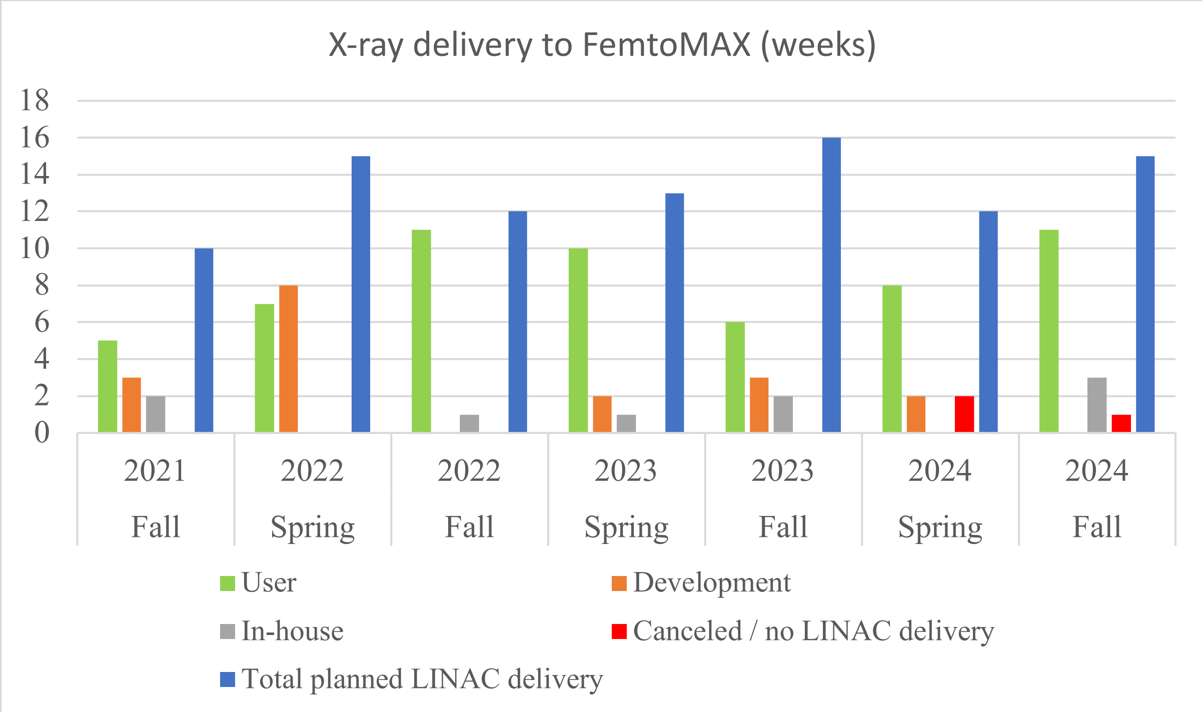

Figure 27. Beamtime distribution at the FemtoMAX beamline.

For the X-ray scattering set-up different data collection modes can be set. This includes single shot experiments, fast data collection mode at 10 Hz and reference data collection mode where every other X-ray pulse is used as a reference. Different sample excitation modes can be applied to all endstations and all set-ups.

3.4 FemtoMAX & LINAC development: towards brighter and smaller X-ray beam

FemtoMAX is the only beamline at MAX IV using the LINAC as a source to produce X-rays. The beamline and LINAC groups meet for joint meetings regularly to discuss possible LINAC/FemtoMAX developments. In 2019, a device called transverse deflecting cavity (TDC) was designed. This is now built next to the FemtoMAX front-end and is in commissioning since 2023. FemtoMAX (at 10 Hz and 100 Hz in the future) and the TDC (10 Hz only) cannot operate at the same time due to different design specifications.

In discussion with the LINAC, FemtoMAX has proposed to increase the electron bunch charge from 100 pC to 200 pC, as a standard operation mode. In this mode, experiments will benefit from the increased X-ray flux at the sample position. The LINAC at MAX IV can deliver this increased charge at FemtoMAX and was tested in the early commissioning stage of the FemtoMAX beamline. Starting 2024 nominal charge in the LINAC is increased to 160 pC which is limited by the charge budget that is set by radiation safety team. Increased X-ray flux did not affect X-ray beam size (60 x 60 µm) or pulse duration (50 fs). Further developments are ongoing to reach 200 pC goal and smaller x-ray beam size at the sample position (20 x 60 µm).

3.5 Typical beamtime process

The FemtoMAX user base is very diverse therefore standard routines for a typical beamtime and the responsibility for the local contact are still being refined. The typical beamtime process is as follows:

Contact is established between the beamline local contact for the proposal and the principle investigator. Details about the experimental geometry, experimental safety, data analysis, and other important experimentally related topics are confirmed, this communication being either by e-mail or online video meeting. Normally the local contact takes the responsibility to inform the FemtoMAX team about the experiment and a plan is made for which team members will help support the experiment.

During the start of a beamtime, the laser pump excitation is normally set up on the first Monday by either David Kroon or Carl Ekström and the X-rays the next day, by the local contact. Typical experimental parameters such as beam sizes, X-ray energy, laser fluence, and photon flux are measured and logged in electronic log book. The following days of the beamtime are required to find and improve the signal, perform spatial and temporal overlap between the pump and probe beams and to tune the final experimental conditions in general. The users are also training so that by the end of the week, they can operate the beamline independently and to collect the first data sets before the weekend. They then give the beamline staff feedback from their analysis at the start of the second week.

3.6 Data analysis

The raw data, as well as diagnostics from the FemtoMAX beamline is normally collected and saved in HDF5 format. Every new scan that is made creates a main HDF5 file that contains the links to all the single steps in the scan which further contains the single shot values and raw data of the experimental configuration. In most cases the raw data are single shot images from a large area detector, such as the Pilatus detector. Each single shot of data must then be further sorted into time bins to get down to the femtosecond time resolution. FemtoMAX has written MATLAB and Jupyter Notebook scripts for primary data analysis. Users are encouraged to use those or write their own scripts for data analysis. A typical simplified procedure of data analysis at the FemtoMAX beamline is shown in figure 28.

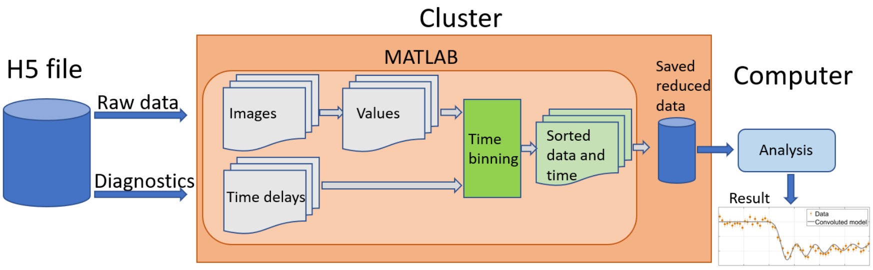

Figure 28. Schematics of the data analysis at the FemtoMAX beamline using MATLAB and computer cluster.

The production of reduced and sorted data demands heavy parallel computing, which means that it is always necessary to use the MAX IV computer cluster to read, reduce and sort acquired data.

In 2023, the beamline implemented online data analysis pipelines where data is analysed as it is being collected to simplify decisions during the ongoing experiment.

3.7 Community outreach

The list below outlines ways to increase the beamline scientific output and keep users up to date concerning beamline instrumentation and methods. The local contact for planned beamtime experiments and the beamline spokesperson (J. Larsson) for in-house research are responsible for reporting and dissemination (if allowed) outside MAX IV.

1. Follow standard documentation routines for efficient beamtime usage.
2. Promote Fast Access at FemtoMAX for new experiments (sample screening only) to increase the likely success of an experiment.
3. Regularly encourage users to give talks in MAX IV and in external workshops/conferences on data from FemtoMAX.
4. Regularly encourage and support users to publish data collected at FemtoMAX.
5. FemtoMAX encourages staff in-house research.
6. Typically, FemtoMAX supports research groups and their experiments via regular user call or inhouse activities. In addition to allow innovation and development of key scientific cases for FemtoMAX, the beamline may invite experiments from guest researchers, with the permission of the Science Director.
7. FemtoMAX participates regularly at conferences, workshops and yearly FEL's user meetings highlighting FemtoMAX development and user science examples.
8. FemtoMAX will contribute to the MAX IV newsletters to highlight important developments and instrumentation upgrades. The beamline will update the FemtoMAX webpage prior to every proposal round.

4 User engagement to achieve the FemtoMAX Science Roadmap presented in section 3.1

5 Summary, user outreach strategy.

FemtoMAX beamline have 4 out 5 end stations ready for user experiments. The last one (spectroscopy set-up) is planned to be ready to accept regular users in 2024. The beamline instrumentation supports a broad range of experimental capabilities that covers a number of reaserch fields, as listed above. A summary per endstation for all experiments performed at the FemtoMAX beamline is shown in table 5.

Table 5. Summary of all beamtime used vs endstation at FemtoMAX.

Endstation name / installation date	Number of weeks performing experiments (2021 fall - 2024 fall)	Number of papers	Average impact factor	Status
(1) GIXS/2017	22	3	4.9	Commissioned via regular proposal call. Ready
(2) Tilt/2017	6	1	2.7	Commissioned via regular proposal call. Obsolete
(3) Kappa/2023	2	0	NAN	Commissioned via regular proposal call.
(4) G-chamber/2022	2	0	NAN	Commissioned via regular proposal call. Ready Paper in manuscript.
(1) Fluorescence/2022	4	3	4.9	Commissioned via regular proposal call. Ready
(5) Spectroscopy/2021	6	0	NAN	Commissioning only. Feasibility not confirmed. Technical paper in manuscript.
(1, 5) Scattering from liquids/2021	1	0	NAN	Feasibility confirmed, not ready.
(1, 4) SAXS/2023	1	0	NAN	Feasibility confirmed. Ready Technical paper in manuscript.

On average the beamline is scheduled for 10 weeks (5 x 2 week slots) every half year resulting to 4 PAC approved user experiments for two weeks and 1 slot for in-house research or collaborative research. A left-over scattered weeks 1 or 2 are dedicated for commissioning experiments, in-house development, training and maintenance or studies on fast scintillating materials. Most of the end stations have been commissioned via regular user call. We see that each need about 6 weeks (3 experimental in-house or commissioning runs) to get to an operational state where experimental results get published.

A strategy to build scientific community by making joint experiments has been chosen. The experimental complexity at FemtoMAX differs a lot for dissimilar user groups. The most complex and costly (economically) are cryo experiments using GIXS chamber that requires at least 2 attempts at FemtoMAX (not including beamtime at other facilities) to produce one high impact factor (impact factor > 5) publication. To configure a different set-up takes up to a day, which does not affect user beamtime as it is done on Mondays. A standard experiment such as SAXS, fluorescence or spectroscopy has a potential to produce a publication every beamtime. A balance between challenging and standard experiments is a goal that has not been achieved at this stage.

The beamline staff focuses to attract national and Baltic region researchers first. The beamline has identified three approaches broadening the user base. Firstly, the beamline staff will contribute to a higher degree than before to relevant seminars, workshops and conferences (see table 6) to make the beamline visible in the scientific community. Secondly, 1 group from the previously identified potential user groups will be personally invited every half year to perform a joint experiment. They will be encouraged to preform new experiments or use our most recent set-ups. Thirdly, the beamline plan to be active in networking within collaborations such as Röntgen-Ångström Cluster, EU research and development projects (PRISMAS, LEAPS).

Table 6. FemtoMAX annual conference calendar and beamline representatives for year 2024.

Name	Place	Representative
European XFEL and DESY Photon Science Users' Meeting. January 22 – 26, 2024.	Germany	Thai Pam
Northern Lights on Food Conference V - Boosting structural food science, May 27 – 29. Lund	Sweden	Andrius Jurgilaitis
DanScatt XFEL Workshop 2024, May 29 and 30, 2024, Aarhus University	Denmark	Andrius Jurgilaitis
Danscatt Annual Meeting 2024 - 30 and 31 May, 2024, Aarhus University	Denmark	Carl Ekström
Nordic Nanolab User Meeting, June 3 – 4, Oslo	Norway	Andrius Jurgilaitis
Science@FELs, from 17 – 21 June 2024, Paris	France	Carl Ekström
The 23rd international conference on ultrafast phenomena, 14–19 July 2024, World Trade Center, Barcelona, Spain	Spain	Not decided
15th SRI conference, from 26 – 30 August in Hamburg	Germany	David Kroon
MSE 2024: Materials Science and Engineering (MSE) Congress 2024 September 24-26, 2024, Darmstadt.	Germany	Not decided
SSRL/LCLS Annual Users' Meeting 2024. September 22-27	USA	Not decided

With the current staffing and instrument specifications the beamline cannot support more users per call cycle than it does today. To reach a full user program at FemtoMAX where regular and new user groups contribute to the experiments will take 2 – 5 years. Under current conditions a steady beamline operation with constant scientific output is expected by year 2029. This period can be shortened if one or several conditions is fulfilled: 1) repetition rate of the LINAC is increased, 2) beamline staffing is increased, 3) scientific networking and outreach is increased, 4) beamline scientific direction is refined, 5) performing standard experiments only. Economical, time and user impact estimates are presented in table 7.

Table 7. A summary of the impact and its result to expected outcome.

Prio.	Type	Time needed to implement	Economical aspect	User impact	Worst case scenario at the beamline
1	Scientific outreach	1 – 3 years	Low/medium	High	There is a risk of dissatisfying new user groups due to a lack of available beamtime or unforeseen circumstances.

2	High rep. rate (>50 Hz)	3 – 6 years	High	High	None. Beamline work routines needs a review if high rep. rate operation results in shorter beamtimes.
3	Staffing	1 – 3 years	Medium	Medium	None
4	Scientific direction refinement	1 year	Low/Medium	Medium	Narrowing FemtoMAX scientific case will make beamline less competitive.
5	Standard experiments	1 year	Low	Low	Standard measurements might not result in high impact scientific output.

FemtoMAX beamline is one of several places where time resolved X-ray scattering experiments in repetitive mode with femtosecond time resolution is performed. The technical flexibility of the beamline enables the staff to adapt the user set-ups and tune X-ray energies over a wide range during the actual beamtime. The FELs in operation today cannot match this flexibility and tunability. The fact that many users are not able to use the full flux provided by FELs due to sample damage and instead perform experiments at low repetition rates while rastering samples[4] raises the question what actually is needed to perform a time resolved experiment in general?

Considering the technical base including multiple large area detectors, endstations and data analysis infrastructure FemtoMAX aligns well with FEL facilities. FemtoMAX have not reached it's full potential yet and continues to discover new feasibility experiments, where some of them have been performed and published already at FEL[5,6]. Those results are a must to have when building user community centered around FemtoMAX.

A beamline project overview with key goals towards achieving a user friendly operation and a broader user community is presented in figure 29. The time line starts with the first user call in year 2021. The timeframe is set for the next 5 years.

[4] Room temperature XFEL crystallography reveals asymmetry in the vicinity of the two phylloquinones in photosystem. Scientific Reports. 2021; 11: 21787 (14 pp.).
[5] Levantino, M., Schirò, G., Lemke, H. *et al.* Ultrafast myoglobin structural dynamics observed with an X-ray free-electron laser. *Nat Commun* **6**, 6772 (2015).
[6] Bacellar C, Rouxel JR, Ingle RA, Mancini GF, Kinschel D, Cannelli O, et al. Ultrafast energy transfer from photoexcited tryptophan to the haem in cytochrome c. Journal of Physical Chemistry Letters. 2023; 14(9): 2425-2432.

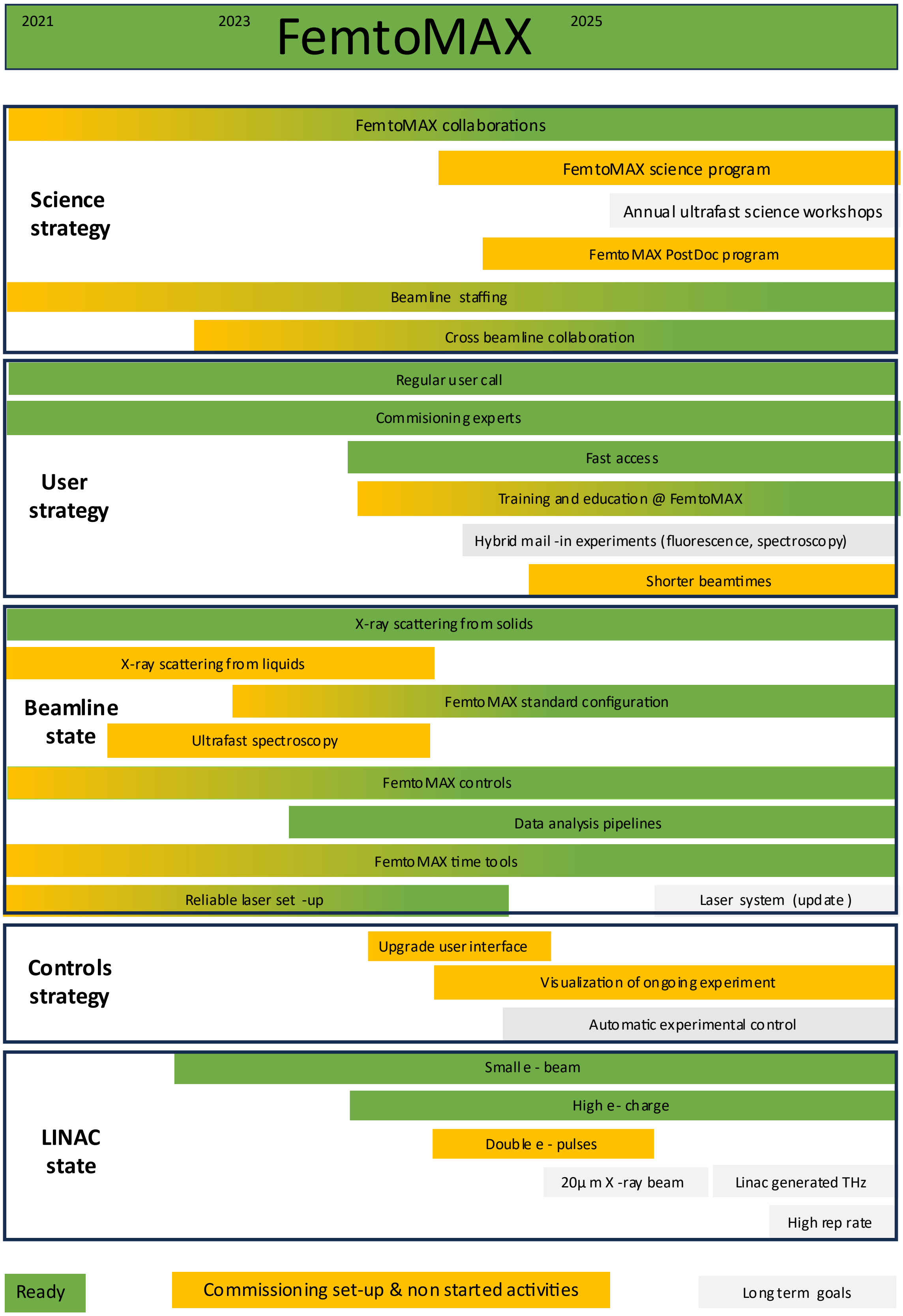

Figure 29. Overview and outlook of the FemtoMAX beamline development.

6 Long term beamline developments to improve beamline competitiveness.

FemtoMAX beamline will benefit a lot from a tailored LINAC development towards meeting the beamline's needs. These are long term (> 5years) investments that are expensive and requires many person work hours require significant effort before the projects are implemented. We see the following projects to be beneficial and aligned to the FemtoMAX science roadmap:

a) LINAC double X-ray pulse operation

The MAX IV LINAC team can accelerate double e-bunches produced by splitting and delaying the main laser pulse in to two before it hits a photocathode. The two pulses generated are similar in charge and are accelerated on the same RF field inside the acceleration cavity. A delay of a 50 ns between pulses can be achieved. Such LINAC operation mode is preferred for ultrafast spectroscopy experiments at FemtoMAX. Spectroscopy experiments are long in time and therefore every second pulse is used for signal normalization to eliminate X-ray beam fluctuations, thus decreasing the data collection rate from 10 Hz to 5 Hz. A double pulse structure where the first pulse is always used for normalization and the second to track laser pump response at different delays will align the data collection rate to the LINAC repetition rate.

b) LINAC based THz

The implementation of a double pulse mode is necessary for THz pump and X-ray probe experiments. Here THz radiation is emitted from a metal target hit by the relativistic electron beam. The position of the transverse deflecting cavity (TDC) is the ideal position for installation of an Al foil. This metal foil would work as a target and can be inserted into the electron beam as required. Intense THz radiation generation using short electron bunches has been generated at other LINAC based facilities[7], however, the transport of the THz beam is not trivial. The TDC is a short distance from the sample point and so we are likely to achieve efficient THz beam transport. To implement this capability a fast electron bunch at BC2 (bunch compressor) kicker is needed. Here one pulse will be delivered to the TDC branch to generate THz pulse and the other one to the FemtoMAX branch to generate X-ray pulse, see figure 30 for details.

[7] Ziran Wu, Alan S. Fisher, John Goodfellow, Matthias Fuchs, Dan Daranciang, Mark Hogan, Henrik Loos, Aaron Lindenberg; Intense terahertz pulses from SLAC electron beams using coherent transition radiation. Rev Sci Instrum 1 February 2013; 84 (2): 022701.

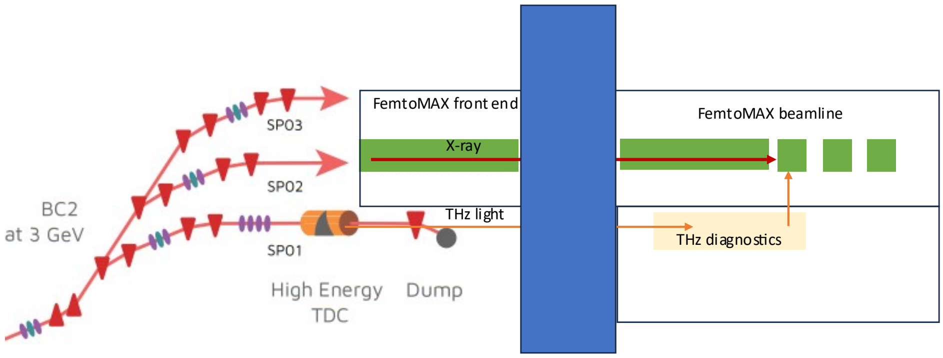

Figure 30. Conceptual lyout to use LINAC genearted THz light at the FemtoMAX beamline.

7 Points of concern

7.1 Beamline issues

7.1.1 Old beamline equipment

Several key components for the beamline have become old and need to be replaced. These are optical and electronic components that can be expected to live 5 – 8 years. Many date from 2013. The first request for further funding within the MAX IV operation budget was made in 2019 for replacement of timing oscilloscope and laser by 2023. The oscilloscope provides 200 fs timing information for each laser/X-ray pulse. The expected cost is 2.5 – 3 MSEK. The laser system is no longer serviced by the company and we spend significant effort to keep it running. The corresponding laser system at the LINAC was replaced 3 years ago with the motivation of keeping the linear accelerator running. Since we are the only beamline benefitting from delivery from the linear accelerator we believe it is equally important to have a new laser for FemtoMAX while the old one can be kept as a hot spare until it takes it last breath. The cost for this is about 8 MSEK.

A final key component is the Pilatus X-ray detector which is special in the sense that it can count more than one photon per pixel per shot using time over threshold technology (technology named by Dectris). At present, it is not a high-risk component, but it may become so in the future.

7.1.2 Common laboratory resources

The MAX IV laboratory is maintained, developed and operated by dividing technical expertise into support groups. The support groups cover standard facility operations like economy, HR, vacuum, design, automatization, safety, communications, beamline controls and floor coordinators. During the initial construction and operation phase, efficiently using these common resource groups proved difficult and a prioritisation of projects was undertaken in 2019 to help deliver operational beamlines. A recent restructuring and creation of a new Technical Division in March 2023 is expected to help prioritise user operation, however, a budget shortfall and recruitment freeze means that beamlines are still delayed in achieving full operation. FemtoMAX is increasingly affected by this especially by being the only beamline on the SPF.

As might be expected at a facility like MAX IV, there are different levels of projects, dealing with projects which have different levels of complexity, size and costs (big beamline construction projects to simple operation-based tasks requiring less than a week's work). To manage this, there are more than one project organisation directing the work of the Support Groups, many of which are within the Technical Division. All large beamline projects, or project the coordination of several resource groups, are handled via the Central Project Organization (CPO); smaller scale, operation focussed projects via BPAG within the Beamline Office (BO). The start of an approved beamline project ranges from a few weeks up to 2 months. While the structure is good, it is clear that there are not enough resources for the amount of work needs to be done.

FemtoMAX came into user operation with one detector only, slow data collection and no data analysis pipelines. All this has been solved while supporting users but the price has been overloaded beamline staff with no time for inhouse research, commissioning or developments.

7.1.3 Running user operations with under specified beamline parameters

The design parameters for FemtoMAX user operation are shown in figure 31. Beamline operation started at 2 Hz in 2014. Beamline alignment and commissioning work has been done at 2 Hz. The beamline opened for user operation in 2021 with 100 pC and 10 Hz repetition rate.

Operating energy	3 GeV
Maximum on-crest energy	3.7 GeV
Max RF rep rate	100 Hz
Bucket charge	100 pC
Normalized emittance	<1 mm mrad
Bunch length @ 3 GeV	<100 fs
Peak current	>3 kA
Operating RF	3 GHz
Linac gradient	20 MV/m
No of klystrons	18
No of acc structures	39
Injector length	300 m
Electron gun	FERMI type

Figure 31. FemtoMAX beamline design parameters.

The user community that work at FELs expect to perform scattering experiments using very thin (poorly reflecting) samples, observe diffuse scattering due to acoustic phonon

redistribution or changes in a liquid phase. The increase of flux of a factor 10 by operating at 100 Hz will enable these experiments to be carried out at FemtoMAX. It is already possible to observe such effects at 10 Hz, but it is not possible to carry out systematic experiments within a reasonable time. As an example we now require 10 minutes to get a single timepoint for the diffuse scattering that highlights the precursor to laser-induced melting of InSb. However, 100 time points in a scan is 1000 minutes or 15 hours which equates to one working day in real terms. 5 – 10 scans may be needed to vary parameters to find optimum conditions. The timescales are similar for liquid scattering in water or to refine the structural changes in a protein structure during THz irradiation.
Many experiments at FemtoMAX are performed @ 10 Hz repetition rate (100 pC) have been performed successfully, however results are not published yet and is expected to be posted late 2024 – early 2025. Year 2023 LINAC boosted electron bunch charge from 100 pC to 160 pC and reduced electron beam size (1.5 smaller) effectively increasing X-ray flux per area/shot at the FemtoMAX sample position. Charge increase has been received positively by FemtoMAX staff and users. High charge LINAC operation is risky due fast degrading LINAC cathode, since it falls outside designed cathode operational parameters, therefore lifetime is compromised. This situation resulted in the first cancelled user beamtime year 2023. In table 8 is presented data collection times at FemtoMAX from previous beamtimes. Here one can see how LINAC charge and repetition rate affects user data collection times.

Table 8. Femtomax flux per pulse vs data collection times vs noise at different charge values in the LINAC.

Charge (pC)	**Rep. rate (Hz)**	**Photons/shot on the sample (DCM @ 8 keV)**	**Amount of data (shots)**	**Data collect. time (min)**	**Noise level (%)**
60	10	54 000	5k, 10k, 20k	23, 43, 83	1, 0.7, 0.5
100	10	88 000	5k, 10k, 20k	14, 26, 50	1, 0.7, 0.5
150	10	135 000	5k, 10k, 20k	9, 17, 33	1, 0.7, 0.5
Original design parameters					
100	100	88 000	5k, 10k, 20k	2, 3, 5	1, 0.7, 0.5
FemtoMAX request					
200	100	175 500	20 k	3	0.5
Predicted future scenario					
150	50	135 000	20 k	7	0.5

Typical time resolved curve requires 50 – 100 different parameters consisting of different time delays between laser and X-rays, energy settings, laser power settings or magnetic field direction. This results to 2 – 4 days of data collection only at 10 Hz and 100 pC. Situation like this leaves no margin for technical or human errors leaving users with incomplete data after 2 weeks of beamtime at the FemtoMAX beamline.

7.1.4 FemtoMAX SWOT analysis

FemtoMAX beamline science productivity is low and has been raised as a point of concern. A SWOT analysis has been performed to identify different factors affecting beamline performance, benchmarking against other beamlines and to develop strategic planning.

Details and action plans reflecting on the SWOT analysis will be commented on the reviewer request only.

Table 9. SWOT analysis of the FemtoMAX beamline.

Strengths	Weaknesses
X-ray beam stability, tender x-rays, scan energy, beamline versatility, commitment and dedication, strong LINAC support, enough time for experiments, low staff turnover.	Defined roles and guidelines for the user experiment, beamline versatility, low staffing and staff availability, non-commissioned beamline equipment, shared accelerator with ring operation and beamline installation, high running cost.
Opportunities	**Threats**
Learn from FEL experience, standard set-ups, strong LINAC collaboration, shorter beamtimes, (10 day offer for beamtime) mix challenging and standard experiments, attract external researchers/Postdocs, new way of working.	Many working FELs, long beamtimes (workload on user/staff), no time for in-house development, vulnerability, soft x-ray laser, outdated equipment, running costs and beamline upkeep.

7.2 FemtoMAX history

The original scientific case for FemtoMAX was written in 2009 – 2010 and submitted in the application to "Knut och Alice Wallenbergs Stiftelse" in order to fund the first 7 beamlines. The scientific case was written for 100 Hz.

The facility building and accelerator infrastructure was designed for the higher repetition rate. All equipment has been specified, procured and tested to operate at 100 Hz. In the period 2015 – 2020 , the Linear accelerator was operated at 2 Hz enabling only commissioning of equipment and experiments where Bragg reflections from solid single crystals were monitored. In 2015 – 2017 there was only a surplus undulator from MAX II providing low flux.

With the upgrade to 10 Hz in 2020, it became possible to carry out experiments on thin films and to look at tails of Bragg reflections or weak reflections in solid single-crystal materials. The data acquisition time for such experiments is about 1 week allowing us to schedule beamtimes extending for two weeks which is reasonable for a user group. It was decided to launch call for users even if the performance of the beamline was far from the. The electron beam size at the time was a factor 10 too large and the post-sorting software which is part of the data acquisition system did not work well enough to reduce the temporal resolution which was 500 fs.

Only recently (March 2022) the electron beam size 60 x 60 μm and the data acquisition software have been optimized to achieve these parameters. The cross correlator giving sub-100 fs temporal resolution has recently been commissioned. The experiments carried out so far could be done significantly faster at 100 Hz allowing for beamtimes of one week, but the most important case is the new experiments it opens up for. FemtoMAX is a competitive source for scattering measurements on solid samples and possibly liquids.

Since the science case was written several pump-probe stations at FELs have become operational. Mainly LCLS 2010, European X-FEL 2016 and SwissFEL 2018. However, the pulse structure at European X-FEL is not optimized for pump-probe experiments from solids and it is likely that proposals in other areas which require the high average flux and can handle the pulse structure will get priorities. In some cases, like serial crystallography FemtoMAX is not competitive, but for pump-probe experiments in solids where diffract and destroy in a single shot is not viable, sample damage demand attenuation of the beam to a level of below or to about 100 times more photons than at FemtoMAX. In this case the stability (X-ray beam position and intensity) at FemtoMAX will give a competitive advantage.

8 Developments: ongoing, planned, and possible

8.1 FemtoMAX roadmap

To be competitive and attractive time resolved X-ray beamline, the FemtoMAX team sets short- and long-term goals listed below. Estimated costs risks are presented in parentheses.

Short-term planning (1-2 years)

1. *Firm data collection and data analysis pipelines.* (Typically, 1 – 2 TB of data is recorded per day shift @ 10Hz using one detector only. Multiple detectors are a common choice for the user. Analysis pipelines are essential for decision making during time resolved experiments.
2. *Finalize beamline time tools.* 1st ready (ping), 2nd in commissioning (cross correlator), 3rd in development (streak camera).
3. *Establish standard beamline configuration* for non-challenging in air diffraction and scattering experiments.
4. *Joint LINAC developments* to increase flux at the FemtoMAX: high electron bunch charge (200 pC), double electron bunch structure @ 10 Hz, low jitter and high temporal resolution.

Key performance indicators:
1. Effective beamtime use outside office hours. Positive user experience.
2. 2 – 4 technical beamline papers.
3. 20 % increase oversubscription.

Mid-term planning (3-4 years)

1. *All end-stations/set-ups ready for user operations.*
2. *Appropriate beamline staffing.*
3. *Education and collaboration via EU co-funded programs.*
4. *Establish science program via collaborations with Lund University and Lund Nano Lab.*
5. *Inhouse science program and cross-beamline collaboration.*
6. *Cryo system upgrade (~ 1 – 2 MSEK).*
7. *X-ray pulse parameter change on user demand: pulse duration (10 – 100 fs), charge (100 pC, 200 pC) and pulse structure (1 or 2 pulses).*

Key performance indicators:
1. 1 – 3 technical beamline papers, ~ 10 scientific papers/year.
2. 100 % increase oversubscription.

Long-term planning (> 4 years)

1. *High repetition rate* (> 50 Hz).
2. *New laser system* (OPCPA) ~10 MSEK.
3. *Beamline upgrade*.
4. *X-ray beam size* < 20 µm.

8.2 LINAC roadmap

Linac development towards Roadmap goals

- Reliable operation
  - Reduce interruptions (MTBF and MTTR)
  - Monitor beam quality
  - Deliver specific bunch length thanks to the TDC
- 100 Hz
  - Needed by FemtoMAX
  - More stable operation of the injector, less conditioning time, less downtime for ring injection.
- Low jitter – precise synchronization
  - Relative electron energy
  - Bunch arrival time
  - Bunch VS experimental laser arrival time
  - Precision time stamping
- High charge
  - Cathode exchange (this summer)
  - Upgrade of laser transport optics
  - Move the laser UV generation into the linac tunnel
- Multi-bunch mode
  - Double pulses ~100 ns separation
  - Pulse trains 4-16 pulses per RF shot (=1.6 kHz maximum rep rate together with 100 Hz)
- Ultra short pulses
  - Non-linear compression
  - Simulations show sub fs pulses
- Minimized transverse beam size
  - Optics setup through undulators
  - emittance reduction

Linac status – Sara Thorin **User Meeting FemtoMAX Jan 2024**

9 Charge questions

MAX IV asks the review committee to evaluate the material presented in the written report and the oral presentations and discussions and address the following charge questions:

1) Technical realization of the beamline:

a. Does the beamline provide adequate capabilities, and does the beamline team address areas of necessary improvement?

b. Does the beamline offer unique capabilities to the user community?

c. How does the beamline compare to leading beamlines in its field worldwide?

d. Is different endstations, set-ups and sample environments seen as an advantage of the FemtoMAX beamline compared to other beamlines worldwide.

2) User communities, science program, and impact:

a. Is the beamline attracting and supporting the relevant user communities?

b. Is there sufficient focus between the different activities?

c. Do the capabilities meet the needs of the relevant scientific communities (as laid out in the original science case)?

d. Are the staff research and development projects of appropriate quality and in line with the current and future direction of the science program at the beamline?

e. Are user and in-house science programs productive and making a sufficient impact in their science fields?

f. Is the beamline missing opportunities regarding user communities, science programs, or research directions?

g. Does the beamline / MAX IV employ an adequate outreach and training program?

3) Beamline operation:

a. Is the user support at the beamline of high quality and allowing for a productive user program with high impact?

b. Is the beamline or the facility missing out on opportunities for further improving user productivity?

c. Are sufficient support labs and related facilities available to enable high-quality research at the beamline?

d. Is the facility setting the right priorities in providing high-quality supporting infrastructure, services, and procedures?

4) Future directions:

a. Does the beamline have a well-laid-out and actionable development plan?

b. With the user community and national and international developments in mind, are the right priorities set out for these developments?

c. Is the beamline / MAX IV having an adequate funding strategy and making use of funding opportunities?

d. Are there additional opportunities (funding, development, science directions) that the beamline or the facility should take into account?

e. Are the (envisioned) operation and science programs at the beamline well-adjusted?

10 Appendix A, data control system

The current control system for data collection uses the Sardana Framework, which is a software suite for the Supervision, Control and Data Acquisition in scientific installations. It was initially developed at ALBA, Spain, and currently is supported by a larger community including MAX IV, Alba, DESY and Solaris. At MAX IV, sardana scans can be started using two different tools: Spock or ScanGui. FemtoMAX uses custom made scans in order to synchronize the detectors and laser delays with the x-ray bursts incoming from the linear accelerator.

Spock is a command line interface based on IPython with a direct link to the Sardana MacroServer Door, see figure 38. Thus, it can use standard python commands and scripting alongside tango and sardana commands and macros and it also has access to Sardana MacroServer environment variables.

```
Door_FemtoMAX [2]: burstscan dummy_mot_01 0 1 3 5
Operation will be saved in /data/staff/femtomax/kits-testing/streakcamera-%05d.h5 (HDF5::NXscan from FemtomaxNXscanH5FileRecorder)
Operation will be saved in None (['daq'] from HttpPostRecorder)
Scan #103806 started at Sun Nov 12 17:11:26 2023. It will take at least 0:00:19.225403
                                                        BSP02-O
                                                          DIA
                                                        OSCA-01
 #Pt No   dummy_mot_01  pcap_xray_counter  oscc_02_seq  rawwaveform1  oscc_03_seq     dt
   0            0              (5,)        h5file:///data/staff/femtomax/kits-testing/scan-103806/oscc_02_seq/step-00000000.hdf5::data/    <nodata>      <nodata>    1.0915
   1        0.333333           (5,)        h5file:///data/staff/femtomax/kits-testing/scan-103806/oscc_02_seq/step-00000001.hdf5::data/    <nodata>      <nodata>   7.43716
   2        0.666667           (5,)        h5file:///data/staff/femtomax/kits-testing/scan-103806/oscc_02_seq/step-00000002.hdf5::data/    <nodata>      <nodata>    13.789
   3            1              (5,)        h5file:///data/staff/femtomax/kits-testing/scan-103806/oscc_02_seq/step-00000003.hdf5::data/    <nodata>      <nodata>   20.1383
Operation saved in /data/staff/femtomax/kits-testing/streakcamera-103806.h5 (HDF5::NXscan)
Operation saved in None (['daq'])
Scan #103806 ended at Sun Nov 12 17:11:52 2023, taking 0:00:26.278603. Dead time 175.9% (setup time 0.2%, motion dead time 3.1%)
```

Figure 32. Output window from the FemtoMAX control system.

Scangui is a graphical interface linked to the Sardana MacroServer Door. It allows the configuration of the experiment and can start individual scans or a series of scans in a sequence. The standard interface of the ScanGUI allows the execution of scan macros and configuration of the experiment.

Additionally, custom macros can be created by the beamline staff and users to fit specific experimental needs.

10.1 Trigger gate controller and timing scheme

In FemtoMAX, the triggering scheme is done using PandABox, which is a FPGA based system that implements in hardware time resolved schemes. This solution was designed to produce valid triggers for the various different data acquisition equipment at the beamline.

The validity of the triggers relies on the availability of signals from the linear accelerator and should ensure that the data acquisition devices capture data synchronized with real incident (electron/x-ray) beam, see figure 39. Achieving such synchronism is challenging since the availability of the beam can be affected by different issues. The main issues are related: a) to the electron beam, b) the X-ray and c) the laser beam.

a) *Electron Beam Gate*

The LINAC is not always delivering to the SPF, but has instead 3 typical operation modes:

- SPF delivery
- R1 top-up
- R3 top-up

In each case, injection events from the appropriate timing system (SPF, R1, R3) are routed to trigger the appropriate LINAC electron gun.

The FemtoMAX event receiver (EVR), BSP02-C100009-CAB04-CTL-IOC-01, listens to all events propagated over the SPF timing system only, and is configured to output a hardware signal (LV-TTL) on each injection event.

Injection events are still propagated through the timing systems even when not routed to the guns. As such, only when the LINAC electron gun is being triggered by the SPF timing system (i.e. SPF delivery mode) does each injection event on the SPF timing system correspond to an actual electron injection into the LINAC. Triggering the FemtoMAX DAacq on every SPF timing system injection event would therefore result in no-beam data acquisition whenever the LINAC is not in SPF delivery mode.

Furthermore, even when the LINAC is in SPF delivery mode, several LINAC operational parameters (e.g vacuum valve states, screen insertions, etc.) may result in the electron beam not reaching FemtoMAX.

To mitigate these issues, the LINAC operational state, including its operational mode, must gate DAcq triggering.

b) X-ray Gate

Even when the electron beam from the LINAC does reach FemtoMAX, several beamline operational parameters (e.g vacuum valve states, screen insertions, etc.) may result in the x-ray beam not reaching the DAcq hardware. To mitigate this, the beamline operational state must gate DAcq triggering.

c) Laser Beam Gate

Finally, even when the x-ray beam does reach the DAcq hardware, successful data acquisition is often dependent on laser beam incidence from the FemtoMAX laser system. Several beamline laser parameters (e.g. oscillator mode-locking, laser shutter state) may preclude this. To mitigate this, the beamline laser state must also gate DAcq triggering.

10.2 FemtoMAX trigger scheme (trigger gate)

The FemtoMAX beamline has a wide variety of data acquisition (DAcq) equipment for experimental purposes, e.g. area x-ray detectors, CCD based cameras, oscilloscopes, etc. Much of this equipment must be triggered by hardware signals in order to properly synchronize data acquisition with the incident beam from the LINAC and laser beam from the FemtoMAX laser system.

The trigger gate currently accepts the following hardware signal inputs (TTL):

- SPF timing system injection events (TTLI01): Supplied by the FemtoMAX EVR
- Gate signals:
    - LINAC PLC gate (TTLI02): Supplied by the LINAC PLC (IO node in I-C080008-CAB02). High when the LINAC is in SPF delivery mode and LINAC operational parameters are conducive to beam at FemtoMAX. Full details of the constituent PLC signals and logic can be found in the relevant functional description.
    - Beamline PLC gate (TTLI03): Supplied by the beamline PLC (IO node in BSP02-C080003-CAB02). High when beamline operational parameters are conducive to beam at FemtoMAX. Full details of the constituent PLC signals and logic can be found in the relevant functional description.
    - Laser modelock gate (TTLI04): Provided by the beamline laser oscillator controller. High when the FemtoMAX laser is modelocked.
- SPF timing system RF clock (CLK): Supplied by the FemtoMAX EVR (@ $f_{rf,spf}/2 \approx 38.5$ MHz). Required to synchronize the PandABox clock to the SPF timing system for low jitter in output triggers.

Ten general purpose hardware signal outputs (TTL, TTLO01–TTLO10) provide gated trigger signals to the FemtoMAX DAcq:

- Diagnostic cameras (TTLI01): Zylas, BSP02-O-DIA-CAM-{01,02,05,06,07,09,10,11,12}
- Diagnostic oscilloscopes (TTLI02): R&S, BSP02-O-DIA-OSC{A,B}-01
- 'Ping' oscilloscope (TTLI03): Lecroy LabMaster, BSP02-C080016-DIA-OSCC-02
- Pilatus detector (TTLI04): BSP02-E-DIA-DETPI-01
- Laser oscilloscope (TTLI05): Lecroy WaveRunner, BSP02-L-DIA-OSCC-01

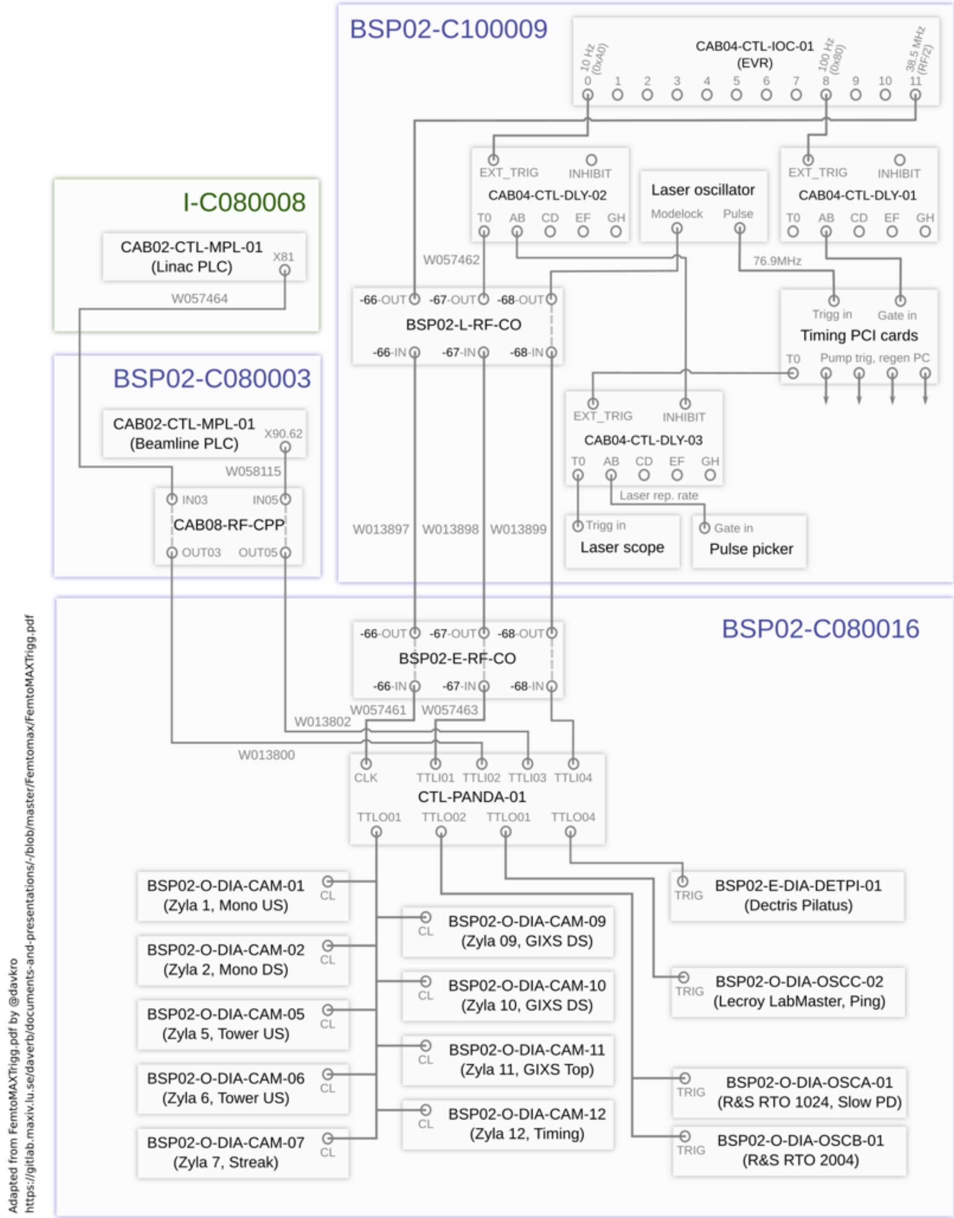

Figure 33. The FemtoMAX triggering scheme.

In the PandaBox the triggering scheme is implemented according to figure 40 and does not use any custom FPGA block. In this scheme the signal from the SPF is gated to the sensor inputs until they reach the count of n triggers, for each step. Each TTL output is connected to a detector or group of detectors and can have a configurable delay.

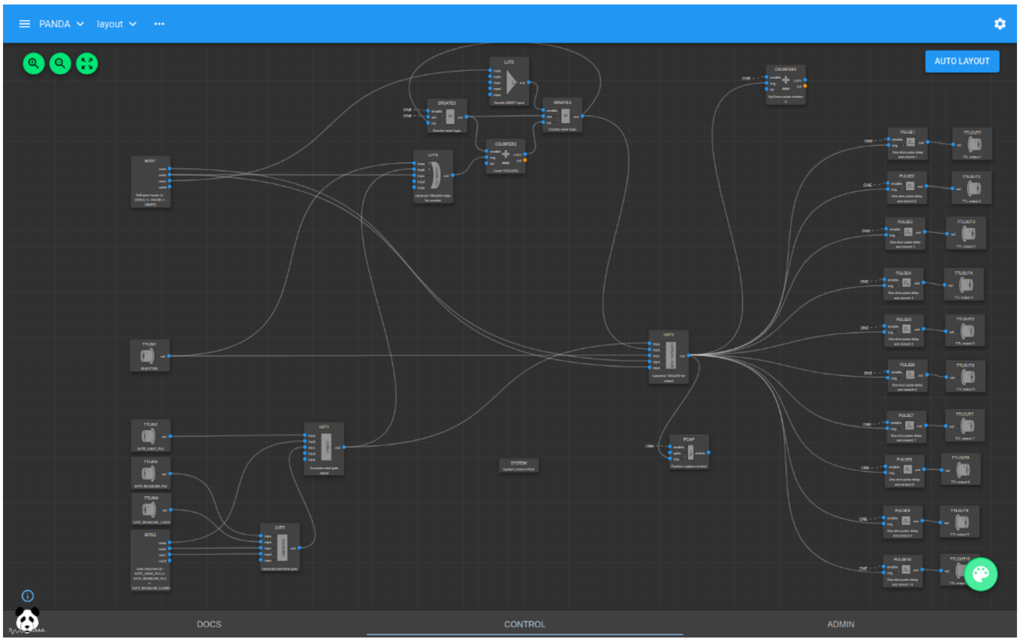

Figure 34. Map showing the connectivity of the control signals in the PandaBOX.

The trigger gate software provides the following functionality:

- Injection signal gating
  - On LINAC PLC gate input
  - On beamline PLC gate input
  - On beamline laser gate input
  - Individual software overrides (bypasses) for all gate inputs
- Trigger output
  - Finite trigger output ('scan mode')
  - Abort trigger output
  - Continuous trigger output ('debug mode')
  - Pause/continue trigger output
- Individual delays for each trigger output
  - Coarse delay
  - Fine delay (~8 ns resolution over ~240 ns window)

11 Appendix B

Table 10. FemtoMAX beamline post beamtime user feedback.

2019	The KITS team took half a day to show us video feed from a simple camera installed at the hatch, making us lose valuable time. The beamline team had no permission to do it themselves. We had to repeat safety test on paper after arrival, despite already doing it online. FemtoMAX team, technical support and LINAC control room staff were very friendly and helpful, fixing our problems ASAP. Despite some time lost, the feasibility test was successful and even some scientific data were collected! --- Access: My access card stopped working on the last night and the first Saturday I could not access the sample preparation lab. Support staff could help me both times. The paper version of safety training felt unnecessary after the online version. Data processing computer had Windows with an outdated browser, could have been better with a Linux station. KITS could only fix a few problems encountered during the visit. There are fluctuations in the beam intensity and the 2 Hz repetition rate severely limits the full potential of the beamline. My scores reflect that of a beamline in standard user operation and the attainable full potential of the beamline. For a beamline that is still commissioning mode I was astonished by the capabilities that exceeds beamlines like ID09 of the ESRF for scattering experiments. The MX X-ray diffraction data is comparable to a dedicated MX station such as BioMAX and possibly exceeds the best MX data available from XFELs. It was difficult to determine the exact energy of the beam and I believe that workign with higher photon energies are not established yet. The 2 Hz operation is a severe limitation of the beamline increasing a data collection to 20 hours rather than less than 1 hour at 100 Hz. Sample stage was higher than convenient, icing is a problem with the cryostream and long data collections. It would have been an advantage to be able to position the detector closer to the sample. Positioning of the beam on the sample can be improved by better placed cameras and marking the fluorescent area of X-ray sensitive paper. The motors failed at inconvenient times with time out error (sardana bug?). Synchronization of data collection and shutter opening and closing would be more convenient and save sensitive sample at future 100 Hz operation. The pump laser was prone to drift in timing and losing synchronization, again a severe problem for long data collections caused by the limitations of 2 Hz operation. Stopping repeated measurement in scans when X-ray is unavailable can be improved. Some images did not undergo tot conversion (Dectris software or KITS problem). Our data processing was performed almost entirely in the user space (installed and licensed by the user), the computational resource at the cluster was not overutilized, more memory would be advantage. The terminal could have been more useful as a Linux station. Currently there is very limited online information about the beamline operation online or written, but the beamline is undergoing rapid development, therefore it is understandable. The instruction given by the beamline staff were clear and easy to follow. In short, the staff is extremely competent to perform technically very challenging experiments such as femtosecond pump-probe experiments and go very much beyond what can be reasonably expected from collaborators and not to mention user support. Structural support from the MAX IV management is needed to provide compensation to the staff for working inconvenient times.
2021	There is a wish that the machine group would announce that they would like to work on accelerator well in advance - not calling to the beamline and 15 minutes later the beam was taken

	away. Some experiments need more time and their interruption would mean for users starting over. This would be great help for users in planning their research in most efficient way. We succeeded with everything nearly as planned. The beamline operation was smooth and reliable. We are grateful for the beamline staff for their help and care. With their professional help we managed to work efficiently and reached the goals. Their contribution was especially important because we brought a new experimental setup with us and this was implemented for the first time. Thank You very much! --- about beamline stability: FemtoMAX is absolutely impressive in terms of stability when it works properly. One possible improvement would be to solve the issue of temporal desynchronization between the various parts of the experiment. This would increase a lot the real time dedicated to measurement. --- Beam size too large at the time. THz set-up and alignment was an heroic effort that led to great results. Make beamline control system and software more user friendly.
2022	Main problem is with IT infrastructure: No compression in beamline h5 files making data files absurdly large, straining bandwidth everywhere. Access to the HPC cluster is not straightforward, ssh X tunneling makes data processing frustratingly slow due to slow graphical update. Old linux kernels on the beamline make backup difficult, modern compressing filesystems not supported. No progress on these issues since last year. Unfortunately, the high speed oscilloscope broke down which limited to the maximum achievable time resolution. The geometry of the endstation geometry was much better this time and we could process the data to acceptable quality to atomic resultion. We still have to find more accurate beam energy and detector distance. It is a challenging task a priori and there are only a few things one can do to improve the beamline to make indexing and integration easier. Very impressive improvement on the diffraction sample environment. With the optimization of the environment and improvement in stability the experiment reached the target resolution, further major improvement is not necessary in the foreseable future. A translation stage for the detector may be considered, but only if it does not compromise the stability and definition of the experimental geometry. Pump-probe timing and pumping geometry has been substantially developed since the commissioning experiment. There is still further potential for improvement and we recommend the beamline to invest primarily in this direction. Very successful experiment 12 lysozyme crystals were analysed mostly full rotation. Signal to noise to 1.2 Å resolution is already acceptable (>2) with more accurate description of the geometry this will be further improved. Congratulation for the beamline staff for the impressive improvement over one year!
2023	The experiment was not as successful as we expected probably because of the complexity of the experimental setup. In particular, because of the difficulties in the overlap between the reduced lateral dimensions of the laser and XRD footprint (pump-probe experiments). ---

	I would recommend to have a block access to the FemtoMAX. Our scintillator research of ultrafast processes uses the same time-resolved luminescecnce spectroscopy method, thus to describe and rewrite in each beamtime call is not a big problem, but does not bring any additional value . Therefore, having a valid proposal for longer period (a year or two) would be reasonable because we are looking maybe one or two experimental sessions during this longer period. It depends how much new materials will be proposed by us and by the CCC collaboration partners (scintillator research community) at CERN . --- FemtoMAX laser was not running well. Low power, poor spatial mode. --- The files from the detector were too big and this caused some of the scans not to be saved properly, which make my data a little bit more difficult to analyze. The problem remained unsolved. Amazing facility staff. They were very helpful and they were very easy to reach when a problem occur. They were always willing to help. --- IT usage was not so smooth, though the IT support person was very kind and supportive. There was beam loss at times and flux was less than expected.

12 Appendix C

Factors impacting S/N

There are two fundamental factors impacting the S/N ratio. The *first* factor is the total amount of photons scattered from the sample, which in the case of a given sample is proportional to the amount of incident photons. The *second* factor is the pulse-to-pulse intensity fluctuations and the ability to compensate for these fluctuations. In practice, Poisson statistics means that the S/N ratio is proportional to the square root of the number of detected photons for the first factor and proportional to the square root of the number of shots for the second factor.

Additional factors that could impact S/N

The main experimental detectors (Balor, Pilatus) can be used to detect photons with the right energy range to discriminate against cosmic rays, soft X-ray leakage etc provided that the high efficiency monochromators (DCM and multilayers) are used. The present intensity monitor (relevant for the second factor) has electronic noise which has not been possible to eliminate. The use of large zero dimensional detectors such as APDs and diodes will generate electronic noise and does not provide the capability for discrimination against cosmic rays, gamma ray events generated by the LINAC unless the count rate drops below 1/3 of the repetition rate (photon counting mode with pile-up compensation). Long term intensity drifts and are non-Poissonian deviations, but these can in general be compensated for by long term averaging (provided that some kind of intensity monitor is used).

Impact of sample damage due to X-rays.

This is relevant for all scattering (or spectroscopy) on solids, nanostructures and films. Liquids and samples in solutions can in generally be replenished between shots at 100 Hz so that each X-ray pulse hits new sample.

InSb nanowires damage at around 10^8 incident photons on a beam size similar to that of FemtoMAX. The same is true for many films and solids. This can be understood as each X-ray photon generate about 1000 carriers. For a beam size of 100 micrometres, and a typical absorption depth of 100 nm, 10^{20} carriers per cm^3 . If the flux and carrier density is increased by an order of magnitude several per cent of all the bonding electrons have been excited which generates a coulomb explosion that permanently destroys the sample.

At an FEL there is either the option to attenuate the X-ray beam to 10^8 photons per pulse or to move to a fresh spot for each sample data point which lowers the effective repetition rate to a few Hz and consumes sample at a high rate.

Data quality vs S/N

There is range of solids and films where 0.1% or more of the incident photons are scattered providing the signal. In experiments for solids and films we typically observe several percent changes due to the laser interaction. We need 0.5 – 1 % noise level to reach a S/N of 5-10 which is needed for publication quality data.

FemtoMAX provide 1e6 photons per pulse. As the scattering was assumed to be 0.1% ,1000 photons detected per pulse. At 100 Hz we acquire 100 pulses in 1s and in a temporal scan with 100 points it takes 2 minutes to acquire a scan with 100000 detected photons giving a contribution to the noise which is about 0.3%.

The second contribution is from pulse to pulse fluctuations which is about 5% at the SPF. For 100 pulses the contribution is about 0.5 %. Using improved intensity monitors it may be possible to reduce to the 1% for a single shot as described for the FEL below.

Comparing to theoretical numbers for Swiss-FEL (Bernina) with 10^{12} incident photons and 10^9 detected photons we only need to consider pulse-to-pulse fluctuations which can be compensated[8] to 1 %, but the temporal structure, and the frequency content also vary using the SASE where at 100 Hz, the contribution is about $\frac{1\%}{\sqrt{100}} = 0.1\%$. A realistic comparison with Bernina for a solid involves 10^8 incident photons and 10^5 detected photons which gives photon statistics on the order of 0.3% in a single shot. This means that the main issue at an FEL is still the pulse-to-pulse fluctuations. At 10 Hz the corresponding numbers for FemtoMAX are 1.5% noise due to fluctuations and 1% due to photon statistics which is more than 10 times worse than a FEL.

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[8] *J. Synchrotron Rad. (2019). 26, 1092-1100*