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Review

Status of the crystallography beamlines at the MAX IV Laboratory*

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Abstract. The MAX IV Laboratory in Lund is currently operating two storage rings, the 1.5 GeV MAX II and the 700 MeV MAX III, as well as constructing the new facility MAX IV, which will house a 1.5 GeV and a 3 GeV ring. At the MAX II synchrotron there are three hard X-ray beamlines at which crystallography can be performed: I711, I811 and I911. Beamline I711 is mainly used for powder diffraction. I811 is an EXAFS station at which surface XRD can also be carried out. I911 is a beamline with five experimental stations on a single superconducting wiggler source, of which two are currently used for macromolecular crystallography, namely the monochromatic station I911-2 and the tuneable station I911-3, which is equipped with a state-of-the-art goniometer and robotic sample changer. We will give an overview of the capabilities of these beamlines, focusing particularly on the macromolecular crystallography beamline I911 and some recent scientific highlights produced there. We will also give a brief overview of new beamlines for crystallography that are under construction or planned for the MAX IV facility.

1 Introduction

The MAX IV Laboratory in Lund, formerly known simply as MAX-lab, was inaugurated in 1987. It is a Swedish national laboratory hosted by Lund University and financed principally by the Swedish Research Council (VR), although users come from all parts of the world. The MAX IV Laboratory initially consisted of only one storage ring, MAX I (circumference 32 m, energy 550 MeV) which was further augmented with two rings, MAX II (1.5 GeV, 96 m circumference) in 1997 and MAX III (700 MeV, 36 m circumference) in 2007. The MAX III ring is, among other things, a test bed for the novel multi-bend achromat magnet technology to be employed at the new MAX IV synchrotron from 2016 onwards. At the peak of its usage the MAX I ring had seven experimental stations and greatly stimulated Swedish synchrotron research, but it is now used only to a limited extent for nuclear physics experiments. Access to beamlines at the MAX IV Laboratory is open to all researchers via an internationally peer-reviewed application system, through the laboratory's Digital User Office (DUO). Beam time is allocated according to three models: a) regular proposals for specific projects, valid for half a year to one year in the operational period of late August to late June; b) block allocations for combined projects, sometimes involving several user groups, valid for two years; c) a rapid access scheme, for the macromolecular crystallography MX beamlines only, within which applications can be submitted at any time, typically giving access within a few weeks for a one-off experiment. The rapid access option is particularly useful for new users of the MAX II MX beamlines. 5% of the beamtime available at I911-2 and I911-3 is reserved for fast access projects. In 2013, 43% of the laboratory's users were from Sweden, 19% from Denmark and 38% from other countries. The facility had about 900 individual users, of whom around 500 described themselves as physicists, about 200 as chemists and 200 as life scientists. In 2014, 108 days of beam time were made available to

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users at I711, but this was used only for powder diffraction. At I811, 141 user days were allocated in total, of which 27 days were for crystallography. At I911, the two stations I911-2 and I911-3 allocated 370 days to users in 2014, of which all but a few days were dedicated to macromolecular crystallography. See below for details of the beamlines.

The MAX IV Laboratory as an organization currently also comprises a further two storage rings under construction at the new MAX IV site in the north-east of Lund: a 1.5 GeV ring (96 m circumference) and a 3 GeV ring (528 m). The 3 GeV ring will be based on novel multi-bend achromat technology [1] that will increase the intensity by orders of magnitude with respect to the current MAX II ring, as well as offering world-leading emittance (the current target is 0.25 nmrad). Beamlines at MAX II will remain in operation until mid-December 2015, at which time the present facility will be closed down in order to concentrate resources on commissioning of MAX IV, whose first beamlines are planned to begin operation in mid-2016. Among these, the BioMAX beamline for macromolecular crystallography, whose design has been described in detail elsewhere [2]. Further beamlines where crystallography experiments can be performed are planned at MAX IV and will be described briefly.

2 Beamlines usable for crystallography

2.1 Overview

2.1.1 Beamlines

The third-generation MAX II storage ring, with an energy of 1.5 GeV and a circumference of 90 m, became operational in 1997 [3] and currently has a total of 10 operational beamlines. Among these, there are three hard X-ray beamlines at which crystallography experiments can be performed: I711, I811 and I911. Beamline I711 is mainly used for powder diffraction experiments, while I811 is used for X-ray absorption and surface diffraction experiments. Two of the five experimental stations at beamline I911 are equipped for macromolecular crystallography, while two of the other monochromatic stations, I911-1 and I911-4, are used for X-ray education experiments and small angle X-ray scattering [4], respectively, and the fifth station, I911-5, has been retired. The crystallography beamlines have been highly productive and have attracted users from all around the world. They are particularly important research tools for the Scandinavian research communities.

2.1.2 Ancillary facilities

The present MAX-lab is equipped with an efficient facility for low-volume, high-throughput crystallization of proteins and other biological macromolecules using minimal sample volumes (`http://www.maxlab.lu.se/crystal`). The facility has been in operation since 2006 and is open to all academic users. The facility is equipped with advanced liquid handling robotics for generation of crystallization screens, dispensing of crystallization drops down to 50 nl in size, as well as automated storage and visualization of crystallization experiments using both visible and UV light, the results of which are stored in an online database viewable through any web browser. The facility also includes equipment for biophysical characterization of proteins using differential scanning fluorimetry and dynamic light scattering. The crystallization facility is open for all local and national users in Sweden, as well as international users upon request. Finally there is a general laboratory for all users of the hard X-ray beamlines I711, I811 and I911 including an anaerobic box, ultra-pure water, centrifuge, furnace, fume hoods, refrigerators, freezers and general laboratory utensils.

2.2 Brief description of each beamline

The key parameters of each crystallography beamline are listed in table 1.

Beamline I711 is used for single crystal and powder diffraction. I711 was originally also used for macromolecular crystallography [5], but this kind of work has since 2004 largely been carried out at I911 (see below). I711 is to a large extent a copy of station 9.6 at the Daresbury synchrotron in the UK, and is built around a 13-period, 1.8 T, multipole-wiggler designed to operate in the 0.98–1.4 Å (12.6–8.8 keV) region. The beam is focused in the vertical direction by a 1.2 m long Pt-coated glass mirror 10 m from the source. This is followed by an asymmetrically cut Si(111) single-crystal monochromator, which provides a photon flux of around 10^{11} photons/s at a fixed wavelength of 1 Å, in a beam size of approximately $0.3 \times 0.3\,\mathrm{mm}^2$. The monochromator is bent to focus the beam in the horizontal direction. The monochromator is followed by a 2Θ arm, 5 m long, with an angular travel range between 2° and 40°. However the station is now used at fixed wavelength (1.000 Å), so the 2Θ angle is no longer varied.

The experimental setup at I711 is a Newport 4-circle diffractometer with kappa geometry, located 5.5 m downstream of the monochromator. This diffractometer is capable of doing both single crystal and powder diffraction using a large-area Titan CCD detector from Agilent, with a 165 mm radius. The detector arm is currently being fitted with a Pilatus

Table 1. Key parameters of current crystallography beamlines at the MAX IV Laboratory.

	I711	I811	I911-2	I911-3
Source	Multi-pole wiggler, period = 174 mm, 27 poles, $B_{max} = 1.8$ T	Superconducting multi-pole wiggler, period = 61 mm, 49 poles, $B_{max} = 3.5$ T		
Monochromator	bent Si(111) crystal, horizontally focusing	double-crystal pairs that can be altered between Si(111) and Si(311). Second crystal bendable for horizontal focusing.	bent Si (111) crystal, horizontally focusing	double-crystal Si(111) monochromator. The first crystal is water-cooled.
Mirror (first)	vertically focusing cylindrical mirror.	water-cooled vertically bendable cylindrical mirror ($R = 2000$–6700 m)	multilayer mirror, curved to focus in the vertical ($R = 400$ m)	water-cooled vertically collimating cylindrical mirror ($R = 7300$ m).
Mirror (second)	–	vertically bendable cylindrical mirror ($R = 800$–5300 m).	–	toroidal mirror for horizontal and vertical focusing ($R = 3300$ m, $R = 27$ mm).
Wavelength (range, Å)	1.00	0.6–5.0	1.04	0.75–2.0
Wavelength resolution	$E/\mathrm{d}E \sim 10^3$	$E/\mathrm{d}E \sim 10^4$	$E/\mathrm{d}E \sim 10^3$	$E/\mathrm{d}E \sim 10^4$
Photon flux on sample	1×10^{11} ph/s in 0.3×0.3 mm^2	10^{11}–10^{12} photons/sec @ 9 keV.	1×10^{11} ph/s in 0.3×0.3 mm^2 (measured)	3×10^{11} ph/s in 0.3×0.3 mm^2 at 1 Å (measured)
Spot size on sample	Focused spot size 1.0×0.5 mm^2 (h/v), can be collimated further to 0.8×0.8, 0.5×0.5 or 0.3×0.3 mm^2	0.5×0.5 mm^2	0.3×0.3 mm^2 (measured); can be collimated to 0.2×0.2 mm^2 using slits	0.3×0.2 mm^2 (h/v) FWHM (measured). Can be collimated to 30, 50, 70, 100 μm using apertures

detector and a Ge(111) multi-analyzer crystal system for high-resolution powder diffraction. The sample to detector distance can be varied from 70–375 mm. The CrysAlis software package is available for analysis of single-crystal data, and powder data are processed using Fit2D. The beamline is equipped with a Cryojet from Oxford Instruments producing a cold jet of nitrogen gas in the temperature range 80–490 K ± 0.1 K. Such devices are most commonly used for preventing radiation damage on protein crystals but the Cryojet has also been used successfully for other applications such as thermal expansion studies.

Beamline I811 is used for X-ray absorption spectroscopy (XAS), single-crystal X-ray diffraction and surface X-ray diffraction (SXRD) research in the photon energy range 2.4–21 keV (0.6–5 Å) [6]. It is based on a 3.5 T, 49-pole superconducting multi-pole wiggler [7] that provides up to 10^{15} photons/s into the beamline. The wiggler photon beam is first vertically collimated by a cylindrical Rh-coated silicon X-ray mirror, then passed through a double-crystal monochromator, and finally refocused on the sample by a second Rh-coated mirror. The monochromator has two exchangeable pairs of Si(111) and Si(311) crystals in order to cover a large energy range. The first monochromator crystal is water cooled to accommodate the high power of the wiggler beam, while the second crystal is sagittally bent for horizontal focusing on the sample. The beam-spot size on the sample is approximately 1×1 mm^2 in focused mode, and a flux of 10^{11} photons/s (in the range 5–10 keV) can be expected on the sample. At 9 keV the beam energy resolution on the sample is 2 eV ($\Delta E/E = 2.2 \times 10^{-4}$).

Experimental stations for XAS and SXRD are in user operation. The XAS station is equipped with ion chambers for measuring the sample absorption in transmission, as well as detectors for collecting the fluorescence yield on diluted samples. The beamline detection limit, *e.g.*, for iron is approximately 10 mg/kg (10 ppm) metal concentration. Furnaces and sample cells are available for *in situ* XAS experiments, as well as liquid helium cryostats for experiments on sensitive metal-containing biological samples. The SXRD station is based on a Newport N6050-G+K multipurpose

diffractometer that has two sample rotations and three detector rotations. To be able to cover as large a part of reciprocal space as possible for surface and thin-film samples, detector rotations are decoupled from the sample rotations. Grazing-incidence and specular X-ray diffraction experiments are possible, and X-ray reflectivity measurements can also be performed. A hybrid-pixel area detector (Dectris, Pilatus 100 k) located at about 1.2 m from the sample is used for data collection. Vacuum chambers and protective gas chambers with X-ray transparent windows are available for air sensitive samples.

Beamline I911 (fig. 1) has a unique design [8] in which five experimental stations are built around the relatively broad fan of radiation produced by a 47-pole liquid-He cooled superconducting wiggler designed and built at MAX-lab and essentially identical in design to the one used at I811 [7]. When operated at 2.8 T the I911 wiggler has a critical energy of 4.2 keV and a peak brilliance of 2×10^{15} ph/s/0.1%bw/mrad^2/mm^2. The calculated flux through the primary slits is 1.6×10^{13} ph/s/0.1%bw. The four monochromatic side stations are built around the same optics design [8], while the central station is tuneable. Of these five stations, two are currently used for macromolecular crystallography, namely the monochromatic station I911-2 and the tuneable station I911-3. A fixed aperture in the front-end permits 2 mrad of the wiggler beam fan to pass through. Of this beam fan, the central 0.5 mrad is used for I911-3, while the rest is used for the side stations. The optics for each side station consist of a monochromator crystal followed by a curved multi-layer mirror. For the two side stations closer to the source (I911-1 and -5) the monochromator crystals are flat 111 diamonds in Laue geometry. For the two side stations further from the source (I911-2 and -4), monochromation is achieved by bent Si(111) crystals in Bragg geometry [8]. All the optical elements for the four side stations are on a single table (JJ X-Ray, Kgs. Lyngby, Denmark).

2.3 Future plans

Construction is underway for a next-generation light source in Lund, MAX IV, which will consist of two storage rings fed by a 300 m long linear accelerator [9] (fig. 2 and table 2). Due to the innovative multi-bend achromat magnet technology used [1], the larger of the two rings, with a circumference of 528 m and an energy of 3 GeV, will have the lowest emittance of any synchrotron in the world (the targeted value is 0.25 nmrad), which will represent a quantum leap in performance relative to the current facility and will enable science that is unachievable today. The smaller ring will have a circumference identical to that of MAX II, *i.e.* 96 m, an energy of 1.5 GeV and will be oriented towards soft X-ray experiments.

One macromolecular crystallography beamline is currently financed for MAX IV and a second one is planned for the near future but not yet financed. The first beamline, BioMAX [2], will be a multipurpose high-throughput data collection facility for macromolecular crystallography. The uniquely low emittance properties of MAX IV are being exploited in the design of BioMAX to offer variable beam size at the sample (20–100 μm) with very low divergence and high flux ($> 10^{13}$ photons/s). The BioMAX insertion device will be a 2 m long in-vacuum undulator with an 18 mm period and 111 full periods. The minimum gap will be 4.2 mm, giving a K-value of 1.9. BioMAX will be rapidly tuneable in the energy range 5–25 keV and will be equipped with a state-of-the-art sample changer, a low X-ray noise sample environment and a large-area pixel detector that, together with advanced software solutions, will give high data quality and high throughput, including fast feedback from data analysis. BioMAX will be complemented in the near future by MicroMAX, a state-of-the-art microfocus undulator beamline aimed at tackling the most challenging problems in modern structural biology, involving very small sample sizes, large protein complexes, very large unit cells, room temperature data collection and the handling of large partial datasets collected from many samples. The aim of MicroMAX is to deliver a beam in which 10^{13} photons/s can be delivered in a beam as small as $1 \times 1\,\mu$m^2. Given that this represents around a 100-fold gain over BioMAX, particular emphasis will be given to alternative methods of sample presentation, as the flux will be such that multiple crystals will need to be used to obtain complete datasets for many systems. A pink beam option is also being considered, which could potentially further increase the flux up to 10^{15} photons/s.

Four further beamlines are under construction or planned at MAX IV at which crystallography experiments can be performed (fig. 2). NanoMAX, currently under construction, is an X-ray undulator beamline for micro- and nanobeams designed to take full advantage of the exceptionally low emittance and coherence properties of MAX IV. NanoMAX will enable imaging applications, diffraction, scattering, fluorescence and other methods at spatial resolutions down to 10 nm while at the same time allowing larger beam sizes up to around 1 μm, providing the possibility of matching spot size and divergence to varying experimental requirements [10]. This long beamline (100 m) will have two experimental stations, using Fresnel zone plates for focusing of the beam to $\sim$ 10 nm and Kirkpatrick-Baez mirror optics for focusing to $\sim$ 100 nm, respectively. The main experimental techniques will be scanning transmission X-ray microscopy, X-ray diffraction, X-ray fluorescence and coherent diffractive imaging. As at BioMAX, user operations at NanoMAX are planned to commence in late 2016. The FemtoMAX beamline at the MAX IV Short Pulse Facility is designed for ultrafast X-ray experiments on the femtosecond time scale. Short bursts of X-rays will be generated by sending ultrashort pulses of electrons from the MAX IV 3 GeV linear accelerator through an undulator or a wiggler. The highly intense X-ray pulses generated at FemtoMAX will have a duration of 100 fs in a beam of 100 μm full width half

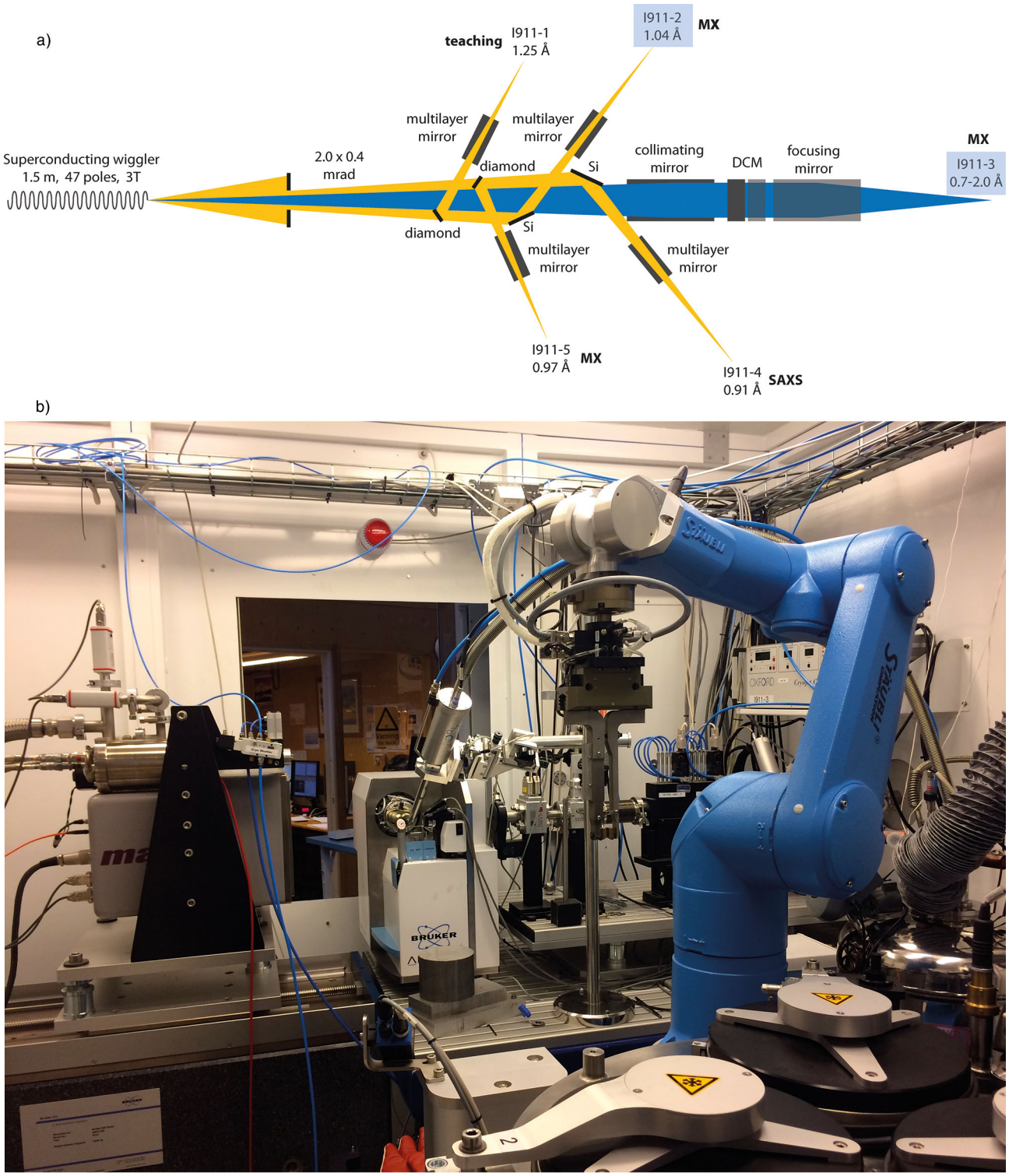

Fig. 1. a) Schematic overview of the I911 beamline at the MAX II storage ring. b) The interior of the I911-3 experimental hutch, showing the CATS sample changer in the foreground and the MD2 diffractometer and marMosaic 225 CCD detector in the background. Behind these can be seen the window through which users can mount samples manually.

maximum. The beamline will be tuneable in the energy range 2–20 keV. A femtosecond laser system will provide optical pulses for exciting the samples and will be synchronized to the incoming X-ray pulses. Three experimental stations are planned at FemtoMAX and among the scientific applications possible will be time-resolved X-ray diffraction experiments from single crystals and other samples.

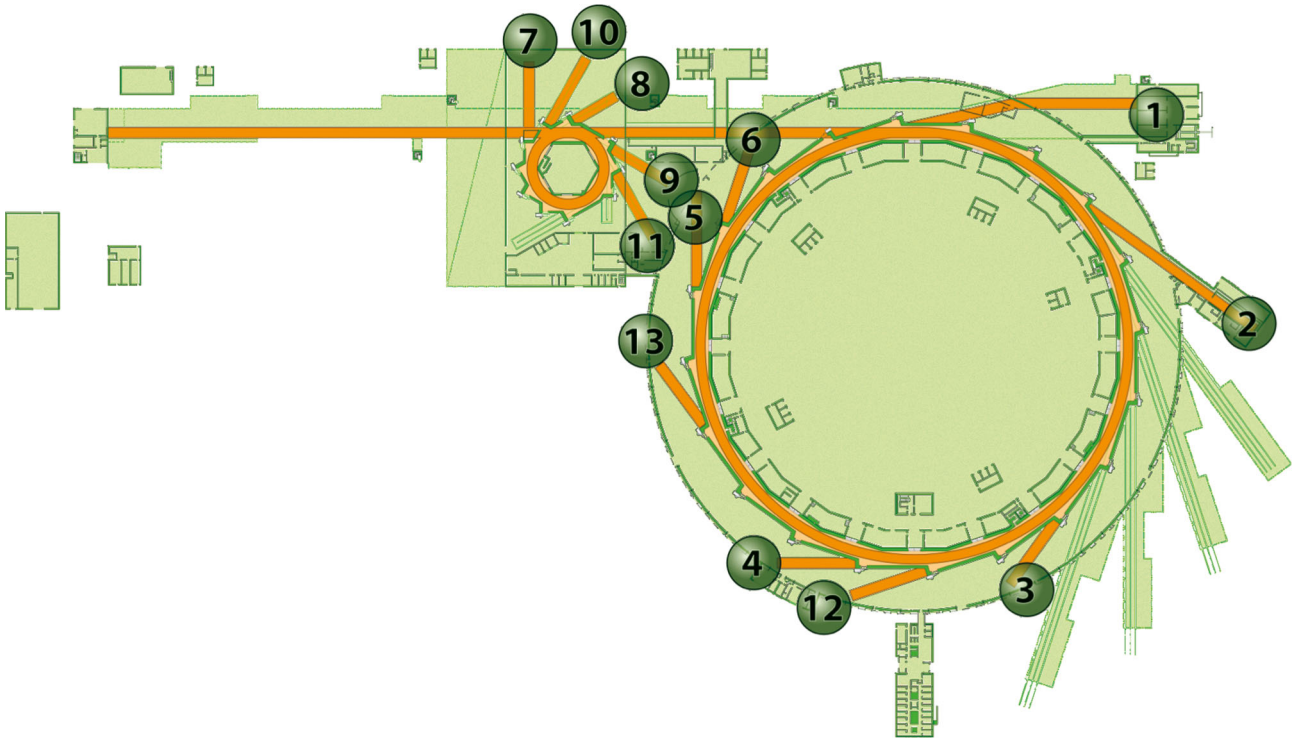

Fig. 2. Schematic overview of the MAX IV facility ring, with currently funded beamlines indicated. Of these the most relevant for crystallography are BioMAX, NanoMAX and FemtoMAX. For a short description of all beamlines, see table 2 (note that the DanMAX beamline is not included in table 2 as its position on the 3 GeV ring has not yet been decided). The 1.5 GeV ring is at the top left and the 3 GeV ring on the right. Figure courtesy of Johnny Kvistholm, MAX IV Laboratory.

Table 2. Description of currently funded beamlines at MAX IV.

Number in fig. 2	Name	Method
1	FemtoMAX	Studies of ultra-fast processes in materials.
2	NanoMAX	Imaging, spectroscopy and scattering techniques with nanometre resolution.
3	BALDER	Hard X-ray absorption spectroscopy with emphasis on in situ and time-resolved studies.
4	BioMAX	Macromolecular crystallography with a high degree of automation and remote access.
5	VERITAS	RIXS combining unique resolving power with high spatial resolution.
6	HIPPIE	High pressure photoelectron spectroscopy.
7	ARPES	Angle-resolved photoelectron spectroscopy for detailed studies of electronic structure.
8	FinEstBeaMS	Estonian-Finnish beamline for materials science.
9	SPECIES	VUV high-pressure photoelectron spectroscopy and RIXS.
10	FlexPES	Photoelectron spectroscopy and NEXAFS.
11	MAXPEEM	Photoemission electron microscopy.
12	CoSAXS	Small-angle X-ray scattering.
13	SoftiMAX	STXM, coherent soft X-ray scattering.
14[(a)]	DanMAX	Imaging and powder diffraction.

[(a)] DanMAX is not shown in fig. 2 as its position on the 3 GeV ring has not yet been decided.

The planned beamline DiffMAX will be dedicated to a range of diffraction-related experiments including powder, surface and grazing incidence diffraction on a wide range of samples. DiffMAX will have a wide energy range, from 5–30 keV, providing both a tuneable monochromatic beam and the possibility to use the full undulator peak to achieve a broad bandwidth beam to enable ultra-fast data collection or the exploitation of very weak signals. Both NanoMAX and DiffMAX will be engineered to accommodate a variety of experimental setups; however due to the precise engineering required for sample orientation at NanoMAX, it will be used for smaller samples while DiffMAX will be used for those of a more standard size, as a very large area will be made available for the implementation of bulky sample environments.

Finally the DanMAX beamline, funded by a consortium of Danish universities and regions and built and operated in close collaboration between MAX IV Laboratory and the consortium, will be equipped with two endstations, of which one can be used for powder diffraction experiments in the energy range 5-35 keV. A particular focus area will be "energy materials" and collaboration with industry.

3 Example of a crystallography beamline: I911

As noted above, there are currently two active user stations for macromolecular crystallography (MX) at beamline I911. The monochromatic station I911-2 has a fixed wavelength of around 1.04 Å and is equipped with a mardtb goniostat on which is mounted a 165 mm marccd detector (Rayonix, Evanston, IL, USA). The goniostat and detector are controlled by the marccd software and the X-ray optics by spec (Certified Scientific Software, Cambridge, MA, USA). The beam can be shaped to 0.2×0.2 mm using the built-in slits of the mardtb. I911-2 is suitable for routine data collection on fairly large crystals, at least 0.1 mm in the largest dimension. The I911-2 experimental area is a very compact mini-hutch with dimensions 1.25 (w) × 3.0 (l) × 2.5 (h) m, with a sliding window for access to the goniostat.

I911-3 is an energy-tunable, automated beamline, built for macromolecular crystallography of small crystals [2]. It is tunable in the range 0.7–2.0 Å, with a flux of around 4×10^{11} ph/s at 1 Å in a beam size of 0.3×0.2 mm. The beamline first became available for users in 2005 and was extensively refurbished in 2010 to improve beam quality and sample handling, including a new goniostat, support tables, sample changer, fluorescence detector and improvement of most of the beam conditioning equipment. Beamline I911-3 can be tuned to wavelengths in the range 0.75–2.0 Å, though it is usually operated in the range 0.9–1.8 Å. The optics consist of a collimating mirror, a double crystal monochromator and a focusing mirror (all by Oxford Danfysik, Oxford, UK, now FMB Oxford, with mirrors and mirror benders from SESO, Aix-en-Provence, France). Full details of the X-ray optics at I911-3 have been published elsewhere [2,4].

Though redesigned and entirely rebuilt in 2010, the experimental hutch at I911-3 is still relatively small compared to those common at other synchrotrons. Because of the compact design, with the sample environment placed just inside a sliding, rapidly interlockable window, users are able to mount crystals through the open window, with fast access from the nearby sample handling table that houses a high-magnification microscope, without having to open a heavy door. However an additional door at the rear of the experimental hutch allows users to enter the hutch and access the sample changer dewar in order to fill it with their samples.

The experimental setup has a MD2 micro-diffractometer [11] with a mini-kappa goniometer MK3 (both from Arinax, Moirans, France). The MD2 has an extended horizontal translation range to allow data collection from crystallization plates. A 5-hole beam defining aperture (BDA) with cleaning capillary and beamstop is implemented in the MD2, with the result that a circular X-ray beam can be produced with diameters of 30, 50, 75, 120 or 150 μm. This ensures a low X-ray background and makes it possible to work with relatively small crystals. The detector is a MarMosaic 225 mm area detector (Rayonix, Evanston, IL, USA) that can be positioned between 55 and 770 mm from the sample. Crystals can be mounted either manually or by using the CATS sample changer [12] (Irelec, Grenoble, France), which has a storage dewar with a capacity of 90 samples. The CATS robot is configured to use exclusively EMBL/ESRF pucks with SPINE standard pins and vials [13], and can change a sample in less than one minute. A 10 mm^2 Bruker XFlash fluorescence detector (Bruker-AXS, Berlin, Germany) can be used either to collect the accurate X-ray fluorescence edge scans necessary to determine the optimal wavelengths for MAD or SAD data collection, or for element analysis using X-ray fluorescence. Almost all data collection is carried out at around 100 K and the samples are cooled by an Oxford Instruments CryoJet N_2 gas cooler (Oxford Instruments, Abingdon, UK). If necessary, the cooler can be operated at any temperature between 100–300 K.

The beamline hardware is controlled by the software spec through a number of different protocols. Communication with the MD2 microdiffractometer uses the MD2 Tango device server. The marmosaic detector is controlled by spec via the marccd program, which is also used to visualize the diffraction images stored on an internal disk of the detector computer. The data frames are immediately synchronized with an 8 TB storage system that interfaces with a rack-mounted 64-bit 8-processor Linux cluster for data processing.

Users at station I911-3 interface with their experiments through the software MxCuBE [14], which allows programming of various data collection strategies as well as collection of fluorescence and X-ray emission spectra. Recently control of the CATS sample changer was integrated into MxCuBE, as well as automatic three-click crystal centering. Both of these were previously managed using separate GUIs, thus integration into MxCuBE enables users to control their experiment from a single interface. Using MxCuBE a crystal can be centered at several different points and the collection of test images or datasets at each of these points can be queued, *e.g.*, for rapid characterization of the crystal quality at different points or avoidance of radiation damage by collecting each wavelength of a MAD dataset from a different crystal volume. Data collection strategies can be automatically generated using BEST [15], although work is still ongoing to implement the optimal beamline parameters, *e.g.*, a correct estimate of flux in order to model potential radiation damage using RADDOSE [16]. Work is ongoing to implement data processing pipelines such as EDNA [17] and XIA2 [18]. The data collection interface is now also integrated with the iSPyB database [19] for sample tracking,

which is increasingly popular with users due to the trend towards increasing numbers of samples per experiment. Experiment control through a single interface and integration with iSpyB are all major steps towards implementation of the remote operation mode that we predict will become the norm at the future BioMAX beamline. The described developments also help to ensure that macromolecular crystallography users have a reasonably homogeneous experience when using beamlines at different European synchrotrons.

Data processing is done on the aforementioned 8-core Linux cluster. The full range of standard macromolecular crystallography software is available, for example MOSFLM/iMOSFLM [20], XDS [21], XPREP (Bruker, Madison, WI, USA), HKL2MAP [22], the CCP4 [23], SHELX [24] and Phenix [25] suites are available for data processing and subsequent structure solution.

4 Examples of science at crystallography beamlines

Stations I911-2 and I911-3 are used principally for macromolecular crystallography, and researchers have applied the method to a wide range of structural biology problems, from fundamental structural studies of the function of soluble and membrane proteins to drug design against a variety of targets and the study of artificial proteins designed to investigate the mechanisms of protein folding. Since the beamline opened in 2005, data collected at I911 have resulted in 438 depositions in the Protein Data Bank [26], according to the BIOSYNC database (`http:/biosync.sbkb.org`) and 315 publications have been reported. Among many other projects, data from I911 have been used consistently in on-going studies of the enzyme acetylcholinesterase (AChE) by researchers from the Swedish Defence Research Agency and their collaborators. AChE is an essential enzyme that terminates cholinergic transmission by hydrolysing the neurotransmitter acetylcholine. Non-covalent AChE inhibitors have applications in treatment of Huntington's and Alzheimer's diseases. In contrast, irreversible AChE inhibitors include organophosphorus-based nerve agents that abolish enzyme activity by covalently binding to the active site. Molecules can be designed that reactivate AChE by binding to the active site and cleaving the covalent bond between the nerve agent and the enzyme. For both of these reasons, study of the binding of small molecules to the AChE active site is of great importance, and data from I911 were used in several recent studies on AChE inhibitors involving varying combinations of high-throughput screening, crystallography, spectroscopy, molecular modelling and thermodynamic profiling [27–29].

The list of work to which I911 has contributed also includes several studies for which the dataset used in the publication and in the PDB entry was not collected at I911 but where critical screening or collection of preliminary datasets was carried out there and for which the beamline is explicitly acknowledged. Among such recent publications is a drug design study against the human protein MTH1 [30]. MTH1 is an enzyme that degrades nucleotides that have become oxidized through the action of reactive oxygen species to prevent their incorporation into DNA, which would result in erroneous base pairing, mutations and cell death. MTH1 is not necessary for normal cells but is important for the survival of cancer cells. MTH1 was validated as a cancer target using siRNA knockout assays. Screening of compound libraries followed by hit expansion led to potent inhibitors of MTH1 and co-crystal structures verified the mode of action by confirming their binding to MTH1. Important recent contributions to the membrane protein literature involving I911 include the structure of a membrane-bound Na^+-pumping pyrophosphatase [31] and several structures of Ca^{2+} and Zn^{2+} pumps from the P-type ATPase family [32,33]. The P-type ATPases constitute a large protein family that pump ions and lipids across cellular membranes. Such pumps, with different transport specificities, are essential for almost all life, among other things by converting metabolic energy into electrochemical gradients that can be exploited for cellular uptake processes, or by mediating cellular signalling. Structural studies have revealed the striking and precise conformational changes associated with transporting metal ions across biological membranes through a central high-affinity ion binding site in the central membrane-spanning segment of the protein. Screening of many hundreds of crystals using the sample changer robotics at I911-3 was critical to the success of the P-type ATPase projects.

The I711 beamline started as a versatile MX facility and was used to produce (then) state of the art protein crystallography data on medically important proteins [34,35]. Later it also proved very useful for the SAXS community, *e.g.* [36], paving the way for the MX and SAXS branches of I911. Nowadays, the beamline is mostly used for powder diffraction experiments. Various user communities come to the beamline to perform experiments in the domains of hydrogen fuel cells [37], lithium batteries [38,39], pharmaceuticals and high pressure [40].

About 90% of the research at beamline I811 is conducted using XAS methods. An example of the potential for life science research of combining XAS at beamline I811 with MX at I911 was recently published by Frankaer *et al.* [41]. They compared structure determinations of Ni and Cu T_6 bovine insulin derivatives by X-ray diffraction and XAS. In this study it was shown that XAS is a route to highly accurate determination of coordination and bond distances around metal centres in the insulin derivatives. I811 has also been used in environmental science. In research on natural waters and soils it is of great importance to understand the structures and speciation of different metal-containing complexes. Fundamental information on the structure and hydrogen bonding in hydrated selenite ($SeO_3{}^{2-}$)

and selenate (SeO_4^{2-}) ions was provided by Eklund and Persson (2014) [42], who quantified the coordination changes in selenite and selenate ion species in water solutions, and determined the hydrogen bond strength in the complexes. A recent representative example of SXRD work at I811 is provided by a study of the influence of uniaxial stress on the electrical conductivity of thin epitaxial lanthanum-strontium manganite films [43].

5 Conclusions

Beamlines where crystallography experiments can be performed have been in operation at the MAX IV Laboratory since 1997 and have made significant contributions to the scientific literature. The construction of the new MAX IV facility with planned inauguration in mid-2016 promises a huge leap in performance that will ensure that the MAX IV Laboratory continues to be a highly productive synchrotron for crystallographers in Scandinavia, Europe and the rest of the world.

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