BioMAX: The Future Macromolecular Crystallography Beamline at MAX IV

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Abstract. This paper describes the preliminary design of the BioMAX beamline at the 3 GeV ring of the MAX IV facility, focusing on the optics and x-ray beam performance. The MAX IV facility will include two storage rings with 1.5 GeV and 3.0 GeV electron energy and a linac serving both as injector for the two rings and feeding a short pulse facility. BioMAX is one of the first seven beamlines funded at the MAX IV facility. It is a multipurpose high-throughput beamline for macromolecular crystallography. The beamline aims to be robust and simple to operate with a beam benefiting from the properties of the MAX IV 3 GeV ring. However it does not aim at the smallest beam or crystal sizes since it is foreseen that it will be complemented with a microfocus beamline aiming at a beam size of 1 μm. The beamline experiment setup will be highly automated, both in terms of sample handling hardware and data analysis, including feedback to the data collection. The BioMAX beamline is planned to be in operation in 2016.

1. Introduction

The MAX IV facility is presently under construction in Lund, Sweden. It will consist of a linac and two storage rings with electron energies of 1.5 GeV and 3.0 GeV. The linac will serve as a full energy injector to the two rings that will operate in top-up mode, and also feed a short pulse facility and a possible future free electron laser. A first set of seven beamlines have been funded. The BioMAX beamline at the 3 GeV ring is presently being designed and the preliminary x-ray design is presented in this paper. The beamline is planned to be in operation in 2016.

BioMAX will be a multipurpose high-throughput beamline for X-ray diffraction data collection and phasing, dedicated to the needs of the macromolecular crystallography community. It will offer high-brilliance, tuneable (0.5–2.5 Å wavelength), monochromatic X-rays with state-of-the-art performance in terms of low beam divergence (<0.1 mrad), high X-ray flux (~10^13 photons/s) and variable beam size (20–100 μm), allowing work with both small crystals and large biomolecular complexes with concomitantly large unit cells. The design allows for a later upgrade with refocusing optics for additional demagnification and/or to increase the stability by using a pinhole at the secondary source.

This high-performance X-ray beam will be complemented by a state-of-the-art experimental setup, including rapid automated sample changing facilities, crystal alignment software, a large area detector with ultra-rapid readout and low noise, cryo-cooling, on-line X-ray fluorescence measurement, on-the-
fly data analysis and remote data collection. The beamline will also be equipped to allow *in situ* spectroscopic measurements on the crystals being used for X-ray data collection.

2. Beamline Design

The main optic elements will be a liquid-nitrogen cooled, channel-cut Si (111) monochromator followed by two mirrors in Kirkpatrick-Baez (KB) geometry focusing at the sample position. This design allows for future addition of a secondary source and refocusing optics. The optics layout is shown in figure 1 and presented in table 1.

2.1. Insertion Device

The insertion device will be an in-vacuum permanent magnet undulator with a magnetic period of about 18.5 mm, a minimum magnetic gap of 4.2 mm and a magnetic lattice length of about 1.5 m. The total power from the undulator is 5.3 kW. The straight section would allow adding a second insertion device of the same length.

2.2. Monochromator

A channel-cut crystal monochromator is chosen since it is mechanically simple in design and operation, e.g. reducing the risk of beam instabilities due to crystal vibrations. The monochromator does not give a fixed exit beam, but with a distance of 5 mm between the crystal surfaces the beam will move less than 1 mm over the full energy range (and e.g. 20 μm in the range 12 to 13 keV). The mirrors and the experimental setup will follow automatically using motorized translations. Limiting the beam acceptance angles to 40 x 40 μrad², the heat load on the monochromator will be 61 W with a peak power density on the monochromator crystal surface of 20 W/mm² at 5 keV.

2.3. Focusing Optics

To fulfill the beamline specifications, only a modest demagnification is required in the horizontal while the vertical source size is already smaller than the specified beam size. We have therefore

![Figure 1. Optics layout of the BioMAX beamline. (a) Initial optics with a monochromator and KB focusing optics. (b) With added secondary source and optional refocusing optics.](image-url)
chosen to position the mirrors at 31 m (horizontal focusing mirror, HFM) and 32 m (vertical focusing mirror, VFM) with the sample position at 45 m. Due to the small vertical source size ($\sigma < 4 \mu m$), the focused beam at the sample will still be small (around 15 $\mu m$ FWHM depending on mirror quality). In addition to the possibility to work out of focus to achieve a larger beam size, the VFM will be retractable from the beam path, giving a larger, homogeneous and extremely parallel beam at the sample position, suitable for evenly exposing larger crystals. In the horizontal direction, the beam size at the sample position will be 60 $\mu m$ (FWHM). A larger beam can be achieved by a slight change in the bending of the HFM, i.e. with the sample out of focus with the risk of having an inhomogeneous beam as a result of mirror imperfections but with the suggested design it is only for horizontal beam sizes larger than 60 $\mu m$ that this will be the case. Smaller beam sizes than the focused 60 x 15 $\mu m$ (horizontal x vertical, FWHM) will be provided by using beam defining apertures close to the sample.

2.4. Harmonic Rejection

Higher harmonics will be rejected by the focusing mirrors, which will have stripes of Rh and Pt coating in addition to an uncoated Si stripe, and a set of harmonic rejection mirrors (HRMs) close to the sample. The HRMs will consist of two flat, uncoated Si mirrors placed close to the sample position, giving improved harmonic rejection e.g. when the vertical focusing mirror is retracted. The double bounce arrangement of the HRMs will facilitate the operation since the beam will be offset but not rotated. The HRMs will be mounted on a rotation stage so the energy cut-off can be adjusted and also allowing the beam to pass undisturbed when the mirror surfaces are parallel to the beam.

2.5. Optional Refocusing Optics

In addition to the initial optics design, we suggest to prepare for the addition of a refocusing stage. It will refocus the beam from a primary focus at 40 m upstream of the sample position. This can be achieved by adjusting the bending radii of HFM and VFM (from around 6.5 km to 4.5 km). The FWHM of the primary focus will be 30 x 10 $\mu m$. The refocusing can be used both to increase the

| Table 1. Characteristics of the optics and x-ray beam at the BioMAX beamline. |
|---------------------------------------------------------------|
| X-ray source | In-vacuum undulator, 18.5 mm period, 4.2 mm minimal gap, 1.5 m magnetic length |
| Energy (wavelength) range | 5 - 25 keV (0.5 - 2.5 Å) using 3rd - 11th harmonics |
| Monochromator | At 28 m, Si (111), channel-cut, vertically deflecting, LN2 side-cooling |
| Energy bandwidth ($\Delta E/E$) | 2 x 10$^{-4}$ |
| Focusing optics | Kirkpatrick-Baez (KB) mirror pair (HFM, VFM) |
| Horizontal focusing mirror (HFM) | At 31 m, flat mirror bent to cylindrical shape, length 400 mm, 3 mrad grazing incidence angle, 0.5 $\mu$rad RMS slope error, 2 Å RMS roughness |
| Vertical focusing mirror (VFM) | At 32 m, flat mirror bent to cylindrical shape, length 400 mm, 3 mrad grazing incidence angle, 0.2 $\mu$rad RMS slope error, 2 Å RMS roughness |
| Harmonic rejection | VFM and HFM with Si/Rh/Pt stripes |
| Optional optics | Harmonic rejection mirrors (HRMs) at 44 m (Si) |
| Focus size at sample (at 45 m) | 60 x 15 $\mu m^2$ (FWHM, horizontal x vertical) |
| Divergence at sample | 40 x 30 $\mu$rad$^2$ (FWHM) |
| Beam size at sample | 10 to 100 $\mu m$ diameter (pinholes, defocusing) |
| ≈1 mm vertically (vertically unfocused) |
| Flux at sample (focused) at 1 Å | 2 x 10$^{13}$ ph/s (through a 50 x 15 $\mu m^2$ pinhole) |
| (vertically unfocused) at 1 Å | 4 x 10$^{12}$ ph/s (through a 50 x 100 $\mu m^2$ pinhole) |
stability and to demagnify the beam further. Slitting down the secondary source to 30 x 10 μm² and using a 5:1 demagnification of the secondary focusing stage would result in a beam with 1.8 x 10¹³ ph/s at 11.4 keV through a 5 x 2 μm² pinhole with 0.3 x 0.2 mrad² divergence. The refocusing stage is not included in the present beamline budget, but the setup of the initial configuration of the beamline will be prepared to make it easy to add a refocusing stage at a later time-point.

3. Beamline Performance

3.1. Methods

We have used Spectra [1] for undulator radiation calculations. Ray tracing has been done using MASH (Peter Sondhauss, MAX-lab internal report January 11th 2011) that uses Shadow [2] for ray tracing and Comsol (www.comsol.se) for finite element analysis.

3.2. Results

The largest heat load effects are at 5 keV where the heat load induced slope errors are within ±4 μrad. The simulations show that the heat load on the monochromator can be handled giving a nice focused beam with good energy resolution. The heat load deformations of the monochromator needs however to be compensated by the focusing mirrors as the energy is changed.

The optics give a nice focal spot of 60 x 15 μm² with around 2 x 10¹³ ph/s at 11.4 keV. The vertical focus size is determined by the mirror slope errors but since the vertical focus size is still smaller than the lower range of the specified beam size (20 μm) this is not a problem. Since the vertical focus size is also small compared to the upper range of the specified beam size (100 μm) and since the small vertical source size enhance the effect of mirror imperfections when working out of focus we suggest including the option of using the vertically unfocused beam. The simulations show that this will give a homogeneous beam with high flux (4 x 10¹² ph/s in a 50 x 100 μm² pinhole).

Figure 2 shows the calculated flux at the sample through a 50 x 15 μm² pinhole and through a 10 x 10 μm² pinhole (dotted lines).

**Figure 2.** Flux at the sample through a 50 x 15 μm pinhole (solid lines) and through a 10 x 10 μm pinhole (dotted lines).

**Figure 3.** Flux at the sample through a 50 x 15 μm pinhole (solid lines), and 5 x 2 μm pinhole for the refocused beam (dotted lines).

The optimizations give a nice focal spot of 60 x 15 μm² with around 2 x 10¹³ ph/s at 11.4 keV. The vertical focus size is determined by the mirror slope errors but since the vertical focus size is still smaller than the lower range of the specified beam size (20 μm) this is not a problem. Since the vertical focus size is also small compared to the upper range of the specified beam size (100 μm) and since the small vertical source size enhance the effect of mirror imperfections when working out of focus we suggest including the option of using the vertically unfocused beam. The simulations show that this will give a homogeneous beam with high flux (4 x 10¹² ph/s in a 50 x 100 μm² pinhole).

Figure 2 shows the calculated flux at the sample through a 50 x 15 μm² pinhole and through a 10 x 10 μm² pinhole. Figure 3 shows the flux at the sample through a 5 x 2 μm² pinhole with the optional refocusing optics.

**Figure 2.** Flux at the sample through a 50 x 15 μm pinhole (solid lines) and through a 10 x 10 μm pinhole (dotted lines).

**Figure 3.** Flux at the sample through a 50 x 15 μm pinhole (solid lines), and 5 x 2 μm pinhole for the refocused beam (dotted lines).

**Acknowledgements**

The BioMAX beamline has been funded by The Knut and Alice Wallenberg foundation and twelve Swedish universities.

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