

## V - MicroMAX

<b>External collaborations</b>	GU, AU, KU, LU, DESY and others.
<b>Funders</b>	Not yet funded.
<b>Official start</b>	Not yet funded
<b>Expected date of completion</b>	DDR review 9 months after start of project.

The field of structural biology has benefited tremendously by structure determinations at synchrotron radiation sources and typically a large fraction of the users and publications at these facilities come from the field of macromolecular crystallography (MX). At MAX IV the BioMAX beamline is the only MX beamline funded so far. BioMAX will cover a wide range of applications within MX and is expected to be the workhorse MX beamline at MAX IV.

MicroMAX will open new possibilities within the field of macromolecular crystallography by 1) providing an X-ray beam with properties that are presently not available elsewhere in the world and 2) by combining this with new experimental methods that are presently being developed at many X-ray free electron lasers (XFELs) and synchrotron radiation facilities. The aim of these new experimental methods is to most efficiently collect the best data from a large number of crystals since these demanding projects with microcrystals inherently will need many crystals to record full datasets due to e.g. radiation damage and sample heterogeneity. These methods are commonly referred to as "serial crystallography". MicroMAX will thus widen the scope of MX to difficult targets such as membrane proteins for which microcrystals are commonly the only obtained crystal form.

As there is rapid development of serial crystallography and in particular new sample delivery systems, MicroMAX must be flexible to take future developments into account. In addition, since it is likely that different sample delivery methods will be optimal for different experiments, it is important to offer a choice. Therefore, the experimental station will include setups for both standard rotational data collection and also for new sample delivery methods such as chips, jet-driven sample delivery, micro-fluidics, acoustics and more. The rotational data collection setup can also be used for samples suitable for BioMAX and in this way MicroMAX is a complement to BioMAX.

MicroMAX will with its performance also give better opportunities for fast room-temperature data collection, especially using the serial approaches. We envision that this will lead to a future development of time-resolved methods.

### *Technical description*

We propose to construct MicroMAX as a dedicated macromolecular crystallography beamline with the capability to focus a high-intensity monochromatic X-ray beam ( $10^{13}$  photons/sec) down to a spot size of  $1 \times 1 \mu\text{m}^2$ . We believe that the combination of a stable, highly focused brilliant X-ray beam that exploits the uniquely low emittance of MAX IV, with attention to detail and serving the highest demands of the life science user community, will drive novel and innovative solutions to the most challenging problems in structural biology.

The beamline can also provide an X-ray beam with a wider energy spectrum ( $\Delta E/E \approx 0.01$ ), "pink beam", which will give  $10^{15}$  photons/sec and open up completely new possibilities. The proposed beamline optics design is based on mirrors to make the beamline rapidly energy tuneable. The beamline flexibility will develop with time but the  $1 \times 1 \mu\text{m}^2$  beam size is expected to be achievable early.

The experimental station will include setups for both standard rotational data collection and for new sample delivery methods. The latter setup will build on the extensive development taking place elsewhere but we anticipate to continue the development further in-house and in collaboration with user groups.

### *Present status*

Concept design review (CDR) is ready. Work with a detailed design review (DDR) is ongoing in order to shorten the time from funding to completion of the project.

### *Expected status end 2018*

With funding in early 2017, insertion device and optics will be in manufacturing, the infrastructure installation starting and the experiment setup will be in development by the end of 2018.

### *Major partners and additional funding*

An application for funding of MicroMAX to the Novo Nordisk Foundation is being prepared for an invited submission in December 2016. This application is being written in a collaboration with user groups from Gothenburg University (R. Neutze), Lund University (P. Gourdon), CPR (KU, G. Montoya), KU (Sine Larsen) and Aarhus University (P. Nissen, G.R. Andersen).

As MicroMAX will be an exploratory beamline where methods are expected to continuously develop, more collaborations are foreseen. Here the established collaboration with Gothenburg University on sample delivery will be important. In addition, MAX IV Laboratory has several collaborations regarding method and instrumentation development relevant for MicroMAX within the framework of the EU project iNEXT, which includes partners at Aarhus University, DESY and EMBL-Hamburg. MAX IV is also a partner in the recently funded EU project EUCALL (EUropean Cluster of Advanced Laser Light sources) and will within this collaboration develop the sample screening standards needed to fully exploit the possibilities at X-ray free electron lasers and serial crystallography beamlines such as MicroMAX. EUCALL is a three-year program that started in October 2015.

### *Changes made since the start*

A project leader (Thomas Ursby) has been appointed for MicroMAX and since autumn 2015 he is working with MicroMAX, starting with the transition from the already available and reviewed concept design (CDR) to a final and detailed design (DDR).

### *Comparison to beamlines world wide*

MicroMAX will be a unique beamline thanks to the quality of the MAX IV 3 GeV. There are many other synchrotron radiation beamlines worldwide (ID13 and ID23-2 at ESRF (France), I24 at Diamond Light Source (UK), P14 at EMBL@PETRA-III and P11 at PETRA-III (Germany), PROXIMA-2A at SOLEIL (France), X06SA at SLS (Switzerland), GM/CA at APS (USA) and BL32XU at Spring8 (Japan) that aim at offering serial crystallography possibilities, however these beamlines have considerably lower X-ray beam performance than MicroMAX.

The following beamlines are under construction or commissioning and will offer competitive serial crystallography facilities, but again the X-ray beam performance will not reach the level of MicroMAX:

- VMXm at Diamond Light Source (UK)
- FMX at NSLS-II (USA)

MicroMAX will also complement serial crystallography beamlines at XFELs. The short pulses and high peak brilliance of the XFELs allow diffraction-before-destruction experiments but their beam time is scarce and will remain highly oversubscribed even when the European XFEL and SwissFEL come into operation. A large fraction of the scope of serial crystallography can more easily be performed at MicroMAX.

### *Future development*

With the rise of more diffraction limited synchrotron sources, we expect the field of micro-crystallography to grow in the coming decade and in particular the experiment setup will further develop. These developments will make time-resolved experiments more accessible and more development on triggering reactions will need to be investigated. MicroMAX is perfectly suitable to cover the time domain from microseconds and slower.