

MS39-P16 VMXi – Development of an *in situ* MX beamline at Diamond Light Source

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For protein crystallographers, one of the bottlenecks in the structure solving process is the harvesting of protein crystals and finding appropriate cryo-protectants. This may be early on in the life of a project where the experimenter wishes to identify whether crystals are salt, protein or some other crystallisable object, or later when protein crystallisation conditions are being optimised to achieve the best possible resolution from the X-ray diffraction experiment. Additionally, some protein samples are either too small to harvest, are too fragile to manipulate, or do not permit cryo-cooling.

At the Diamond Light Source we are developing an *in-situ* MX beamline specifically designed to take the crystallisation support, be it a crystallisation plate, or an LCP plate, and collect useful data which will aid the crystallographer in their experiment. We will be able to remove this bottleneck by providing a very high flux, tunable micro-focus beamline to allow extremely rapid screening and data collection of samples at room temperature.

Users of this beamline will be able to deliver or post their plates to Diamond and have the plates stored at either 20° C or 4° C. The plates will be imaged and the user will identify objects that they wish to investigate. The user will interact with the VMXi beamline via a web interface which will give them the ability to mark objects, determine what kind of experiment they want i.e. screening, data collection, fluorescence etc and will give access to results from data previously collected.

Construction of the experimental area is now complete and the endstation is being designed by in-house engineers to make a very efficient and effective *in-situ* beamline. Due to the staged construction process we are able to keep the I02 beamline operational whilst building and commissioning the new endstation. The new VMXi beamline is scheduled to open in 2016 when I02 will cease operations.

Keywords: in-situ, beamline, macromolecular crystallography

MS39-P17 Single crystal neutron diffractometer for Biological macromolecules iBIX at J-PARC

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Single crystal neutron diffraction is one of the powerful methods to obtain the structure information including the hydrogen atoms. IBARAKI biological crystal diffractometer called iBIX is a high performance time of flight single crystal neutron diffractometer to elucidate the hydrogen, protonation and hydration structures of organic compound and biological macromolecules in various life processes. iBIX is installed on BL03 in Material and Life Science Facility, J-PARC. Since the end of 2008, iBIX has been available to user experiments supported by Ibaraki University. In FY2012, we have succeeded to upgrade the 14 existing detectors and install the 16 new detectors for diffractometer of iBIX. The total measurement efficiency of the present diffractometer was on one order of magnitude from the previous one coupled with the increasing of accelerator power. In the end of FY2012, iBIX could be started to user experiments for biological macromolecules in earnest. In FY2014, the accelerator power of J-PARC is 300kW. We can collect a full data set of biological macromolecules for neutron structure analysis with around 2.0Å resolution in 10 days by using iBIX. The size of sample measured by iBIX is from 1 to 6mm³ in volume. If the accelerator power will become 1MW, the total measurement time or the sample size will be reduced to a one-third. In the beginning of FY2014, we have succeeded to collect the diffraction data sets of 6 biological macromolecules for about 4 months. Some interesting results obtained from these experiments which make the most of the merit of the neutron diffraction experiment will be reported in the poster. We started to upgrade the data reduction method and the diffractometer instruments in order to improve the data accuracy for the integrated intensities of Bragg reflections and to become user friendly system in the next phase, for example background extraction, the data correction method, integration method and profile fitting method. In the case of the diffraction data from larger unit cell crystals measured by iBIX, the some neighbor Bragg spots will overlap partially each other because iBIX was installed on the coupled moderator with the wide pulse shape. It is necessary to de-convolute the overlapped spots in order to obtain the integrated intensity of them. The profile fitting method can be applied for de-convolution of overlapping reflections. We will report also the development status of iBIX in the poster.

Keywords: Single crystal neutron diffraction, Biological macromolecule, pulse neutron