

facility will be available for structural biology researchers for routine use from October 2008. In the near future, we also have a plan to construct a micro focused beam at our BL12B2 beamline. To apply for beamtime or for more details about the NSRRC facilities, visit the General User program website: (<http://portal.nsrcc.org.tw/>). The details of the up-grade installation will be discussed.

Keywords: synchrotron X-ray instrumentation, data collection methods, technology

### P01.02.11

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#### Crystallography at MAX-lab

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MAX-lab, the synchrotron radiation facility in Lund, Sweden is focused on soft X-ray activities. However, on the largest of the three storage rings, the 1.5 GeV MAX II ring, there are three beamlines operating at energies suitable for crystallographic experiments. I711 is a multipurpose beamline and is presently running powder diffraction and SAXS experiments. It is a tunable wavelength station with a range of 0.8-1.55 Å and uses a single monochromator crystal. The material science beamline I811 is primarily used for EXAFS and surface diffraction experiments and is a tunable wavelength station between 0.6-5 Å. It is equipped with a large multiple axis goniometer capable of carrying heavy loads such as UHV chambers. I911 is the protein crystallography beamline a consist of 2 fixed wavelength stations (0.97 and 1.03 Å) and one tunable wavelength MAD station (0.7-2.1 Å). The MAD station is equipped with a kappa goniostat and a MAR 225 CCD and the fixed wavelength stations has MARdtb goniostats with MAR 165 CCDs. The Mar dtb on the 0.97 Å beamline has been redesigned to fit the MAR flatpanel. The three beamlines provide a very wide range of different setups and detectors ranging from the 430x350 mm<sup>2</sup> flatpanel detector to scanning point detectors. A comparison of the stations and setups using powder diffraction data will be presented.

Keywords: synchrotron radiation crystallography, synchrotron powder diffraction, crystallography instrumentation synchrotron radiat

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#### Macromolecular crystallography at Diamond Light Source: Automation and pathogenic sample environment

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At Diamond Light Source [1] the three phase I macromolecular crystallography (MX) beamlines [2] have experienced their first year of user experiments. The current user programme is interspersed

with commissioning and optimisation of the X-ray source (including automation of beam delivery) in conjunction with deployment and improvements in software and hardware to provide intuitive, state of the art MX beamlines. A large component of this work is to automate as many components and experimental processes as possible, from beam conditioning to user interaction. Aspects of automation of MX beamlines include tracking of information of protein crystal samples from before arriving on site, automounting and screening for crystal quality, collecting data and processing the results, and recording the results of all these steps. Of particular note, beamline I03, will provide biological containment category 3 facilities in the near future for work with pathogenic crystals at room temperature. Automation will be an essential component of this development, allowing tracking of crystals and the automounting of 1680 samples before decontamination of the working environment is required. Automation of the routine aspects of MX should aid both experienced and less experienced users and allow them to profit from their short time on the Diamond MX beamlines to maximise their scientific output. This suite of beamlines will provide an excellent environment for the collection of data from both cryogenic and room temperature crystals, using automation to guide the experiment rather than direct it. The current status of all aspects of automation on the phase I MX beamlines at Diamond Light Source will be presented.

[1] <http://www.diamond.ac.uk>

[2] <http://www.diamond.ac.uk/MX>

Keywords: crystallography, automation, synchrotron

### P01.02.13

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#### Approach for automated data collection at the photon factory protein crystallography beamlines

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Fully-automated X-ray diffraction data collection has been strongly demanded by structural biology researchers. The key technologies of the fully-automated data collection are automated sample exchange and automated sample centering. We have developed sample exchange robots named PAM (PF Automated Mounting) system and installed at the Photon Factory macromolecular crystallography beamlines; BL-5A, BL-17A and AR-NW12A, which are designed based on SAM system developed by SSRL macromolecular crystallography group. In order to reduce the time required for the sample exchange, we developed a double-tongs system, Gemini, which can hold two sample pins at the same time. The double-tonged PAM system can exchange samples without leaving the diffractometer area within 10 seconds successfully. Data collection experiments require alignment of the sample to the X-ray beam. We have developed and implemented an automated loop centering function onto our GUI software. It can be automatically executed after the PAM system mounts the sample. Moreover, we are developing an automated crystal centering function based on low-dose diffraction patterns for fully-automated X-ray diffraction data collection. For estimation of the best diffraction conditions, we are developing software, PROCESSOR, which evaluates the diffraction patterns. In order to monitor the X-ray diffraction experiments, we have developed REPORTER software and a PRMo (PF Remote Monitoring) system. The REPORTER collects the states and the results of present experiments, and stores them in a large-scale storage. The PRMo system permits users to access the information

even from the outside of beamlines over HTTPS protocol.

Keywords: automated data collection, robots, macromolecular synchrotron X-ray crystallography

## P01.02.14

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### A proposed suite of macromolecular crystallography facilities for NSLS-II

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A new, highly-optimized 3rd-generation synchrotron radiation (SR) source, the National Synchrotron Light Source -II (NSLS-II), is being planned as a replacement of the existing 2nd-generation SR source NSLS at Brookhaven National Laboratory. When operational, NSLS-II will deliver unprecedented brightness in the soft and hard x-ray spectral regions, e.g. at 8 keV about 10 times that of the brightest SR sources now available. NSLS hosts a strong macromolecular crystallography (MX) program, nearly 40% of its user community. At NSLS-II, MX is expected to be closely associated with other life sciences programs including small angle x-ray scattering, x-ray absorption spectroscopy, x-ray footprinting, and nanoscale imaging. We are preparing plans for a set of MX beamlines that would view canted, tunable undulator radiation sources in multiple straight sections of the storage ring, which would work independently. The experimental apparatus would include diffractometers to handle crystals of microns dimension or smaller, fast-framing active-pixel detectors, automated sample exchange and cryogenic apparatus, VUV/visible spectroscopy, and fluidic-based sample handling systems. These bright sources will extend MX into unexplored realms of sample size, perfection, and state of complexity and environment. Research and development in all of these areas are proposed, including methods for overcoming the effects of radiation damage, in order to exploit the properties of these sources. In addition to these undulator-based beamlines, it is also proposed to implement a set of MX beamlines viewing three-pole wiggler radiation sources, somewhat brighter than current NSLS bending magnet radiation sources. This work is supported by the US Dept. of Energy and the US National Institutes of Health.

Keywords: synchrotron radiation crystallography, synchrotron radiation optics, synchrotron radiation sources

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### A new macromolecular crystallography beamline for softer X-ray at the Photon Factory

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The use of softer X-ray for phase determination in macromolecular crystallography has gained quite some popularity, owing to the interest in utilizing weak anomalous signals provided by light atoms such as sulfur and phosphorus present in native protein and nucleic acid molecules. The method is quite useful especially for the range of macromolecules which are difficult to prepare heavy atom derivatives. The Photon Factory has started to develop a new macromolecular crystallography beamline for softer X-ray at BL-1A of the 2.5 GeV ring, funded by the national project 'Targeted Proteins Research Program'. The beamline is designed to deliver an intense softer X-ray beam at around 4 keV using the first harmonics of a short gap undulator to enhance the weak anomalous signal from light atoms. The optics and the diffractometer are optimized for the softer X-ray beam. The expected beam intensity at around 4 keV is more than  $10^{11}$  photons/sec on the area of 10 square microns at the sample position. The beamline can also cover the energy range of 12-13 keV with the 3rd harmonics, which enables Se- or Hg-MAD data collection from very small crystals with the intense 10 micron beam. The beamline development is particularly dedicated to the crystallographic study of integral membrane proteins and macromolecular complexes, systems of enormous biological significance which are currently difficult to be measured due to crystallization problems. The construction of the beamline is scheduled in the summer of 2009, followed by six months of commissioning. The beamline will be opened to the members of the national project in 2010.

Keywords: biological macromolecular crystallography, protein crystallography with synchrotron, synchrotron X-ray instrumentation

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### AR-NE3A, a new pharmaceutical beamline for macromolecular crystallography at the Photon Factory

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In recent years, advancements in high-throughput techniques for macromolecular crystallography have heightened the importance of structure-based drug design (SBDD) and demand for synchrotron use by pharmaceutical researchers has increased. In order to meet this demand, we are constructing a new high-throughput macromolecular crystallography beamline AR-NE3A, dedicated to SBDD. This is funded in partnership with Astellas Pharma Inc. The light source is an in-vacuum undulator in the PF-AR 6.5GeV ring, providing a high flux X-ray beam. The optics consist of three main components, a collimating mirror, double crystal monochromator with liquid nitrogen cooling system, and a toroidal double-focusing mirror. Ray-tracing simulations suggest that new AR-NE3A affords higher X-ray beam flux at the sample position than existing high-throughput beamlines at the Photon Factory, AR-NW12A and BL-5A. In the experimental hutch, there will be a high precision diffractometer, a fast-readout and high-gain CCD detector and a sample exchange robot which can handle more than two hundred cryo-cooled samples in a Dewar. In order to realize high-throughput data collection required for pharmaceutical researches, we are developing a fully-

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