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.nsrrc.org.tw/. The details of the up-grade installation will be discussed.

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

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Crystallography at MAX-lab

Krister Larsson, Stefan Carlson, Yngve Cerenius, Thomas Ursby
MAX-lab / Lund University, PO Box 118, Lund, Skane, 22100, Sweden, E-mail：krister.larsson@maxlab.lu.se

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 Mardtb 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^2 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

David Hall, Alun Ashton, Jose Brandao-Neto, David Butler, Elizabeth Duke, Gwyndaf Evans, Ralf Flaig, Andrew Foster, Paul Gibbons, Mic Harding, Michael Latchem, Karl Levik, Katherine McAuley, James O'Hea, Geoff Preece, James Sandy, Thomas Sorensen, David Waterman, Mark Williams, Richard Woolliscroft
Diamond Light Source, Diamond House, Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 0DE, UK, E-mail：david.hall@diamond.ac.uk

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

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

Masahiko Hiraki, Naohiro Matsugaki, Yusuke Yamada, Noriyuki Igarashi, Yurii Gaponov, Shokei Watanabe, Kumiko Sasajima, Nobuo pHonda, Soichi Wakatsuki
Photon Factory, IMSS, KEK, 1-1 Oho, Tsukuba, Ibaraki, 305-0801, Japan, E-mail：masahiko.hiraki@kek.jp

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 PReMo (PF Remote Monitoring) system. The REPORTER collects the states and the results of present experiments, and stores them in a large-scale storage. The PReMo system permits users to access the information