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

P01.02.11

Crystallography at MAX-lab
Kristoffer Larsson, Stefan Carlson, Yngve Cerenius, Thomas Ursby
MAX-lab / Lund University, PO Box 118, Lund, Skane, 22100, Sweden, E-mail: kristoffer.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. I11 is a multipurpose beamline and is presently running powder diffraction and SAXS experiments. It is a tunable wavelength station with a range of 0.8-1.5 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 have MARdb goniostats with MAR 165 CCDs. The Mardb 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 mm2 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 radiation

P01.02.12

Macromolecular crystallography at Diamond Light Source: Automation and pathogenic sample environment
David Hall, Alun Ashton, Jose Brando-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 Wooliscroft
Diamond Light Source, Diamond House, Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 ODE, 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.

Keywords: crystallography, automation, synchrotron

P01.02.13

Approach for automated data collection at the photon factory crystallography beamlines
Masahiko Hiraki, Naohiro Matsugaki, Yusuke Yamada, Noriyuki Igarashi, Yuri 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.
A new macromolecular crystallography beamline for softer X-ray at the Photon Factory
Naohiro Matsugaki, Yusuke Yamada, Masahiko Hiraki, Noriyuki Igarashi, Shigeru Yamamoto, Kimichika Tsuchiya, Tsutsumi Shioya, Hideki Maewaza, Seiji Asaoka, Hiroshi Miyachi, Yoshihiro Tahara, Yusunori Tanimoto, Soichi Wakatsuki
High Energy Accelerator Research Organization, Institute of Material Structure Science, 1-1 Oho, Tsukuba, Ibaraki, 305-0801, Japan, E-mail: naohiro.matsugaki@kek.jp

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 flux X-ray beam 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-