automated data collection system. With this system, automatic sample exchange, centering, data collection and data processing are automatically carried out according to a user defined schedule. The construction of the beamline will be completed in the summer shutdown of PF-AR. The beamline commissioning will be finished by the end of March 2009. The first user operation is expected in April 2009. Here, we will present the general outline and current progress of this project.

Keywords: synchrotron radiation, structure-based drug design, automated data collection

**P01.02.17**  
*Acta Cryst.* (2008). A64, C176

**Beamline developments for structural biology at the Photon Factory**

Noriyuki Igarashi, Naohiro Matsugaki, Yusuke Yamada, Masahiko Hiraki, Soichi Wakatsuki
Institute of Materials Structure Science, Photon Factory, 1-1 Oho, Tsukuba, Ibaraki, 3050801, Japan, E-mail: noriyuki.igarashi@kek.jp

Structural Biology Research Center at the Photon Factory currently operates 4 structural biology beamlines. AR-NW/12A, BL-5A and BL-17A are insertion device (ID) beamlines, while BL-6A is a conventional bending magnet beamline. Among these ID beamlines, AR-NW12A and BL-5A are high-throughput structural biology beamlines. A micro-focus beamline BL-17A was newly constructed and opened to general users in 2006. It was designed for micro-crystal structure analysis. In addition, the intense lower energy beam at around 6 keV is used for structure determination by SAD phasing with light atoms. In the next two years, two more beamline construction plans are scheduled. A new high-throughput beamline will be built at PF-AR NE3A in summer 2008 and opened to users in April, 2009. The beamline is expected to show a higher performance than current high-throughput beamlines. The beamline will be mainly dedicated to drug design. Another new beamline will be built at PF BL-1A in FY2009. The goal is to deliver brilliant lower energy beam at around 4-5 keV (dedicated to sulphur SAD experiment) and more photon flux at around 12keV than that of BL-17A. After completion of these two new beamlines, we will operate three high-throughput, two micro-crystallography and one conventional beamlines. For further high-throughput protein crystallography, we facilitate automation of beamline operation, with developments of sample changer robots, automatic sample centering system and unified beamline control software. These developments based on stable beamlines and reliable network will allow for the goal of full integrated structure determination pipeline. Here, we will introduce overview of our beamline developments and our future plans. As for details of topics, please refer to our other presentations.

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

**P01.03.18**  
*Acta Cryst.* (2008). A64, C176

**Experiences with automated crystal screening at the JCSG**

Christine B. Trame1,2, H-J. Chiu1,2, S. Oommachen1,2, M. Miller1,2, A. Cohen1, I. I. Mathews1, J. Song1, A. Deacon1,2
1Stanford Synchrotron Radiation Laboratory, Joint Center for Structural Genomics, MS 99, 2575 Sand Hill Road, Menlo Park, CA, 94025, USA, 2Joint Center for Structural Genomics (JCSG), E-mail: cctrame@slac.stanford.edu

The Stanford Automated Mounting (SAM) system plays a crucial role in the JCSG crystal screening effort. Promising crystals are identified for data collection and screening results are used to optimize crystallization conditions. Typically, 2500+ crystals from ~70 protein targets are screened each month. We have developed several software and hardware tools to help us efficiently perform this activity. A cassette/dewar tracking system allows us to manage our crystal inventory. A 2D barcode reader is under development to verify the cassette identity prior to screening. A protocol was established to check the vacuum integrity in our shipping dewars to give an early warning of a failing dewar. A crystal sorting interface has been implemented in BLU-ICE, allowing us to consolidate our crystal inventory and to archive crystals that have been used for data collection. The interface also transfers crystals between SSRL cassettes and ALS pucks, which is particularly useful when we collect data at other synchrotron facilities. For the last 3 years during the SSRL summer shutdown, a Rigaku MM-002 X-ray microsource generator was used for screening. In 2007, we upgraded to a MM-002+ system, which we installed inside the BL-1-5 hutch. The mounting for the source allowed us to take advantage of all the existing beamline hardware, including the SAM system. Typical screening exposure times were 5min per 0.5 degree. The MM002+ achieved double the throughput (>100 crystals/day), compared with the MM002 source. The diffraction resolution obtained with the microsource correlated well with the same crystal exposed using a SR source. The JCSG is funded by NIGMS/PSI, U54 GM074898. SSRL is funded by DOE BES, and the SSRL SMB program by DOE BER, NIH NCRR BTP and NIH NIGMS.

Keywords: SAM, JCSG, MM002+
CATS offers both fast and reliable sample changing and in-situ screening of crystallization plates. Decision making procedures for automatic indexing, strategy calculation, data processing, and quick assessment of structure solution are also being integrated into the beamline control software (RemDAQ). An overview of beamline instrumentation and automation software will be presented.

Keywords: beamline, protein crystallography, automation

P01.03.20


Beamline automation and mail-in data collection at SPring-8 structural biology beamlines
Go Ueno1, Kazuya Hasegawa2, Nobuo Okazaki2, Hironori Murakami1, Takaaki Hikima1, Seiki Baba2, Kunio Hirata2, Atsushi Nisawa1, Takashi Kumasaka12, Masaki Yamamoto1
1RIKEN SPring-8 Center, Division of Synchrotron Radiation Instrumentation, 1-1-1 Koto Sayo-cho, Sayo-gun, Hyogo, 679-5148, Japan, 2SPring-8/JASRI, 1-1-1 Koto Sayo-cho, Sayo-gun, Hyogo, 679-5198, Japan, E-mail ueno@springs8.or.jp

In the past years, with enforcing the structural genomics research, the automation of beamlines at synchrotron radiation facilities has been dramatically advanced worldwide. Here in SPring-8, the automatic system to execute successive diffraction experiments with sample auto-changer SPACE [1] was developed at RIKEN Structural Genomics Beamlines [2]. The operation software BSS [3] provides the intuitive GUI and centralized control of beamline instruments with the client-server architecture. The beamlines have been routinely operated with the automatic system in last five years, contributing to the rapid crystal screening and efficient data collection for a vast amount of samples for structural genomics research. Besides, the same architecture has been similarly implemented to many of other structural biology beamlines at SPring-8, providing users a common look and feel at all beamlines. The web-based database D-Cha [4], developed to support mail-in data collection, provides GUI to specify the experimental conditions for crystals stored in SPACE sample trays send to beamline. Collected data can be readily checked out by users through the web browser. Distant users benefit much by conducting the mail-in data collection with D-Cha and remote control will be discussed.

Keywords: automation, remote control, robots

P01.03.22


New approaches to room-temperature synchrotron data collection in macromolecular crystallography
Mehmet Aslantas1, Vivian Stojanoff2, Engin Kendi3
1Kahramanmaras Sutcuimam University, Physics, Kahramanmaras, 46100, Turkey, 2Brookhaven National Laboratory, National Synchrotron Light Source, Upton 11973, NY, USA, 3Physics Engineering Department, Hacettepe University, Beytepe 06800, Ankara, Turkey, E-mail: aslantas@ksu.edu.tr

Cryogenic techniques significantly reduce radiation damage on biological samples, extend crystal lifetimes, and improve data quality during data collection at high-brilliance Synchrotron sources. But avoiding cryo-induced structural changes, high mosaicity, and freezing problems of some protein crystals are brought into focus as a challenge to be overcome with room-temperature data collection at Synchrotron sources. In this study, at first the quality of the crystals grown by Counter Diffusion method and the lowest mosaicities obtained from X-ray diffraction studies performed at room temperature will be presented. Secondly, an improvement in data quality significantly was obtained from lysozyme derivative crystals at the optimum wavelength in contrast to the previous studies will be given. Comparison of cryogenic structure with the room temperature structure makes known a number of differences. Therefore, finally structural comparison of lysozyme crystals grown by Counter Diffusion and Hanging Drop methods, respectively, at room- and cryo-temperature will be discussed.

Keywords: macromolecular synchrotron X-ray crystallography, data collection method, temperature

P01.03.23


The PXRR integrates six beamlines for macromolecular crystallography at the NSLS into one resource
Dieter K Schneider1, Lonny E Berman2, Annie Heroux1, Allen M Orville1, Howard H Robinson1, Anand M Saxena1, Alexei Soares1, Robert M Sweet1
1Brookhaven National Laboratory, Biology Department, Bldg. 463, Upton, NY, 11973, USA, 2Brookhaven National Laboratory, National Synchrotron Light Source 725D, Upton, New York 11973, USA, E-mail: schneider@bnl.gov

Driven by the needs of visiting and remotely participating scientists,