

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

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Beamline automation and mail-in data collection at SPring-8 structural biology beamlines

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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 automatic beamline operation, without visiting SPring-8. Presently, development of some new features, such as automatic crystal screening, real-time monitoring of radiation damage, automatic crystal centering etc. are attempted by associating the beamline operation with the automatic diffraction image analysis.

[1] Ueno et al., (2004). *J. Appl. Cryst.* 37, 867-873.

[2] Ueno et al., (2006). *J. Struct. Funct. Genomics.* 7, 15-22.

[3] Ueno et al., (2005). *J. Synchrotron Rad.* 12, 380-384.

[4] Okazaki et al., (2008) *J. Synchrotron Rad.* 15, 288-291.

Keywords: protein crystallography with synchrotron radiatio, automated data collection, remote access for crystallography

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Beamline automation and remote access at NSRRC BL-13

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SAM (Stanford Auto-Mounter) was installed and commissioned at NSRRC BL-13C endstation, and will be opened to the users in the following seasons. The controlling software is Blu-Ice from Stanford, which is very user-friendly and easy to use. Remote control will be opened at the end of 2008, which will be beneficial especially for international users. The web tool will be WebIce from Stanford. In the future, a mail-in service system will be established, and Phoenix/DNA will be included in our automation system for high-throughput structural determination.

Keywords: automation, remote control, robots

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New approaches to room-temperature synchrotron data collection in macromolecular crystallography

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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

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The PXRR integrates six beamlines for macromolecular crystallography at the NSLS into one resource

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