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.
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[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 aproaches 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 mosaiciticies 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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Driven by the needs of visiting and remotely participating scientists,

the PXRR has introduced rapid access modes that optimally match data collection requirements with the capabilities of its six beamlines. Data collections begun on a bending magnet station may continue on one of our two undulator facilities. This mobility, supported by 20hour / 7day operator assistance and an experiment and data tracking data base, allows the PXRR to increasingly specialize beamlines to better accommodate new methods. In addition to our popular mail-in crystallographic collaborations, we also have begun supporting remote data collection. Three of our beamlines support cryogenic automounters and are particularly well suited for high volume screening and remote operations. A new micro-diffractometer has just been installed on our premier X25 ID beamline to support data collection from a 20-50 micrometer x-ray beam. To support concurrent x-ray diffraction and spectroscopic analysis, we have installed an in-beam single crystal spectrophotometer at beamline X26-C. These new capabilities, and other proposed developments, motivate our planning of an entirely new experimental MX facility to exploit the unique capabilities anticipated at NSLS-II. This work is supported by the NCRR of the US National Institutes of Health, and the OBER of the US Department of Energy.

Keywords: macromolecular synchrotron X-ray crystallography, microdiffraction, optical spectroscopy

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SAXS and macromolecular crystallography at the SIBYLS beamline (12.3.1) of the Advanced Light Source

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Critical processes in cells are coordinately regulated by the assembly of large, dynamic, multi-protein complexes, and structures of these macromolecular machines are key to a detailed molecular and mechanistic understanding of all living systems. To achieve accurate structural information of biologically relevant molecular complexes, the Structurally Integrated Biology for Life Sciences (SIBYLS) beamline (12.3.1) at the Advanced Light Source (ALS) has been developed as a dual endstation synchrotron beamline. The SIBYLS beamline has been equipped with both Small Angle X-ray Scattering (SAXS) and Macromolecular Crystallography (MX) endstations. These two techniques when combined at a single beamline allow SIBYLS users to combine a) advances in the efficient identification and development of diffraction quality crystals by micro-fluidic, chip-based automated crystallization screening plus computationally-based, highly controlled and reproducible humidity conditions for improved crystal diffraction, b) automated sample mounting and screening supplemented with automated data collection, analysis, and phasing, c) knowledge-based, stepwise integration and improvement of solution X-ray scattering technologies for robotically-assisted high throughput characterization of protein conformation and assembly, and d) consequent advances in the integration of these two X-ray diffraction methods. Together the SAXS and MX endstations of the SIBYLS beamline provide for the scientific community experimental and computational technologies and facilities to define biologically relevant structures, conformational states, and assemblies of molecular machines.

Keywords: macromolecular structure determination, SAXS, synchrotron X-ray instrumentation

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The new micro-focus beamline at SSRL: Current capabilities and future possibilities

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The new macromolecular crystallography beam line, BL12-2, at the Stanford Synchrotron Radiation Laboratory (SSRL) is designed for studying small crystals and otherwise weakly diffracting samples. The beam line is also optimized for automated screening and MAD data collection and can be controlled remotely from anywhere in the world. The beam line delivers a flux of ~4.2e+11 p/s at 100 mA, (12658eV), and a focus of 7um vertically and 70 um horizontally. The intense beam supplied from an in-vacuum undulator insertion device has an energy range from 5,500 to 18,000 eV and is performing beyond design specifications. Highly stable, intense beams are essential tools in the elucidation of important macromolecular structures from small crystals generally considered too small for conventional beam lines and from weakly diffracting samples such as membrane proteins and large complex molecular machines. Improving crystal growth parameters is often a challenging bottleneck in the structural solution of these important proteins. With the coupling of the capabilities of BL12-2 and the implementation of the Stanford Auto-Mounting (SAM) robots at SSRL, users from across the world have access to this state-of-the-art resource. The beam line configuration and operation will be described which includes an innovative mirror positioning feedback system that delivers a highly stable, focused beam at the sample position. Future implementation of an in-line sample imaging system and micron precision air bearing goniometer, will allow data collection from smaller crystals. The beam line construction has been funded by the California Institute of Technology through a generous gift from the Gordon and Betty Moore Foundation. General users will have access to 60% of the available beam time.

Keywords: small crystals, protein crystallography, remote access

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NorthEastern Collaborative Access Team (NE-CAT) beam lines at the advanced photon source

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The NorthEastern Collaborative Access Team (NE-CAT) has been established to design and operate synchrotron X-ray beamlines for its institutional members as well as provide an important research resource for the national research community. The NE-CAT facility at the Advanced Photon Source will consist of four beamlines. Three of the beamlines are based upon use of a novel canted undulator source with two undulators in a single straight section. A bending magnet beamline completes the set of four beamlines. Currently there are two operational undulator beamlines: 24ID-C - fully tunable in the energy range from 6 to 25keV with a focused beam size of 20x60 microns and 24ID-E - fixed energy at ~12.66keV or 14.84 keV (with