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 small variability to cover Se and Br edges). The 24ID-E beamline is equipped with a MD2 microdiffractometer, which is used to provide stable and well collimated beam from 5 to 100 microns in diameter and capable of visualizing micron-sized crystals. These operational beamlines are currently open to general APS users. Installation of a bending magnet beamline is now in progress and expected to be completed by the end of this year. NE-CAT is a consortium of scientists organized to design, construct and operate a structural biology sector at the APS. This facility will be used to focus on NE-CAT research on structural studies involving technically challenging crystallographic projects. In order to meet these needs, an ALS robot for screening a large number of crystals is now being commissioned, a microfocus diffractometer MD-2 is installed on 24ID-E beamline and several novel hardware and software ideas will be implemented. Funding for NE-CAT is provided through P41 grant from the National Center for Research Resources and from the NE-CAT member institutions.

Keywords: macromolecular synchrotron X-ray crystallography, microdiffraction, synchrotron X-ray instrumentation

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A beamline for anomalous diffraction at SOLEIL : Proxima 1

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The PROXIMA 1 beamline, built on the SOLEIL synchrotron radiation source, has been in routine operation for users since the beginning of 2008. Using a U20 in-vacuum undulator magnet source, the beamline produces high intensity, well collimated photons for biocrystallography in the range 5-15 keV. Monochromatization and focusing are separate functions. The channel-cut monochromator crystal is cooled to 90 K by a novel cryogenic system, and permits simple and rapid tuning in the above energy range. A Kirkpatrick-Baez bimorph mirror geometry produces a focal spot of 125 micron x 75 micron at the sample. Mirrors and goniostat are mounted on a heavy table provided with vertical translation in order to compensate beam height variations. Work is in progress to optimise the size and divergence of the X-ray beam to different sample and detector geometries. A 3-circle kappa-geometry goniostat (Rigaku Crystal Logic) is installed on the beamline and permits data collection around either the phi or omega axes, permitting a wide variety of data collection strategies. Data are routinely collected with Bijvoet pairs appearing close together in time or using inverse beam geometry. An ADSC Q315r detector can be positioned at crystal to detector distances of between 80 mm and 1 m. The beamline design has been developed in order to favour highly stable beam conditions, resulting in an rms beam stability (in vertical and horizontal) of approximately 1 micron even without the use of feedback control of optical elements. The beamline has been used for a number of structural projects with both MAD and SAD phasing, highlight results of which will be presented.

Keywords: anomalous diffraction, synchrotron radiation, biocrystallography of proteins

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Pushing the envelop of sulfur SAS structure determination at UGA/SER-CAT

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The SER-CAT beamlines were designed and optimized for collecting multiwavelength anomalous dispersion (MAD) data on crystals of seleno-methionyl derivatized protein at the selenium X-ray absorption edge (~12 keV). However, single-wavelength anomalous scattering (SAS) methods have opened up the possibility of structure determination from native crystals based on the weak sulfur anomalous scattering signal enhanced by data collection using soft (6-8 keV) X-rays. Over the past three years, SER-CAT has embarked on a program of soft X-ray beamline optimization focused on identifying and correcting instabilities in the system at low energies which can significantly contribute to noise level in the SAS data produced. This is important to the success of sulfur-SAS structure determination since the signal is still only about one-third of that produced by selenium at its absorption edge, even when the SAS signal is enhanced using soft, X-rays having wavelengths around 2Å. The results of these studies have produced an undulator beamline (22ID) that is highly stable at lower energies and suitable for sulfur SAS data collection and phasing. Using 22ID we are now in the process of developing methods for successful sulfur SAS data collection and phasing for crystals that have, to date resisted this approach due to data resolution, crystal symmetry or sulfur content. Several examples of sulfur SAS structure determination from data collected on 22ID will be presented. Work is supported in part with funds from SER-CAT, the Georgia Research Alliance, the National Institutes of Health (GM62407) and the University of Georgia Research Foundation.

Keywords: synchrotron beamline optimization, soft X-ray data collection, sulfur SAS structure determination

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Probing radiation damage with a 1-micron beam

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Structure determination from crystals of biological macromolecular is often hindered by X-ray induced damage. In practice, data collection is a trade-off between maximizing X-ray flux to the sample to obtain data of the highest possible resolution and minimizing radiation damage. The primary cause of radiation damage at cryo-