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-

temperatures is thought to be from photoelectrons ejected from atoms following the absorption of X-rays. As the photoelectrons traverse the crystal, they lose energy through interactions with atoms in their path resulting in damage. If the X-ray beam is polarized, the photoelectrons are ejected preferentially along the polarization vector. Monte-Carlo simulations [Nave, C., and Hill, M. A. (2005). J Syn. Rad. 12, 299-303] suggest that, when the beam size is only a few microns, most photoelectrons escape the illuminated volume. This leads to the peculiar conclusion that the radiation damage due to photoelectrons may be significantly lower within the illuminated volume than in the volume immediately surrounding the irradiated spot. A second prediction of the calculations is that most of the photoelectron's energy is abruptly dissipated within the last few microns of its trajectory. Recently, a long focal length Fresnel zone plate was used to provide a focused beam of ~1-micron cross section at the sample position, and high quality diffraction data was obtained from protein crystals. The 15.1 keV, 1-micron beam was used to probe the geometrical distribution and extent of radiation damage in protein crystals. These data confirm that radiation damage is greater along the polarization vector than in the perpendicular direction, radiation damage is maximal 3-4 microns from the center of the beam, and radiation damage does not extend beyond 6 microns.

Keywords: radiation damage, microcrystalls, microcrystallography

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Towards protein structure determination using two-dimensional crystals and powders

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Reliable determination of the structure of integral cell membrane proteins (IMPs) is one of the most important problems in biology today. The structure of the vast majority of IMPs remains unsolved however, mainly due to difficulties associated with conventional crystallisation and the concomitant need for preservation of the active form of the protein as it is taken out of its natural environment within the cell membrane. In order to address these problems, we consider the possibility of using two-dimensional (2D) ordered micro-arrays of proteins, i.e., 2D crystals, in X-ray diffraction (XRD) experiments, instead of conventional three-dimensional crystals. In this work, we discuss the potentials and limitations of using 2D protein crystals for XRD based structure determination. We present a systematic approach to data analysis and fitting based on physical description of X-ray scattering by 2D crystals. Scattering by large assemblies of 2D crystals with random preferential orientations is also considered as a model for XRD with 2D crystal powders. We illustrate how 2D crystal powder diffraction data may be used to reconstruct a 2D projection map of the electron density in the unit cell with reference to preliminary results obtained for 2D crystals of bacteriorhodopsin.

Keywords: membrane proteins, two-dimensional protein crystals, X-ray diffraction

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8C2 high resolution powder diffraction beamline at Pohang Light Source and its recent results

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We introduce 8C2 high resolution powder diffraction (HRPD) beamline at Pohang Light Source. This beamline is designed for a powder crystallography, i.e., very high angular resolution and various sample environments. The technical characteristics of the beamline and some performance indicators are listed, such as the incoming photon flux and the angular/energy resolutions obtainable under typical experimental conditions. We present several recent results using synchrotron x-ray powder diffraction data collected from this beamline, not detected by previous powder diffraction experiments.

Keywords: powder crystallography, powder diffraction, synchrotron X-rays

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Accurate powder diffraction standards: Determination of the lattice parameter of LaB_6 SRM(660)

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We use X-ray powder diffraction and synchrotron radiation to determine the lattice parameter of the NIST standard reference material (SRM 660) LaB_6 to be 4.157580 Å with an accuracy of 12 parts per million (ppm), calibrated relative to the lattice parameter of the Si powder standard (a0 =5.430940(11) Å, Si 640b). A discrepancy is observed between the currently accepted lattice spacing of LaB6 and the measured value, of 0.00048(5) Å, or nine standard deviations from the NIST reference. Twelve different measurements of the lattice parameter are made at beam energies between 10 keV and 20 keV. The observed discrepancy in the lattice parameter is consistent for the different energies used. The absolute values of the mean difference between the measured and calculated 2 theta centroids, are highly consistent, between 0.0002o and 0.0004o for energies from 5 keV to 14 keV, and between 0.0005o and 0.0008o for energies from 15 keVto 20 keV. In order to determine the peak positions with high precision, account must be taken of observed peak asymmetry. Significant asymmetry is due to peak broadening and must be taken into account in order to determine accurate peak locations and lattice spacings. Our approach shows significant advantages over conventional analysis. Our analysis of peak broadening is compared with models used in Rietveld analysis.

Keywords: lattice parameters, powder and single crystal diffraction, synchrotron radiation experimental

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A halogen lamp furnace to synthesize nanoparticles: *In situ* X-ray absorption spectroscopy

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