

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

Roger Fourme¹, Denis Duran¹, Eric Girard^{1,2}, Patrick Gourhant¹, Pierre Legrand¹, Majid Ounsi¹, Lucile Roussier¹, Olga Roudenko¹, Andrew Thompson¹

¹Synchrotron-Soleil, BP48 Saint Aubin, Gif sur Yvette, France, 91192, France, ²IBS, UMR 5075 CNRS-CEA-UJF-PSB, 41 rue Jules Horowitz, Grenoble, 91192, France, E-mail: roger.fourme@synchrotron-soleil.fr

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

John P. Rose^{1,2,3}, Chen Lirong², Fu Zheng-Qing^{2,3}, Swindell II James², Zhu Jinyi², Chrzas John^{2,3}, Gonczy John^{2,3}, Fait James^{2,3}, Jin Zhongmin^{2,3}, Wang Bi-Cheng^{2,3}

¹University of Georgia, Biochemistry and Molecular Biology, Department of Biochemistry and Molecular Biology, Athens, GA, 30602, USA, ²Department of Biochemistry and Molecular Biology, The University of Georgia, Athens, GA, USA, ³SER-CAT, Advanced Photon Source, Argonne National Laboratory, USA, E-mail: rose@bcl4.bmb.uga.edu

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

Robert F Fischetti¹, Ruslan Sanishvili¹, Derek Yoder¹, Stefan Vogt², Gerold Rosenbaum³, Richard Benn¹, Steve Corcoran¹, Oleg Makarov¹, Shenglan Xu¹, Venugopalan Nagarajan¹, Michael Becker¹, Sudhirbabu Pothineni¹, Janet L Smith⁴

¹Argonne National Laboratory, BioSciences Division, GM/CA-CAT, 9700 S. Cass Ave, Argonne, IL, 60439, USA, ²X-ray Science Division, Argonne National Laboratory, Argonne, IL, 60439, USA, ³Dept. of Biochemistry, U. of Georgia, and Structural Biology Center, BioSciences Division, Argonne National Laboratory, Argonne, IL 60439, USA, ⁴Life Sciences Institute, Dept. of Biological Chemistry, U. of Michigan, Ann Arbor, MI 48109, USA, E-mail: rfischetti@anl.gov

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-