

**P.01.02.16***Acta Cryst.* (2005). A61, C139**Microcrystallography at ChemMatCARS at the Advanced Photon Source**

Victor G. Young, Jr.<sup>a</sup>, P. James Viccaro<sup>b</sup>, Timothy Graber<sup>b</sup>, Maren Pink<sup>c</sup>, Jeff Gebhardt<sup>b</sup>, Yu-Sheng Chen,<sup>b</sup> <sup>a</sup>*University of Minnesota, Chemistry Department, 207 Pleasant St. S.E., Minneapolis, MN 55455, USA.* <sup>b</sup>*The Center for Radiation Sources, The University of Chicago, 5640 Ellis Ave., Chicago IL 60637, USA.* <sup>c</sup>*Indiana University Molecular Structure Center, Indiana University, Chemistry Department, A421, 800 E. Kirkwood Ave., Bloomington, IN 47405-7102, USA.* E-mail: young@chem.umn.edu.

ChemMatCARS at the Advanced Photon Source (APS) is a high-brilliance synchrotron X-ray based national user facility dedicated to providing experimental infrastructure and support resources to the chemical and materials science community. At the APS, undulator source brilliance is nearly 3 to 4 times that produced by second-generation sources. The superior source brilliance of this third generation synchrotron enables a broader range of micro-crystalline specimens to be investigated. Microcrystallography is now commonly conducted on specimens as small as 1  $\mu$  in its smallest dimension. ChemMatCARS is also a participating partner in the SCrAPS (Service Crystallography at APS) program which allows remote access to our microcrystallography facility. In an effort to provide outreach to the general community potential users are encouraged to submit rapid-access proposals to the General User Program at APS. Please view our web page at <http://www.cars.uchicago.edu/chemmat/chemhome.html>.

**Keywords:** microcrystallography, microdiffraction, synchrotron radiation

**P.01.02.17***Acta Cryst.* (2005). A61, C139**GM/CA Canted Undulator Beamlines for Protein Crystallography**

Robert F. Fischetti<sup>a</sup>, S. Stepanov<sup>a</sup>, S. Xu<sup>a</sup>, O. Makarov<sup>a</sup>, A. Urakhchin<sup>a</sup>, R. Sanishvili<sup>a</sup>, W.W. Smith<sup>a</sup>, D. Yoder<sup>a</sup>, R. Benn<sup>a</sup>, S. Corcoran<sup>a</sup>, S. Devarapalli<sup>a</sup>, W. Diete<sup>b</sup>, M. Schwoerer-Boehing<sup>b</sup>, R. Signorato<sup>b</sup>, L.E. Berman<sup>c</sup>, J.L. Smith<sup>ad</sup>, <sup>a</sup>*Argonne National Lab., USA.* <sup>b</sup>*ACCEL GmbH, Germany.* <sup>c</sup>*Brookhaven National Lab., USA.* <sup>d</sup>*University of Michigan, USA.* E-mail: rfischetti@anl.gov

GMCA CAT has been established to build and operate a macromolecular crystallography facility at the Advanced Photon Source (APS). The facility will consist of three beamlines; two insertion device (ID) beamlines based on the APS dual-canted-undulator geometry and one bending magnet beamline. The independently tunable ID beamlines are presently being commissioned, and crystallographic experiments have begun. The beamlines are rapidly tunable (MAD capable), encompassing an energy range from 3.5 keV to 35 keV (wavelength 3.5 Å to 0.35 Å).

The scientific and technical goals of the CAT emphasize automation for a variety of sample types, sizes and qualities, including weakly diffracting samples as small as 10  $\mu$ m, and unit cells as large as 2000 Å. Several novel features implemented to achieve these goals include "bimorph" mirrors with positional feedback, air-bearing goniometry, miniature piezo translation stages, and high resolution on-axis sample viewing. The control system has been designed to provide capabilities for fast automation. It includes a light weight version of SSRL's BluIce that has been converted into a client of the EPICS distributed control environment. Fast scans have been implemented for all beamline components at the hardware level based on novel motion controllers utilizing fiber links.

**Keywords:** crystallography instrumentation, synchrotron radiation instrumentation, instrumentation and software

**P.01.02.18***Acta Cryst.* (2005). A61, C139**Instrumentation for X-ray Scanning-Diffraction with Sub-micron Resolution**

Manfred Burghammer, Christian Riekel, *Microfocus Beamline (ID-13), European Synchrotron Radiation Facility, Grenoble, France.* E-

mail: burghammer@esrf.fr

Highly focused monochromatic x-ray beams well in the sub-micron range can be produced at third generation synchrotron radiation sources [1][2]. Routine diffraction experiments with sub-micron beams are performed at the ID-13 beamline using X-ray optics such as Kirkpatrick-Baez mirrors, compound refractive lenses and linear Fresnel lenses. The availability of devices delivering beams significantly smaller than 100 nm is already in sight.

Our efforts in order to develop methods and instrumentation for nano-beam diffraction experiments will be presented.

[1] Müller M., et al., *J. Appl. Cryst.*, 2000, **33**, 1231-1240. [2] David C., et al., 2001, *PSI annual report*.

**Keywords:** micro-beam, diffraction, micro-crystallography

**P.01.02.19***Acta Cryst.* (2005). A61, C139**I16: A Magnetic and Material Diffraction Beamline on Diamond**

Alessandro Bombardi<sup>a</sup>, Steve Collins<sup>a</sup>, <sup>a</sup>*Diamond Light source, Rutherford Appleton Laboratory, Chilton-Didcot, OX11 0QX, United Kingdom.* E-mail: Alessandro.Bombardi@diamond.ac.uk

Diamond Light Source will offer a unique opportunity to the research community for X-ray diffraction studies of materials. I16 will be a highly versatile facility for a wide range of science applications. One of the most important of these is the study of bulk and nano-structured magnetic materials. Here, one typically requires high flux, energy tuneability, polarisation selection and analysis, and controllable sample variables, such as temperature and magnetic field. Therefore the beamline will allow to cover very general scattering investigation.

The optical layout of the beamline is presented as well as the large multi axis K-diffractometer equipped with an in-house designed polarization and high-resolution analyser and automatically changeable detectors.

**Keywords:** synchrotron X-ray diffraction, synchrotron instrumentation, magnetic X-ray scattering

**P.01.03.1***Acta Cryst.* (2005). A61, C139**Structural characterization of a small heat-shock protein from *Xylella fastidiosa***

Susely Ferraz de Siqueira Tada<sup>a</sup>, Francisco Javier Medrano<sup>b</sup>, Beatriz Gomes Guimarães<sup>b</sup>, Cristiano Luís Pintode Oliveira, Íris Torriani<sup>b</sup>, Anete Pereirade Souza<sup>a</sup>, <sup>a</sup>*CBMEG, State University of Campinas, Brazil.* <sup>b</sup>*LNLS-Brazilian Synchrotron Light Laboratory, Campinas, Brazil.* E-mail: susy\_fs@yahoo.com.br

The small heat shock proteins (smHSP's) belongs to a family of proteins that function as molecular chaperones by preventing protein aggregation, and are also known to contain a conserved region termed alpha-crystallin domain. The chaperonin smHSP17,9 kDa from the orange phytopathogen *Xylella fastidiosa* was partially characterized in respect to your assembly and structure. This protein was overexpressed in *E. coli* BL21(DE3) strain and after your purification (by affinity chromatography), crystallization tests were performed and a single crystal was obtained, which diffracted at low resolution. At this moment, refinement tests are in progress in different crystallization conditions, in order to obtain a greater crystal. Parallel this, SAXS (Small Angle X-Ray Scattering) measures revealed us that this protein tends to aggregate in oligomeric complexes, fact that is known in the chaperonins family.

An estimate of the molecular weight showed that the formed complexes possess 12±1 monomers. The obtained radius of gyration was about 50,5±0,5 Å with a maximum dimension of 157 Å. It was also verified that the protein has a spherical globular conformation and its tertiary structure is rigid, without flexible domains, what it corroborates some inherent structural characteristics of this protein family.

**Keywords:** protein structural analysis, bacterial pathogenesis, chaperonins