

proteins are 0.097 GPa⁻¹ and 0.076 GPa⁻¹, respectively. It may imply that SoIPMDH, which is from land bacteria, is more sensitive to pressure than SbIPMDH from extremophile.

The SoIPMDH structure shows a dimer that presents an internal hydrophobic cavity surrounded by Pro120, Lue121, Ile125, Lue232 and Lue258 at the dimer interface. Two structurally functional water molecules appeared in the cavity at a pressure of 470 MPa, while no such water molecule could be observed under atmospheric pressure. Previous published works assume that the pressure denaturation of proteins is induced by water penetration into the hydrophobic interior of proteins. Although concrete data are lacking, several theoretical and simulation studies support this theory [2]. The present observation is a direct evidence of the fact that water molecules do penetrate into the inner cavities of proteins under high pressure.

[1] R. Kasahara, T. Sato, H. Tamegai, C. Kato, *Bioscience, Biotechnology, and Biochemistry* **2009**, *73*, 2541-2543. [2] T. Imai, S. Ohshima, A. Kovachenko, F. Hirata, *Protein Science* **2007**, *16*, 1927-1933.

Keywords: high-pressure protein crystallography, high-pressure adaptation, pressure denaturation

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Automation and remote control of the MX beamlines at the canadian light source

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The Canadian Light Source (CLS) is a 2.9 GeV national synchrotron radiation facility located on the University of Saskatchewan campus in Saskatoon. The Canadian Macromolecular Crystallography Facility (CMCF) is composed of two beamlines, the small-gap in-vacuum undulator illuminated beamline 08ID-1 and a second bending magnet beamline, 08B1-1 [1]. Beamlines are equipped with very robust end-stations including on-axis visualization systems and Rayonix 300 CCD series detectors. They are each complemented with a Stanford automounter (SAM) which accepts SSRL type cassettes or universal pucks. MxDC, a beamline control system developed in-house, is integrated with a data processing module, AutoProcess, allowing full automation of data collection and data processing with minimal human intervention [2]. AutoProcess is based on XDS, Pointless, CCP4 and BEST packages. The system also allows remote control of experiments through interaction with a Laboratory Information Management System (LIMS) that was developed at the facility.

The CMCF provides service to more than 60 Principal Investigators in Canada and the United States. Up to 25% of the beam time is devoted to commercial users and the general user program is guaranteed up to 55% of the useful beam time and is run under a peer-review proposal system. The CMCF staff provides "Mail-In" crystallography service to the users with the highest scored proposals.

[1] P. Grochulski, M.N. Fodje, J. Gorin, S.L. Labiuk and R. Berg, **2011** 08ID-1 Beamline, the Prime Beamline at the Canadian Macromolecular Crystallography Facility. *J. Appl. Cryst.* In press. [2] Fodje, M. N., Berg, R., Black, G., Grochulski, P., & Janzen, K. **2010**. Automation of the Macromolecular Crystallography Beamlines at the Canadian Light Source. *PCaPAC*, (130-132). Saskatoon.

Keywords: Macromolecular crystallography, Beamline automation, Remote access

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New possibilities offered to crystallography by 6-axis robotic-arm based systems

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CATS and G-Rob systems were developed on protein crystallography beamline FIP-BM30A at the ESRF. CATS [1] is a high throughput reliable sample changer currently operating on the major synchrotrons worldwide (BESSY, SLS, DLS, APS, ...) and commercialized by Irelec Company (www.irelec-alcen.com). G-Rob, also a 6-axis robotic arm based system, is a fully integrated device for crystallography beamlines (commercialized by Irelec) and laboratories (commercialized by NatX-ray company, www.natx-ray.com). G-Rob is an "all in one" system, since it integrates the following functions:

- sample changer,
- goniometer for frozen samples, capillaries, ... [2],
- crystallization plates/micro-chips screening for *in situ* analysis of diffraction condition and data collection [3],
- beam monitoring.

G-Rob provides unique features. It is automated: thanks to its tool changer, it goes automatically from one application to another. CATS and G-Rob are also highly flexible: if a new application or a new sample format emerges in the community, a new tool can be designed to implement it. They are highly reliable systems, based on well-known, industrial quality equipments, with reduced maintenance.

Several G-Rob systems, both at synchrotrons or as laboratories in-house systems, are now available (ESRF, EPFL, ...). The first system, in use on beamline FIP-BM30A, was made available to the research community in 2005 and up to now, users have expressed an unprecedented high degree of satisfaction. The crystallization plates screening capability for example appears to be a precious tool in several cases (crystals too small to be fished, or too fragile, or when there is no good cryoprotectant).

Several results obtained on FIP-BM30A are presented, such as *in situ* screening of membrane proteins, ribosome, high pressure protein diffraction, etc. Recent experiments demonstrated also the possibility of the automated structural screening for the Fragment Based Drug Design strategy: the same crystal was reproduced in presence of a library of fragments. Systematic *in situ* data collection has shown some of the fragments present in the active site, without having to manipulate the crystals individually. *In situ* data collection was also used recently to solve the structure of entire viruses (D Stuart et al.). All these experiments take advantage of a new sitting drop plate specially designed for *in situ* X-ray analysis. This plate was developed in collaboration between beamline FIP-BM30A at the ESRF (Grenoble, France) and Greiner BioOne. Movies are available on www.natx-ray.com

[1] Jacquamet et al., *JSR* **2009**, *16*, 14. [2] Jacquamet et al., *Acta Cryst.* **2004**, *D60*, 888. [3] Jacquamet et al., *Structure* **2004**, *12*, 1219.

Keywords: robot goniometer, X-ray screening automation

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Automated characterization of nanotube membranes of large Size By X-Ray scattering

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Carbon nanotubes are nanometer sized channels that have a very high potential for applications such as selective chemical filtration or water desalination. For such purposes, large membranes of parallel nanotubes, where all metal-based catalyst particles potentially obstructing nanotubes have been removed, are needed.

An original experimental setup based on X-ray scattering and fluorescence has been designed to characterize membranes of arbitrarily large surface (cm² to m²) [1]. We are able to determine quantitatively the nanotube alignment in the membrane, the density of nanotubes and to check for the removal of metal-based nanoparticles. We will present the set-up, the models we developed to analyze experimental data and some results obtained on the set-up.

The set-up/modeling can also be adapted to others membranes than those of nanotubes, using small or wide angle scattering depending on the membrane composition.

It should be underlined that although the analysis requires complete orientational modeling within the framework of X-ray scattering theory, the set-up is designed for a non-specialist and could be used for instance on an industrial production line, automatic fitting of the data providing one with two-dimensional mappings of the density, chemical composition and nanotube orientation in direct space (figure).

[1] M. Huard, J. Cambedouzou, D. Petermann, P. Joly, G. Guillier and P. Launois *CNRS patent*, December 2010.

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JBluIce-EPICS beamline control system for macromolecular crystallography

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The report overviews the open-source JBluIce-EPICS control system [1] developed for the trio of highly successful GM/CA-CAT macromolecular crystallography beamlines in Sector 23 at the Advanced Photon Source. To make the control system fast, robust, intuitive for users and easily adaptable to new beamline developments, several technical solutions were implemented. First, the system consists of only two software layers, the EPICS backend providing robust control of distributed beamline hardware, and multiple graphical user interface (GUI) clients powered by Java Eclipse RCP. This provides the GUI with direct access to any advanced hardware features, such as on-the-fly scanning capabilities of motion controllers, and it is easy to add new features. Second, the GUI was chosen to conform to the task-oriented philosophy and to mimic the look and feel of the successful SSRL BluIce. Most users become proficient with the software within minutes. Third, JBluIce clients are designed to operate in parallel with other beamline controls, thus streamlining such staff tasks as beamline preparation and maintenance, operations auditing and user assistance. Further, JBluIce-EPICS deploys multiple plugins that can be written in any programming language, thus involving more staff

in the development.

From the users' prospective, JBluIce provides: one-click change between 5, 10 and 20 µm beam sizes; one-click beamline energy change that may involve switching undulator harmonics, mirror lanes and beam realignment; automated diffraction rastering over multiple user-defined polygon shapes for finding small crystals and 'sweet' spots on poorly diffracting crystals [2], data collection along a vector [2]; automated on-the-fly fluorescent rastering with a shuttle scanning option, a faster and lower-irradiation compliment to the diffraction rastering [3]; fully automated fluorescence measurements for MAD that include signal optimization, fast on-the-fly energy scanning and automated adaption of scan range to chemical shifts [3]; fly-scan minibeam realignment; automated loop and crystal centering; controls for sample automounter; automated crystal screening; data collection auditing; remote access and more.

[1] S. Stepanov, O. Makarov, M. Hilgart, S.B. Pothineni, A. Urakhchin, S. Devarapalli, D.Yoder, M.Becker, C.Ogata, R. Sanishvili, N. Venugopalan, J.L.Smith, R.F.Fischetti *Acta Cryst.* **2011**, D67, 176-188. [2] M. Hilgart, R. Sanishvili, C. Ogata, M. Becker, N. Venugopalan, S. Stepanov, O.Makarov, J.L.Smith, R.F. Fischetti *J.Synch.Rad.* **2011**, submitted. [3] S. Stepanov, M.Hilgart, D.Yoder, O.Makarov, M.Becker, R.Sanishvili, C.Ogata, N.Venugopalan, D.Aragão, M.Caffrey *Acta Cryst.* **2011**, D67, submitted.

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Using GDA for novel data collection methods

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Generic Data Acquisition (GDA, www.opengda.org) is the Java-based data acquisition software developed and used at the Diamond Light Source, the third generation synchrotron light source in the UK. GDA is designed to have a generic and flexible client-server architecture that has proven itself by running on almost all beamlines at Diamond and is now in use at several other synchrotrons.

Graphical user interfaces in the GDA client are controlled with intuitive motions to set up experiments. Standard oscillation experiments with crystals at a single position are now routine. In addition to the standard experiment, we have implemented automated techniques that are useful for evaluating crystals or larger sample holder (grid scan) or for collecting data sets along a three-dimensional crystal (line scan). Aided by the development of rapid detectors and suitable sample stages that allow continuous data collection during scans, these techniques have become even more powerful tools for examining samples in ways that would have been too tedious before their automation. The GDA client also aids in evaluation of the results, with feedback from external software presented graphically to the user. This immediate feedback and automation of the experiment are two ways that the beamline control software can contribute to improving the data collected at beamlines.

Keywords: GDA, software, data_acquisition

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CrysAlis^{Pro}: facilitating variable temperature experiments

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