Poster Sessions

At the companion beamline, AMX, with an intense beam of 5-100 μ m suitable for investigating large complexes, the challenge of making efficient use of beam time dictates a high degree of automation. We plan to deploy a fast specimen automounter supported by a puck-loading machine working through the hutch wall. Further, the projected short data collection times dictate the time-shared use of the beam by several investigators. Already, crystallographers using the NSLS X29 undulator beam have welcomed its short beam time allocation method, and those at the similar X25 line, now equipped with a Pilatus 6M detector, experience what may evolve into (or return to) an asynchronous data collection method (collect now, analyze later).

At the SM3 beamline, emphasis will be on the acquisition of absorption, fluorescence, and Raman spectra interleaved or nearly simultaneously with X-ray diffraction measurements. Several of us have redeveloped the NSLS X26C beamline so that complementary structural information obtained by these methods now routinely provides new insights into enzymatic cycles as well as into the effects of radiation damage.

At the NYX beamline, the intellectual successor to NSLS beamline X4A, micro beams of 5-50 μ m and of very high energy resolution ($\Delta E/E$ of 5x10⁻⁵) will benefit the work of structural biologists focusing on challenging problems at the forefront of the field.

Additional life sciences beamlines will complement the four programs summarized above. Visit [1] for complete information.

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[1] NSLS-II: http://www.bnl.gov/nsls2/default.asp ; Approved beamlines: http://www.bnl.gov/nsls2/2010BeamlineProposalResults.asp

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Construction of new time-of-flight single crystal diffractometer SENJU at J-PARC

Ryoji Kiyanagi,^a Kenichi Oikawa,^a Itaru Tamura,^a Takashi Ohhara,^b Takuro Kawasaki,^a Koji Kaneko,^a Hiroyuki Kimura,^c Miwako Takahashi,^d Tamiko Kiyotani,^e Akiko Nakao,^b Takayasu Hanashima,^b Koji Munakata,^b Masatoshi Arai,^a Yukio Noda,^c Ken-ichi Ohshima,^d ^aJ-PARC center, (Japan) Atomic Energy Agency (JAEA), Tokai, (Japan). ^bResearch Center for Neutron Science & Technology, Comprehensive Research Organization for Science and Society (CROSS), Tokai, (Japan). ^cInstitute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, (Japan). ^dInstitute of Materials Science, University of Tsukuba, Tsukuba, (Japan). ^eShowa Pharmaceutical University, Tokyo, (Japan). E-mail: ryoji.kiyanagi@ j-parc.jp

A new time-of-flight single crystal diffractometer, SENJU, is being constructed in Materials and Life Science Experimental Facility (MLF) at Japan Proton Accelerator Research Complex (J-PARC). This instrument aims to pursue precise crystal and magnetic structure analyses including local structures. Target materials will be inorganic and organic materials with lattice constants up to 50 Å. The measurable sample size will be 0.1 mm³ on account of the high flux neutrons from the pulsed source. A wide spectrum of the pulsed neutron, together with wide coverage of scattering angles up to 4 sr, also makes possible the observation of Bragg reflections in a wide reciprocal space at once, which eases detections of clues of phase transitions such as super lattice reflections. In addition, a nearly symmetrical peak shape owing to a poisoned decoupled moderator will realize accurate analyses of diffuse scattering. The diffracted neutrons will be detected with newly developed scintillation detectors ($256 \times 256 \text{ mm}^2$) with the spatial resolution of 4 mm.

Available sample environments will include low temperature, high magnetic field and high pressure. A superconducting magnet has a wide opening angle for diffracted neutrons and a large bore around sample area. A dilution refrigerator (~ 50 mK) can be mounted onto the magnet. Other ancillary equipment can be also utilized in combination with another.

Softwares were also developed based on the software "STARGazer" that has been developed for iBIX at J-PARC. New features such as controlling goniometers and ancillary equipment, live-monitoring of measurements and the reconstruction of a intensity distribution in 3D reciprocal space were introduced.

Although the schedule has been delayed because of the devastating disaster, SENJU will be in commission in 2012.



Keywords: single crystal, structure, neutron,

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New developments for the phase 1 macromolecular crystallography beamlines at diamond light source

Ralf Flaig, Alun Ashton, Michael Engel, Dave Hall, Katherine McAuley, James Nicholson, Pierpaolo Romano, Juan Sanchez-Weatherby, James Sandy, Thomas Sorensen, Mark Williams, Graeme Winter, *Diamond Light Source, Harwell Science and Innovation Campus, Chilton, Didcot, OX11 0DE, (UK)*. E-mail: ralf.flaig@ diamond.ac.uk

Diamond Light Source [1] is the UK third generation synchrotron facility located south of Oxford. In the first Phase the structural biology community was served by the macromolecular crystallography (MX) beamlines I02, I03 and I04 starting with the user programme in early 2007. These widely tuneable (5-25 keV) SAD/MAD beamlines were complemented in Phase 2 with a MAD capable microfocus beamline I24 (7-25 keV) and a fixed-wavelength high-throughput station I04-1 (13.53 keV). In Phase 3 the long wavelength beamline I23 (3-12 keV), which is in the planning and construction stage, will complement the MX beamline portfolio [2].

High quality results, with over 520 structures submitted to the PDB, have been obtained from the Phase 1 MX beamlines during their operation so far. In order to improve efficiency we have improved the automation system, including a quicker sample exchange with the sample transfer robot and automatic loop finding and centering procedures. All three beamlines can now also be fully operated