even from the outside of beamlines over HTTPS protocol.

Keywords: automated data collection, robots, macromolecular synchrotron X-ray crystallography

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A proposed suite of macromolecular crystallography facilities for NSLS-II

Lonny E Berman[1], Marc Allaire[1], Mark Chance[3], Wayne Hendrickson[4], Annie Heroux[2], Babu Manjasetty[3], Allen Orville[2], Howard Robinson[2], Anand Saxena[2], Dieter Schneider[2], Wuxian Shi[3], Alexei Soares[2], Vivian Stojanoff[1], Robert Sweet[2]

[1]Brookhaven National Laboratory, National Synchrotron Light Source, Bldg. 725D, Upton, New York, 11973, USA, [2]Brookhaven National Laboratory, Bldg. 463, Upton, New York 11973, USA, [3]Case Western Reserve University, Cleveland, Ohio, USA, [4]Columbia University, New York, New York, USA, E-mail：berman@bnl.gov

A new, highly-optimized 3rd-generation synchrotron radiation (SR) source, the National Synchrotron Light Source -II (NSLS-II), is being planned as a replacement of the existing 2nd-generation SR source NSLS at Brookhaven National Laboratory. When operational, NSLS-II will deliver unprecedented brightness in the soft and hard x-ray spectral regions, e.g. at 8 keV about 10 times that of the brightest SR sources now available. NSLS hosts a strong macromolecular crystallography (MX) program, nearly 40% of its user community. At NSLS-II, MX is expected to be closely associated with other life sciences programs including small angle x-ray scattering, x-ray absorption spectroscopy, x-ray footprinting, and nanoscale imaging. We are preparing plans for a set of MX beamlines that would view canted, tunable undulator radiation sources in multiple straight sections of the storage ring, which would work independently. The experimental apparatus would include diffractometers to handle crystals of microns dimension or smaller, fast-framing active-pixel detectors, automated sample exchange and cryogenic apparatus, VUV/visible spectroscopy, and fluidic-based sample handling systems. These bright sources will extend MX into unexplored realms of sample size, perfection, and state of complexity and environment. Research and development in all of these areas are proposed, including methods for overcoming the effects of radiation damage, in order to exploit the properties of these sources. In addition to these undulator-based beamlines, it is also proposed to implement a set of MX beamlines viewing three-pole wiggler radiation sources, somewhat brighter than current NSLS bending magnet radiation sources. This work is supported by the US Dept. of Energy and the US National Institutes of Health.

Keywords: synchrotron radiation crystallography, synchrotron radiation optics, synchrotron radiation sources

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A new macromolecular crystallography beamline for softer X-ray at the Photon Factory

Naohiro Matsugaki, Yusuke Yamada, Masahiko Hiraki, Noriyuki Igarashi, Shigeru Yamamoto, Kimichika Tsuchiya, Tatsuro Shioya, Hideki Maezawa, Seiji Asaoka, Hiroshi Miyauchi, Toshihiro Tahara, Yasunori Tanimoto, Soichi Wakatsuki

High Energy Accelerator Research Organization, Institute of Material Structure Science, 1-1 Oho, Tsukuba, Ibaraki, 305-0801, Japan, E-mail：naohiro.matsugaki@kek.jp

The use of softer X-ray for phase determination in macromolecular crystallography has gained quite some popularity, owing to the interest in utilizing weak anomalous signals provided by light atoms such as sulfur and phosphorus present in native protein and nucleic acid molecules. The method is quite useful especially for the range of macromolecules which are difficult to prepare heavy atom derivatives. The Photon Factory has started to develop a new macromolecular crystallography beamline for softer X-ray at BL-1A of the 2.5 GeV ring, funded by the national project 'Targeted Proteins Research Program'. The beamline is designed to deliver an intense softer X-ray beam at around 4 keV using the first harmonics of a short gap undulator to enhance the weak anomalous signal from light atoms. The optics and the diffractometer are optimized for the softer X-ray beam. The expected beam intensity at around 4 keV is more than 10^{11} photons/sec on the area of 10 square microns at the sample position. The beamline can also cover the energy range of 12-13 keV with the 3rd harmonics, which enables Se- or Hg-MAD data collection from very small crystals with the intense 10 micron beam. The beamline development is particulary dedicated to the crystallographic study of integral membrane proteins and macromolecular complexes, systems of enormous biological significance which are currently difficult to be measured due to crystallization problems. The construction of the beamline is scheduled in the summer of 2009, followed by six months of commissioning. The beamline will be opened to the members of the national project in 2010.

Keywords: biological macromolecular crystallography, protein crystallography with synchrotron, synchrotron X-ray instrumentation

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AR-NE3A, a new pharmaceutical beamline for macromolecular crystallography at the Photon Factory

Yusuke Yamada, Noriyuki Igarashi, Matsugaki Naohiro, Hiraki Masahiko, Kikuchi Takashi, Mori Takeharu, Toyoshima Akio, Kishimoto Shunji, Wakatsuki Soichi

High Energy Accelerator Research Organization, Institute of Material Structure Science, 1-1 Oho, Tsukuba, Ibaraki, 205-0801, Japan, E-mail：yusuke.yamada@kek.jp

In recent years, advancements in high-throughput techniques for macromolecular crystallography have heightened the importance of structure-based drug design (SBDD) and demand for synchrotron use by pharmaceutical researchers has increased. In order to meet this demand, we are constructing a new high-throughput macromolecular crystallography beamline AR-NE3A, dedicated to SBDD, This is funded in partnership with Astellas Pharma Inc. The light source is an in-vacuum undulator in the PF-AR 6.5GeV ring, providing a high flux X-ray beam. The optics consist of three main components, a collimating mirror, double crystal monochromator with liquid nitrogen cooling system, and a toroidal doublu-focusing mirror. Ray-tracing simulations suggest that new AR-NE3A affords higher X-ray beam flux at the sample position than existing high-throughput beamlines at the Photon Factory, AR-NW12A and BL-5A. In the experimental hutch, there will be a high precision diffractometer, a fast-readout and high-gain CCD detector and a sample exchange robot which can handle more than two hundred cryo-cooled samples in a Dewar. In order to realize high-throughput data collection required for pharmaceutical researches, we are developing a fully-automated data collection system. With this system, automatic sample exchange, centering, data collection and data processing are automatically carried out according to a user defined schedule. The construction of the beamline will be completed in the summer shutdown of PF-AR. The beamline commissioning will be finished by the end of March 2009. The first user operation is expected in April 2009. Here, we will present the general outline and current progress of this project.

Keywords: synchroton radiation, structure-based drug design, automated data collection

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Beamline developments for structural biology at the Photon Factory

Noriyuki Igarashi, Naohiro Matsugaki, Yusuke Yamada, Masahiko Hiraki, Soichi Wakatsuki
Institute of Materials Structure Science, Photon Factory, 1-1 Oho, Tsukuba, Ibaraki, 3050801, Japan, E-mail：noriyuki.igarashi@kek.jp

Structural Biology Research Center at the Photon Factory currently operates 4 structural biology beamlines. AR-NW12A, BL-5A and BL-17A are insertion device (ID) beamlines, while BL-6A is a conventional bending magnet beamline. Among these ID beamlines, AR-NW12A and BL-5A are high-throughput structural biology beamlines. A micro-focus beamline BL-17A was newly constructed and opened to general users in 2006. It was designed for micro-crystal structure analysis. In addition, the intense lower energy beam at around 6 keV is used for structure determination by SAD phasing with light atoms. In the next two years, two more beamline construction plans are scheduled. A new high-throughput beamline will be built at PF-AR NE3A in summer 2008 and opened to users in April, 2009. The beamline is expected to show a higher performance than current high-throughput beamlines. The beamline will be mainly dedicated to drug design. Another new beamline will be built at PF BL-1A in FY2009. The goal is to deliver brilliant lower energy beam at around 4-5 keV (dedicated to sulphur SAD experiment) and more photon flux at around 12keV than that of BL-17A. After completion of these two new beamlines, we will operate three high-throughput, two micro-crystallography and one conventional beamlines. For further high-throughput protein crystallography, we facilitate automation of beamline operation, with developments of sample changer robots, automatic sample centering system and unified beamline control software. These developments based on stable beamlines and reliable network will allow for the goal of full integrated structure determination pipeline. Here, we will introduce overview of our beamline developments and our future plans. As for details of topics, please refer to our other presentations.

Keywords: macromolecular synchrotron X-ray crystallography, microbeam analysis, automated data collection

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Experiences with automated crystal screening at the JCSG

Christine B. Trame[1,2], H-J. Chiu[1,2], S. Oommachen[1,2], M. Miller[1,2], A. Cohen[1], I. I. Mathews[1], J. Song[1], A. Deacon[1,2]
[1]Stanford Synchrotron Radiation Laboratory, Joint Center for Structural Genomics, MS 99, 2575 Sand Hill Road, Menlo Park, CA, 94025, USA, [2]Joint Center for Structural Genomics (JCSG), E-mail：cbtrame@slac.stanford.edu

The Stanford Automated Mounting (SAM) system plays a crucial role in the JCSG crystal screening effort. Promising crystals are identified for data collection and screening results are used to optimize crystallization conditions. Typically, 2500+ crystals from ~70 protein targets are screened each month. We have developed several software and hardware tools to help us efficiently perform this activity. A cassette/dewar tracking system allows us to manage our crystal inventory. A 2D barcode reader is under development to verify the cassette identity prior to screening. A protocol was established to check the vacuum integrity in our shipping dewars to give an early warning of a failing dewar. A crystal sorting interface has been implemented in BLU-ICE, allowing us to consolidate our crystal inventory and to archive crystals that have been used for data collection. The interface also transfers crystals between SSRL cassettes and ALS pucks, which is particularly useful when we collect data at other synchrotron facilities. For the last 3 years during the SSRL summer shutdown, a Rigaku MM-002 X-ray microsource generator was used for screening. In 2007, we upgraded to a MM-002+ system, which we installed inside the BL1-5 hutch. The mounting for the source allowed us to take advantage of all the existing beamline hardware, including the SAM system. Typical screening exposure times were 5min per 0.5 degree. The MM002+ achieved double the throughput (>100 crystals/day), compared with the MM002 source. The diffraction resolution obtained with the microsource correlated well with the same crystal exposed using a SR source. The JCSG is funded by NIGMS/PSI, U54 GM074898. SSRL is funded by DOE BES, and the SSRL SMB program by DOE BER, NIH NCRR BTP and NIH NIGMS.

Keywords: SAM, JCSG, MM002+

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Automation of the protein crystallography beamline X06DA at the swiss light source

Meitian Wang, Roman Schneider, Claude Pradervand, Wayne Glettig, Mauro Roccamante, Takashi Tomizaki, Ezequiel Panepucci, Andreas Isenegger, Elke Zimoch, Herbert Kalt, Hubert Baechli, Qianhong Chen, Clemens Schulze-Briese
Paul Scherrer Institut, Swiss Light Source, Paul Scherrer Institut, Villigen, Aargau, CH-5232, Switzerland, E-mail：meitian.wang@psi.ch

X06DA is a new protein crystallography beamline at Swiss Light Source, which receives X-rays from a 2.9 Tesla super-bending magnet. The beamline is envisioned to fulfill the requirements of both industrial and academic users by combining a high degree of automation with high performance. In order to achieve maximum efficiency, beamline automation is implemented from optics alignment, energy changing, sample changing and centering, through to crystal screening, data collection, data processing and structure solution. A Bartels dual channel cut monochromator (DCCM) combined with collimating mirror and toroidal focusing mirror ensures rapid energy changing with a true fixed beam position at sample. A novel and compact goniometer (PRIGO) will offer freedom to position a crystal in many unique orientations (Chi: 0 - 70° Phi: 0 - 360°) while minimizing the collision risk with other beamline instruments. By combining DCCM and PRIGO, energy interleaved data collection with optimal crystal orientation could be carried out to fully exploit anomalous signals for SAD and MAD phasing. Furthermore, a versatile automatic sample changing system (IRELEC