agents against Gram-positive pathogens. Here we report new binding and structural studies of FapR from Staphilococcus aureus in complex with both its DNA operator and effector molecules, providing important hints to understand the mode of action of this conserved bacterial repressor.

Keywords: protein-DNA interactions, regulation of fatty acid biosynthesis, X-ray crystallography

MS.09.1

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Seeing the first stages of protein crystal nucleation through to a full powder pattern

Robert Von Dreele
Argonne National Laboratory, Advanced Photon Source, 9700 S. Cass Ave., Argonne, IL, 60439, USA, E-mail：vondreele@anl.gov

The nucleation and growth of protein crystals is the crucial process in any protein structure analysis. Powder diffraction provides a possible means for study of this process because crystallinity can readily be established by diffraction, and a time series of diffraction patterns can be used to explore the crystal growth. Analysis of this data shows not only the time dependence of the amount of crystallized material but also the dimensions of both the crystallites and the crystal unit cell. This talk will show an example of the crystallization of hen egg white lysozyme examined in real time by powder diffraction.

Keywords: powder crystallography, protein crystallization, kinetics of growth

MS.09.2

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Serial crystallography: Use of a micro-jet for diffraction of protein nano-crystals or molecules

David A Shapiro[1,3], Dan Deponte[2], Bruce Doak[2], Petra Fromme[2], Gary Hembree[2], Mark Hunter[2], Stefano Marchesini[1,3], Kevin Schmidt[2], John Spence[2]
[1]Lawrence Berkeley National Laboratory, Advanced Light Source, 1 Cyclotron Road, MS2-400, Berkeley, CA, 94720, USA, [2]Arizona State University, PSF470, Tempe AZ, 85287-1504, USA, [3]Center for Biophotonics Science and Technology, University of California at Davis, 2700 Stockton Blvd, Suite 1400, Sacramento, CA 95817, USA, E-mail：dashapiro@lbl.gov

We propose a method of acquiring protein powder diffraction data from the smallest available protein crystals that can be acquired through batch precipitation. A continuous micro-jet is used to deliver a solution of hydrated protein nano-crystals to an x-ray beam. This method requires neither the crushing of larger polycrystalline samples nor any techniques to avoid radiation damage such as cryo-cooling. Radiation damage is completely avoided because of the very small dose each crystallite receives as it is only briefly exposed to x-rays. We have commissioned an apparatus to record protein powder diffraction in this manner and in this talk present the first such patterns from photosystem-1 crystals with sizes less than 500 nm. These preliminary patterns show the lowest order reflections, which agree quantitatively with theoretical calculations of the powder profile. The results also serve to test our flow-focusing aerojet injector system, with future application to femtosecond diffraction in Free Electron X-ray Laser schemes, and for Serial Crystallography using a single-file beam of aligned hydrated molecules.

Keywords: serial crystallography, nanocrystals, radiation damage

MS.09.3

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Femtosecond laser etching of protein crystal to process and to isolate the single crystal

Yoichiroh Hosokawa[1,2], Masafumi Kashii[2,3], Hiroshi Y. Yoshikawa[2], Hiroaki Adachi[2,3], Yusuke Mori[2,3], Hiroshi Masuhara[1,2]
[1]Nara Institute of Science and Technology, Graduate School of Materials Science, 8916-5 Takayama, Ikoma, Nara, 630-0192, Japan, [2]Osaka University, 2-1, Suita, Osaka, 565-0871, Japan, [3]SOSHO Project (Crystal Design Project), 2-1, Suita, Osaka, 565-0871, Japan, E-mail：hosokawa@hskw.jp

Preparation technique of single protein crystal with suitable shape is needed for precise X-ray diffraction (XRD) measurement giving three-dimensional structure of protein. We have applied an infrared femtosecond laser to isolate and process protein crystal with irregular shape. When the intense femtosecond laser is focused on the protein crystal, electronically excited state of protein molecule is generated densely and the energy is distributed to vibrationally excited states of the molecules in time scale shorter than ns. On the other hand, the time scale for the morphological change of the crystal is longer than ns. Because of the time gap between the photoexcitation energy distribution and the morphological change, a stress is confined at the laser focal point in the time scale shorter than ns. As the result, the etching of the protein crystal by the femtosecond laser is initiated mechanically by the stress increase, though the etching by the other lasers is generally attributed to explosive sublimation explained by conventional heat generation process. The excellence of the femtosecond laser etching is that the cutting is enhanced by a cleaving behavior resulting to stress propagation from the laser focal point. Conclusively the protein crystal has hardly thermal damage by the femtosecond laser irradiation, which was checked by XRD measurement of the small cut component. Furthermore, debris of protein crystal generated by the femtosecond laser etching can be utilized as seed crystal. We confirmed that crystallinity of daughter crystal grew from the seed crystal was fine or comparable in comparison with the mother crystal. These techniques are applicable to select a single crystal from multiple growth forms, even when the size is micrometer-order.

Keywords: protein crystals, pulsed laser ablation, femtosecond laser

MS.09.4

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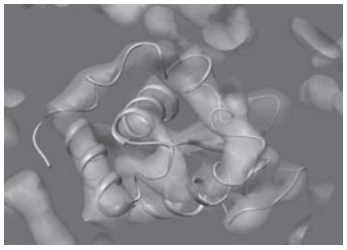
Features of the secondary structure of protein molecules from powder diffraction data

Sebastian Basso[1], Celine Besnard[1], Jon P Wright[2], Irene Margiolaki[2], Fabrice Camus[1], Gavin C Fox[2], Andy Fitch[2], Phil Pattison[1,3], Marc Schiltz[1]
[1]Ecole Polytechnique Federale de Lausanne, Laboratoire de Cristallographie, EPFL - Cubotron IPMC/BSP, lausanne, Vaud, 1015, Switzerland, [2]European Synchrotron Radiation Facility (ESRF), [3]Swiss-Norwegian Beamlines (SNBL) at ESRF, E-mail：sebastian.basso@epfl.ch

The determination of crystal structures greatly depends upon the availability of good quality single crystals, the growth of which is currently one of the major bottlenecks in macromolecular

crystallography. Recently, an interest has grown for protein powder diffraction which is becoming a well-established method in the field of structure refinement and molecular replacement. With the use of two examples it is shown that de novo solutions to the phase problem can be obtained at low resolution via phasing methods such as the isomorphous replacement method. Using synchrotron radiation, high quality protein powder patterns have been collected in which pH- and radiation-induced anisotropic lattice changes were exploited in order to reduce the challenging and powder specific problem of overlapping reflections. The Single Isomorphous Replacement method enabled the computation of molecular envelopes and the mapping out of the solvent channels in the crystal. Electron density maps in which features of the secondary structure of the lysozyme protein molecule can be discerned, were then obtained using the Multiple Isomorphous Replacement method (as illustrated in the image).



Keywords: powder diffraction, protein structure determination, isomorphous replacement

MS.09.5

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Characterization of spider silks weaved by different species living in the Black sea region of Turkey

Pinar Batat[1], Semra Ide[1], Tuncay Turkes[2], Orhan Mengen[3], Yusuf Ozcan[1], Omer Celik[4], Manfred Kriechbaum[5], Mustafa Sargon[6]
[1]Hacettepe University, Physics Engineering, Faculy of Enginnering, Physics Engineering Department, Beytepe, Ankara, 06800, Turkey, [2]Nigde University, Faculty of Science, Department of Biology, Nigde -Turkey, [3]Hacettepe University, Faculty of Science, Department of Biology, 06800 Beytepe-Ankara, Turkey, [4]Harran University,Faculty of Science and Art, Dept. of Physics, 63300 Sanliurfa, Turkey, [5]Institute of Biophysics and Nanosystem Research Austrian Academy of Sciences, 8010 Graz, Austria., [6]Hacettepe University, Medicine Faculty,Dept. of Anatomy, 06100 Sihhiye- Ankara, Turkey, E-mail：batat@hacettepe.edu.tr

Spider silks have attracted many researchers on account of their superior (Physical, chemical, biological and pharmacological) properties [1-4]. Our research group has begun to investigate spider silks with a project (TUBITAK, TBAG-107T017) after pre-studies[5]. The aims of this project are structural investigation of spider silk samples (in dragline and coccon forms) and obtaining some systematical information according to the different species(habitats, feeding and type of silk, etc.) First of all, our biologist group started to look for endemic species in The Backsea region of Turkey. They are indicating that, this geographic region is including very different spider species. During these researches, a lot of species, their draglines and egg-coccons were collected from their natural habitats. On the other hand, several living cavities (simulating their natural habitats) for the collected species were also constructed by our biologists in laboratory conditions. After these studies, a lot of silk samples produced by different species from Araneidae and Gnaphosidae familia were available. With this presentation, we would like to summarize our studies about structural investigation and characterization of the mentioned silks. Approximately, 15 samples were chosen and studied by using SEM, TEM, SWAXS, and XRD experimental methods. Alanine and glycine regions can be detected in XRD and SWAXS patterns due to their nanostructured and crystalline aggregations. XRD and SWAXS data have shown that the majority of these silks contain beta-plated sheet crystals that form from bilateral repeated aminoacid sequences rich in small aminoacid residues. At the end of the presentation, structural views, stabilizations and crystalinities of the samples will be compared.

Keywords: spider silk, Black Sea region, nanostructures, SWAXS, XRD, Araneidae, Gnaphosidae

MS.10.1

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Automation of the APS 11-BM high-resolution and high-throughput powder diffractometer

Brian H Toby[1], Jun Wang[1,2], Sytle Antao[1], Xuesong Jiao[1], Robert B Von Dreele[1]
[1]Argonne National Laboratory, Advanced Photon Source, 9700 S. Cass Ave, Argonne, IL, 60439, USA, [2]NSLS, Brookhaven National Lab, Upton NY USA, E-mail：brian.toby@anl.gov

The 11-BM powder diffractometer at the Argonne Advanced Photon Source operates with resolution on the order of $2x10^{-4}$ delta-Q/Q and collects an average diffraction pattern in ~1 hour. Equipped with a robotic sample changer, we expect this instrument to collect 20 or more datasets per day, primarily for remote users. Managing this level of use with minimal staffing has required that we optimize handling of sample metadata, as well as instrument control and data reduction. This talk will outline the database and web interface for 11-BM, which interfaces to the APS proposal and safety approval systems, as well as the instrument control system. A description of how users supply sample information and retrieve diffraction data via the web will be presented. The current instrument control software, which automatically calibrates the instrument, as well as streamlines data reduction, will also be discussed. Other topics to be presented include our current development plans, which will implement publication tracking and simplify sample storage and return/disposal. Progress on methods for automated review of diffraction data for internal consistency will also be presented.

Keywords: synchrotron powder diffraction, robots, automated data collection

MS.10.2

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Start to finish: Algorithms and parameters for successful robotic data collection

Lee M Daniels, Claire Wilson, Russ Athay
Rigaku Americas Corp, 9009 New Trails Dr, The Woodlands, TX, 77381, USA, E-mail：lee.daniels@rigaku.com

Data acquisition automation implies robotics, and the appearance of new commercial robotic systems (such as the Rigaku ACTOR-SM) for small-molecule samples now requires algorithms that are robust and reliable but also flexible. To achieve fully automated crystal mounting, centering, data collection and processing (and optionally structure solution and refinement), a large number of parameters are necessary. Also, the system should be able to make intelligent decisions about whether to keep a given sample or to move on to the next one. These decisions can be made by applying the technique of *ranking* in order to aid in the decision process, for example to choose the best crystal from a group or to avoid wasting time collecting data on a sample that is unlikely to provide viable results. The choice of a minimum rank will depend on the purpose of the experiment;