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Keywords: automation, crystallization, imaging

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Possibilities and limitations of X-ray diffraction using high energy X-rays on a laboratory system

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Recent interest in nanomaterials has increased the need to analyze structures on a local (nano) scale. However, the atomic structures of nanoparticles and nanostructured materials are not accessible by conventional methods used to study crystalline materials, because of the short ordering range in these materials. One of the most promising techniques to study nanostructures using X-ray diffraction is total scattering pair distribution function (PDF) analysis. This technique is successfully applied in a number of application areas in materials science and technology. The PDF analysis technique makes use of high quality, high energy X-ray scattering data, usually obtained at synchrotron facilities, available in several national and international research centers around the world. Despite the advantages and data quality that measurements at synchrotron beam lines offer to the researcher, in practice it can be difficult and time-consuming to get access to the facilities required. In order to be prepared as good as possible and to make optimal use of the valuable experiment time offered, it is highly desirable to perform selective measurements on candidate samples in the own research laboratory. New developments in XRD technology have been directed towards the possibility of performing nanocrystallography experiments on a standard laboratory X-ray diffraction system. In this presentation we will report on the possibilities and limitations of the use of high-energy X-rays on a homelab system.

Keywords: nanocrystalline materials, pair distribution function, X-ray diffraction

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Super high resolution powder diffractometer at J-PARC

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Neutron Science Division of High Energy Accelerator Research Organization (KEK) is constructing a Super High Resolution Powder Diffractometer (SuperHRPD) at Materials and Life Science Experimental Facility (MLF) of Japan Proton Accelerator Research Complex (J-PARC). SuperHRPD is designed to have the world best resolution $\delta d/d$ = 0.03%, which changes quite slowly in its covered d-range. SuperHRPD is located at about 100 m from a thin side of a decoupled poisoned moderator, which has been developed to produce a high-resolution & good S/N data to achieve the 0.03 % resolution within 100 m flight path. It has a 32 m curved guide and 50 m straight guide section between the instrument and the moderator. To prevent frame overlap caused for a long flight path, the disk choppers were installed in two places of the beam line. The measurement in various wavelength ranges is possible by using these disk choppers, and the adjustment of the choppers are scheduled. To install the beam line of long flight path, we constructed beam line building (MLF SuperHRPD BL building) and annex experimental hall (MLF SuperHRPD building) on the east side of MLF experimental hall. As soon as these buildings were completed in the end of 2007, a guide tube, various shielding blocks, etc. were set up. The *Sirius* diffractometer chamber, which had been used in the previous neutron facility, KENS, at KEK was installed at the SuperHRPD beam line (BL08). At the end of May in 2008, the first neutron was produced successfully at a spallation neutron source in MLF, and the high resolution Bragg reflections were obtained using the *Sirius* diffractometer chamber. The obtained data will be used in designing a new diffractometer chamber for BL08, which will be installed in the summer of 2009.

Keywords: neutron instrumentation, neutron powder diffraction, time-of-flight powder diffraction

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4SEASONS: A high-intensity chopper spectrometer for inelastic neutron scattering at J-PARC/MLF

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4SEASONS is one of the chopper spectrometers for the spallation neutron source in Materials and Life Science Facility (MLF), Japan Proton Accelerator Research Complex (J-PARC). It is intended to provide very high counting rate up to 300 meV neutron energy with medium resolution ($\Delta E/E_i$~6% at E=0) to efficiently collect weak inelastic signals from novel spin and lattice dynamics especially in high-T_c superconductors and related materials. To achieve this goal, the spectrometer equips advanced instrumental design such as an elliptic-shaped converging neutron guide coated with high-Q_c (m=3-4) supermirror, long-length (2.5m) ^{3}He position sensitive detectors arranged cylindrically inside the vacuum scattering chamber. Furthermore, the spectrometer is ready for multi-incident-energy measurements by the repetition rate multiplication method with a special Fermi chopper (the MAGIC chopper), and polarization analysis with ^{3}He spin filters. 4SEASONS is now under construction and will be ready to use in December 2008. In this paper, we show the design of 4SEASONS and current status of its construction. 4SEASONS is supported by Grant-in-Aid for Specially Promoted Research (No. 17001001) from MEXT of Japan.

Keywords: neutron inelastic scattering, neutron instrumentation, pulsed neutron scattering

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Preparation and imaging of lipidic cubic phase based protein crystallization experiments

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Protein crystals grown by the cubic phase method diffract well and have been useful in determining high-resolution structures of several membrane proteins. The lipidic cubic phase methodology employed produces crystallization experiments that pose additional challenges to inspection. A versatile microscope platform, with automated x-y stage and various illumination and imaging options, has been developed with specific application to protein crystal detection. The DETECT-X microscope is a fully automated protein crystallization imaging instrument that operates in polarization, oblique angle and trans-illumination and UV-epi illumination fluorescence mode. Protein crystallization trials in traditional crystallization trays can be imaged in a fully automatic fashion. In its unique birefringence imaging mode the DETECT-X microscope produces false-color coded images of crystalline matter depicting the orientation of the slow optical axis of protein crystals and their orientation independent birefringence. Images that demonstrate the unique protein crystal imaging capabilities of the DETECT-X microscope are presented. The combination of the different observation modes allows the imaging of protein crystals that have strong contrast with respect to their facets as well as the interior body of the crystal. Colorless, transparent protein crystals appear colored. This enhanced contrast, along with UV epifluorescence, allows researchers to (i) see protein crystals through a layer of precipitate, (ii) discern between amorphous precipitate and non-facetted sphaerulites or precrystalline matter, (iii) identify crystal twins, and (iv) distinguish between protein and salt crystals.

Keywords: membrane protein crystallization, birefringence microscopy, lipidic mesophases

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Protein crystallization at the laboratory of molecular biology: Robotics, procedures and developments

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LMB scientists can undertake initial crystallization experiments and also crystal condition refinements for each new protein sample using automated protocols. The LMB protein crystallization facility is high-throughput and includes various robots. The protocols are straightforward and setting up plates is easy. The standard initial screening protocol is comprised of 17 MRC sitting-drop plates pre-filled with a wide variety of commercially available screen kits. Process is fast and requires only small volume of protein. The 17 plates are set up within an hour using 272 ul of sample. 10,000 plates have been set up in 2007 for initial screening alone. Refinement, custom matrices and scale-up screens are made in any type of plate. A refinement screen in MRC plate is made in three minutes on the Sciclone i1000 workstation. New methods and tools are continuously developed and integrated into our crystallization facility. For example, The MRC multi-wavelength imaging system allows assessment of crystals regardless of clarity of the drops. The LMB screen database is a Web based tool to perform basic data mining about the initial screens. To further aid users, liquid handling advances, new micro-plates and specialized gas-tight and strong-binding plate seal developments have enabled the adoption of automated procedures for seeding, for experiments under oil and for crystallization at high temperature. A novel crystallization screen called Morpheus (commercialized by Molecular Dimensions) as also been developed recently. Each crystallization condition incorporates a broad range of small ligands that were found highly successful in co-crystallizations reported in the PDB.

Keywords: robotics, protein crystallization, Morpheus screen

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Structural studies of urate oxidase via powder diffraction

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Modern developments of the powder diffraction technique have allowed the investigation of systems with large unit cells like proteins [1]. Polycrystalline protein precipitates are frequently obtained under a variety of crystallisation conditions and thus powder methods can be employed for structural characterisation of small proteins when single crystals are unavailable. Urate Oxidase from Aspergillus flavus (Uox) is a protein used to reduce toxic uric acid accumulation and also in the treatment of hyperuricaemia which occurs during chemotherapy . In this study, we investigate the effects of pH, salt and polyethylene glycol (PEG) concentration on the structural characteristics of Uox uncomplexed and complexed with 8-azaxanthin (AZA). Powder diffraction data were collected at both room temperature and cryocooled conditions at the ESRF (Grenoble, France). A previously unknown orthorhombic phase of uncomplexed Uox was observed and novel crystallization methods were established. In the case of Uox complexed with AZA a different orthorhombic phase is identified. Correlations between the crystallisation conditions with the structural and micro structural characteristics of Uox will be presented.
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Keywords: proteins, powder diffraction, synchrotron radiation

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A new performing space group determination algorithm

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