The three Phase I MX beamlines have been built for state of the art high-throughput data collection on crystals of biological macromolecules and are now well in their fourth year of operation. High quality results have been obtained. Further improvement of the beamlines is ongoing with a focus of automating and streamlining as many components and experimental processes as possible, from beam conditioning to user interaction and data analysis but maintaining experimental flexibility.
Therefore, we are redesigning the end-station table, beam conditioning components and sample environment with the aim to add new and improved features. The system is also designed for ease of maintenance and keeps adaptability to future scientific requirements for the structural biology community. Delivery of the new end-stations is due to begin towards the latter half of 2010.
Further plans include the provision of an improved software user interface, fast sample screening, remote access and category 3 pathogenic sample handling (I03). An update on these developments will also be presented.

[1] http://www.diamond.ac.uk.
[2] http://www.diamond.ac.uk/Home/Beamlines/MX.html.

Keywords: Diamond Light Source, Macromolecular Crystallography, Beamlines

FA1-MS01-P04

Surfaces of Attenuation of Acoustic Waves in Cubic Crystals. Akhmedzhanov F.R.[a], Saidvaliev U.A.[b].
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In contrast to the propagation velocity the anisotropy of attenuation of high-frequency acoustic waves in cubic crystals is investigated insufficiently.
In this work the acoustic attenuation in $Bi_{12}GeO_{20}$ and $Bi_{12}SiO_{20}$ crystals has been investigated on the basis of experimental data on the attenuation of acoustic waves propagating along the main crystallographic directions. Measurements were carried out using Bragg diffraction of light by acoustic waves at room temperature in the frequency range from 0.4 to 1.5 GHz.
According to the known perturbation theory, the attenuation coefficient can be defined in terms of the effective viscosity. Since the viscosity tensor has the same symmetry as the elastic stiffness tensor, three independent constants must be determined for the crystal class 23, to which belong the investigated crystals. All the viscosity components were determined by substituting effective viscosity values obtained from measured attenuation data into the mode viscosity equations.
The obtained viscosity components were used for calculation of the anisotropy of attenuation of three wave modes propagating along any selected direction using equation:

$$\alpha = \omega \cdot \eta_{eff} / 2\rho \cdot V^3$$

where ω is the circular frequency, η_{eff} is the effective viscosity for selected direction, ρ is the density and V is the propagation velocity.
Calculations have been carried out for acoustic waves propagating in (001) and (110) crystallographic planes.
At the same time the contribution of dielectric loss in the total attenuation coefficient of piezoactive waves was assessed for these crystals [1]. It is shown that the dielectric loss can produce a significant influence on the magnitude and anisotropy of the attenuation coefficient for piezoactive longitudinal and transverse waves in $Bi_{12}SiO_{20}$ crystals.

[1] Shaposhnikov I.G., *ZhETF*, 1941, 11, 332.

Keywords: acoustic elastic properties, anisotropic properties, attenuation coefficients

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Microfocus Beamline for Macromolecular Crystallography MX2@PETRAIII. G. Bourenkov, M. Cianci, S. Fiedler, M. Roessle, T.R. Schneider.
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The undulator beamline MX2 in Sector 9/P14 of the upgraded PETRA III storage ring is a part of the integrated structural biology facility constructed by European Molecular Biology Laboratory at DESY, Hamburg. The purpose of the beamline is to deliver high-quality diffraction data in structural studies of large macromolecular complexes and membrane proteins relying on the usage of small or inherently heterogeneous crystals.
The beamline will provide the focal spot size down to about 4x1 μm^2, matching the dimensions of the smallest macromolecular crystals used for structure determination to date, as well as matching the requirements for spatially resolved sub-crystal diffraction applications on macroscopically disordered crystals. The beam size at the sample position will be adjustable by defocusing in two dimensions, up to ~300x300 μm^2 to permit *in-situ* optimization of signal-to-noise conditions for larger samples. This will be achieved by using an adaptive bimorph focusing mirrors (SESO/BASC/JTEC) in Kirkpatrick-Baez geometry with an ultra-precise surface of the vertical focusing mirror. Microfocusing conditions will be realized at beam divergence <0.5 mrad, sufficient for resolving large unit cells up to ca. 800 Å. For even larger unit cells and for optimal signal-to-noise conditions (e.g. for crystals with very low mosaic spread), further reduction in divergence down to 50 µrad will be achievable. The possibility of using unfocused beam will also be preserved.
The energy range of the beamline will cover most of the absorption edges commonly used for anomalous scattering phasing (Fe-K edge to U-LIII edge), in line with state-of-the-art MAD capabilities. In the high energy range, 17-35 kEV, optimal diffraction signal *versus* sample lifetime conditions are anticipated.
The end station will be equipped with a EMBL-MATTEL microdiffractometer MD2 and a high-efficiency mosaic CCD detector (RAYONIX). The setup was commissioned at DORIS beamline BW7A, and is proven to provide highly accurate data (e.g. for SAD phasing with anomalous signals <0.5%). The MD2 provides repeatability of mechanical positioning better then 0.2 µm, with a sphere of confusion 0.25 µm in a single-axis, and 0.7 µm in a multi-axis mode (r.m.s. values). Later upgrade to a multi-axis diffractometer with even higher precision is planned. Integrated data collection and processing software is being developed on the basis of TINE

(DESY) control system, MxCuBE (ESRF) and EDNA (www.edna-site.org).

Keywords: Synchrotron beamlines, instrumentation, microcrystals

FA1-MS01-P06

Structural biology of the nogalamycine biosynthetic pathway. Magnus Claesson, Gunter Schneider. *Mol. Struct. Biol., Karolinska Institutet, Sweden.*
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Anthracyclines are polyketide antibiotics with a high cytostatic potency and are used in the treatment of a wide range of tumor types. The usage is however limited by a cumulative cardiotoxicity, giving rise to severe side effects during and after treatment. There is therefore a need for new polyketide antibiotics, with reduced toxicity and maintained therapeutic effect.
As part of an on-going effort in the laboratory to characterize the biosynthetic pathways of anthracyclines, five genes encoding glycosyltransferases from two *Streptomyces* species have been cloned. One of these was successfully produced in soluble form and purified to homogeneity. Crystallization screening yielded crystals at several conditions and one of these conditions was scaled up, providing one data quality crystal from which data was collected. Crystal reproduction was optimized, however due to size limitations of the crystals no additional data quality crystals could be obtained. Reductive methylation was successfully utilized to improve crystal quality and reproducibility. Methylation appears not to have given rise to any new crystal contacts or changes in crystal packing, and the crystals were obtained in roughly the same conditions. The beneficial, but rather elusive, effect of the methylation seems to be a reduction in protein diversity, where the chemical treatment causes instable protein to aggregate. Furthermore the remaining protein is less likely to aggregate over time and seems less prone to excessive nucleation as compared with the native protein. The structure of this glycosyltransferase has been determined to 2.7Å in complex with a ligand, using molecular replacement.

Keywords: glycosyltransferases, natural products, X-ray macromolecular structure

FA1-MS01-P07

Facilities for Structural Biology and Chemical Crystallography at Diamond. Michael Engel, Elizabeth J. Shotton. *Diamond Light Source Ltd, Harwell Science & Innovation Campus, Didcot, Oxfordshire, OX11 0DE, UK.*
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Diamond Light Source was opened in October 2007. Phase I construction comprised the building, the machine and the first seven experimental stations. As part of Phase I, three macromolecular crystallography beamlines I02, I03 and I04 were built. The three beamlines will be tunable over the wavelength range 0.5 - 2.5 Å, to enable MAD experiments to be carried out with all three beamlines optimised for performance around the Se K-edge. Robotic systems for automated sample handling and crystal centring, and software allowing automated data collection have led to highly efficient and productive beamlines.
Facilities for remote monitoring and beamline operation further enhance the performance, and the implementation of biological containment at category 3 level on beamline I03 will allow pathogens to be studied.
I24, the tunable microfocus macromolecular crystallography beamline, became operational in July 2008 as part of Phase II. With a beamsize of 5-30 microns it enables measurements on small crystals that are not possible on conventional beamlines, due to their small size or mosaicity. With its ability to mount SBS-format plates it also improves the screening of crystals for optimisation of crystallisation conditions.
Two beamlines for structural chemistry have also opened recently. I11 provides high resolution, high throughput powder diffraction and I19 is a small molecule crystallography beamline suitable for studying microcrystals and weakly diffracting samples as well as excited state systems.
Further crystallography beamlines include a fixed wavelength MX station (I04.1) for high throughput experiments (currently under commissioning with 25% user mode) and I23, a long wavelength MX beamline (currently in the design phase).

Keywords: structural chemistry and biology, X-ray crystallography, synchrotron X-ray diffraction

FA1-MS01-P08

Sulfolobus solfataricus Adenine Phosphoribosyl-transferase. Sune F. Husted[a], Kristine S. Jensen[b], Anne Mølgaard[a], Jens-Christian N. Poulsen[b], Anders Kadziola[a], Kaj Frank Jensen[b]. *[a]Department of Chemistry and [b]Department of Biology, University of Copenhagen, Denmark.*
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Phosphoribosyltransferases (PRTases) are a group of enzymes that catalyze the formation of nucleotide 5´-monophosphates as essential precursors in the synthesis DNA or RNA. They all use a common substrate, 5-phosphoribosyl-α-1-pyrophosphate (PRPP), and transfer nucleobases to C1 of the ribose 5´-phosphate moiety of PRPP to form nucleotide 5´-monophosphates under the release pyrophosphate ($P_2O_7^{4-}$). PRTases are involved in both the *de novo* biosynthesis of nucleotides, e.g. orotate PRTase (OPRTase) and in the salvage path-ways, e.g. uracil PRTase (UPRTase), adenine PRTase (APRTase) and hypoxantine-guanine-xanthine PRTases (HGXPRTases; often with mixed specificity). PRTases share a common domain fold (type 1) which defines the specificity for PRPP and a variable domain for recognition of the various nucleobases.
Adenine PRTase structures are known for eukaryotes and bacteria and details of their active sites have been mapped out. APRTase from the thermophile archaean *Sulfolobus solfataricus* is an enzyme with unexpected properties: The substrate binding order is reversed with adenine binding first followed by PRPP. It has a double pH optimum and is potently inhibited by AMP and ADP. Sequentially it does not resemble other APRTases but merely HGXPRTases from eukaryotes, bacteria and archaea. The closest sequence homologues in PDB used for molecular replacement share about 31 % sequence identity for a 143/210 residue stretch of the sequence. The remaining sequence does not resemble any known structure. *Ss*APRTase is to our knowledge the first archaean APRTase to be structurally characterized.