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.


Keywords: Diamond Light Source, Macromolecular Crystallography, Beamlines

FAI-MS01-P04

Surfaces of Attenuation of Acoustic Waves in Cubic Crystals, Akhmedzhanov F.R.*, Saidvaliev U.A.*
*Nawoi state mining institute, Navoi, Uzbekistan.
*Tashkent university of information technology (Samarkand branch), Uzbekistan.
E-mail: farkhad2@yahoo.com

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 Bi12GeO20 and Bi12SiO20 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:

\[ \alpha = \alpha_0 \eta_{eff} \sqrt{2} \rho V^2 \]

where \( \alpha \) is the circular frequency, \( \eta_{eff} \) is the effective viscosity for selected direction, \( \rho \) 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 piezoeactive 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 piezoeactive longitudinal and transverse waves in Bi12SiO20 crystals.


Keywords: acoustic elastic properties, anisotropic properties, attenuation coefficients

FAI-MS01-P05

Microfocus Beamline for Macromolecular Crystallography MX2@PETRAIII. G. Bourenkov, M. Cianci, S. Fiedler, M. Roessle, T.R. Schneider.

European Molecular Biology Laboratory c/o DESY, Notkestr. 85, D-22603 Hamburg, Germany.
E-mail: gleb.bourenkov@embl-hamburg.de

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 \( \mu \)m², 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 \( \sim 300x300 \mu \)m² to permit in-situ optimization of signal-to-noise conditions for larger samples. This will be achieved by using an adaptive bimorph focusing mirrors (SES/Q/BASCTJE) 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 \( \mu \)rad 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-LLII 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 microdiffactometer 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 than 0.2 \( \mu \)m, with a sphere of confusion 0.25 \( \mu \)m in a single-axis, and 0.7 \( \mu \)m 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.

26th European Crystallographic Meeting, ECM 26, Darmstadt, 2010