extending the diffraction limit of samples. In some cases, X-ray data extending out to atomic resolution is obtainable. Methods of data collection as well as example data sets will be presented.

Keywords: data, atomic, collection

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A Design for a New State-of-the-Art Diffraction Facility

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We present the details of a new state-of-the-art diffractometer being constructed in the crystallography laboratory in the University of Durham. The machine is designed for single crystal diffraction experiments, to explore new extremes in sample environments and combinations thereof.

The new machine, accessing areas of structural chemistry that have hitherto been unreachable in the home laboratory, will comprise: a high intensity X-ray beam to enable crystals too small for standard laboratory machines to be studied; a three stage Displex cryo-cooler which will have a temperature range of ~2-300 K, carried on a robust set of circles and a large, motorised CCD detector. The Displex will be capable of housing Diamond Anvil Cells (DACs), both fixed pressure and variable pressure designs. The Displex will be modified to create a laser injection point enabling sample irradiation at a variety of laser wavelengths, while at very low temperatures. The combination of beryllium housing for the sample environment and the large CCD detector require us to devise solutions to separate the beryllium scatter from the desired diffraction. These solutions will be discussed, including preliminary results from a software collimator, currently under development in the crystallography laboratory, University of Durham.

Keywords: machinery design, cryocrystallography, lasers

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Picosecond Lattice Dynamics Probed by Time- and Angle-resolved X-ray Diffraction

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Fast time-resolved X-ray diffraction using intense pulsed X-ray sources such as synchrotron radiations (SRs) has enabled us to take a "snapshot" of atomic arrangements in transient states produced by ultrashort pulse laser irradiation. So far, we have been developed a picosecond pump-probe system at the SPring-8 undulator beamline by synchronizing a mode-locked laser and the SR pulses [1]. By the synchronization system, the transient lattice expansion of gallium arsenide crystals by the laser irradiation has been observed, and was applied to switching of X-ray SR pulses [2].

Here, we report the acoustic phonon oscillations near the surface of a GaAs crystal observed by employing the 40 ps time-resolved X-ray diffraction, combined with angle-resolved measurement of an X-ray beam diffracted in asymmetric geometry.

The experimental results show that femtosecond laser irradiation generates the longitudinal acoustic phonon and lattice expansion along the surface normal. By decomposing the time-dependent angular distribution of diffraction into peak shift and oscillatory part, acousto-optic effect was clearly observed as out-of-phase GHz-oscillations at sidebands around the principal peak shifted due to the lattice expansion.

[1] Tanaka Y., Hara T., Kitamura H., Ishikawa T., *Rev. Sci. Instrum.*, 2000, **71**, 1268. [2] Tanaka Y., Hara T., Yamazaki H., Kitamura H., Ishikawa T., *J. Synchrotron Rad.*, 2002, **9**, 96.

Keywords: time-resolved X-ray diffraction, synchrotron X-rays, lattice dynamics

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Time-resolved Studies with Pulsed X-rays at BioCARS: Present Capabilities and Future Directions

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Static structures for many molecules are available at high resolution but the mechanism by which these molecules function and the structures of intermediate states often remain elusive. Time-resolved crystallography is a unique technique for determining the structures of intermediates and excited states in biomolecular and chemical reactions. Using the Laue X-ray diffraction technique at the high-brilliance third-generation X-ray sources (ESRF, APS, SPring-8, etc.) snap shots are taken of molecules in action with a time resolution of about 100ps, the typical duration of a single X-ray pulse at synchrotron sources. We present the status of a user facility for time-resolved studies at the BioCARS beamline 14-ID at the Advanced Photon Source. During the past years a continuously growing time-resolved user community has developed; projects under investigation include light and chemically triggered reaction mechanism. Results from most recent studies of photo-sensitive proteins will be discussed. An overview will also be given on the current efforts in enhancing the technical capabilities for time-resolved experiments at BioCARS. The technical upgrades will improve resources for complementary optical monitoring of reactions in crystals, update the laser systems, and most importantly improve the X-ray optics to enable single X-ray pulse experiments.

Keywords: time-resolved Laue diffraction, structure and function, synchrotron radiation instrumentation

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Analyzing Mosaic Domain Changes Induced by Cryo-Cooling with Digital Topography

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To better understand how cryo-cooling affects the mosaic domain structure of protein crystals a complex experiment was undertaken. Super fine φ slicing was coupled with digital topography to study diffraction at two temperatures (RT and 100K) on a single crystal, keeping the same orientation and on the same set of reflections.

For the experiment, a single lysozyme crystal was immobilized in a capillary with epoxy to eliminate slippage. The orientation was adjusted until a group of reflections were positioned to minimize Lorentz effects. The reflection group also had an arrangement that allowed them to be collected on a digital topography system in one pass. For the first part of the experiment a super fine φ slicing run was collected followed by a digital topography run at room temperature. Next the crystal was cryo-cooled in the capillary maintaining the same orientation. After cooling, a run of digital topography followed by a super fine φ slicing run was carried out on the same reflections. After processing, the sequences were analyzed to determine how the cryo-cooling had affected the mosaic domains.

The crisp mosaic domains visible in the room temperature data were shattered during cooling, the domain borders became highly irregular and some regions failed to diffract at all. Although exaggerated, the angular relationships between the major domains appeared to be conserved.

Keywords: cryo-cooling, digital topography, fine phi slicing