standard MX synchrotron beamlines. If no anomalous scatter is available within this range, proteins are either labelled by soaking of ions into the crystals or by the exchange of methionine with seleno-methionine. However, both methods are limited in their applicability. Ideally, the phase problem should be solved directly from the unmodified, native protein or RNA/DNA crystal. This can be realized by using the intrinsic anomalous signal from sulphur or phosphorous present in these crystals. However, so far the success of long-wavelength phasing has been mainly limited to well diffracting crystals with high sulphur content due to the lack of optimised experimental facilities.

Beamline I23 at Diamond Light Source will be the first dedicated beamline for long-wavelength phasing experiments from macromolecular crystals. It will operate in a core wavelength range from 1.5 to 4 Å, offering a complementary setup to the suite of already five existing MX beamlines at Diamond. To minimize absorption effects, the complete beamline will be operated in vacuum. An X-ray tomography setup will be integrated into the experimental end station to determine the crystal shape and size as a basis for an analytical absorption correction. A large curved detector will allow access to diffraction data up to $2\theta = \pm 90^{o}$. An overview of the current status of the beamline project will be given, addressing all aspects of in-vacuum long-wavelength MX and the opportunities by extending the wavelength range towards the sulphur and phosphorous K-absorption edges.

Keywords: anomalous scattering, long-wavelength, synchrotron beamline

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Feasibility study of hard X-ray resonator of sapphire using back reflection

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X-ray cavity interference in sapphire resonator was investigated. The sapphire (0 0 30) reflection was chosen as the back diffraction for 14.315 KeV. The advantages of using sapphire resonator are (1) there is only one ordinary reflection under the back diffraction condition, and (2) the absorption is much less than for silicon [1], [2]. These factors could enhance the resonance interference and improve the cavity finesse. Several sets of crystal resonators with different thicknesses and gaps were manufactured and used for the X-ray diffraction experiment. The resonance spectrum in energy was obtained by using a high resolution monochromator consisting of four silicon crystals with the energy resolution of about 0.82 meV. The separation of two adjacent resonance peaks in energy scan, the so-called the free spectrum range, was measured, which is in good agreement with the theoretical value. These results indicate that the hard X-ray resonator of sapphire is potentially useful for X-ray optics, which can be used as a beam conditioner for producing quasi-coherent X-rays.

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Keywords: diffraction, resonator

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On a New "Gram"

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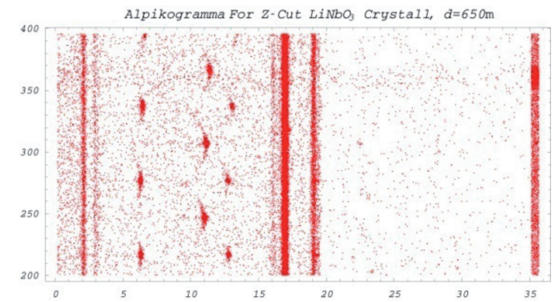
The investigation of phenomenon of radiation of electromagnetic wave by relativistic electrons shows that dynamic maxima are formed.

The dynamic maxima for quartz single crystals were first observed by the authors [1,2] on MAMI microtrone of Mainz University (Germany) for electron energy 255 MeV. In this work, it is reported about a new "gram" for crystal investigation with obvious advantages to the existing ones. In this work, the characteristic sections of dynamic maxima has been named to Alpik-grams in the author's honour.

Further the analogous investigations on SiO_2 sample were made for electron energies of 180 MeV and 280 MeV.

The present work is devoted to the possibility of detailed investigation of crystal structure and determination of the universality of detection of location of both the light and heavy atoms. On the figure below is shown the Alpik-gram of $LiNbO_{3.}$ In the picture, the locations of the dynamic reflections $(3\bar{3}00)$ of lithium niobate (for the energies ~6 keV, ~11keV, ~13 keV) and the characteristic radiation lines K_α-0.52 keV of oxygen and K_α-16.61 keV, K_β-16.615 keV of the niobate are clearly seen.

Thus, by detecting the radiation of the scattered electrons and on the basis of Bragg condition, it is possible to construct the spatial structure of $LiNbO_{3.}$ The suggested method enables to perform both the spectral and structural analysis analogous with Debye-Scherrer patterns and Laue-grams both for light and heavy nuclei.



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Keywords: electron, eadiation, X–ray.

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NE-CAT crystallography beamlines for challenging structural biology research

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The NorthEastern Collaborative Access Team (NE-CAT), located at the Advanced Photon Source (APS), focuses on the design, construction, and operation of synchrotron X-ray beamlines for the solution of technically challenging structural biology problems and provides an important resource for the international research community. Currently there are two operational undulator beamlines: 24ID-C - fully tunable in the energy range from 6 to 22keV (cover most element edges for phasing) and 24ID-E - fixed energy at ~12.66keV (optimized for Se SAD experiments). These operational beamlines are currently open to NE-CAT members and general APS users.

Both undulator beamlines are fully equipped with state-of-the-art instrumentation for its users. MD2 microdiffractometers installed at both the beamlines provide very clean beams from 5 microns to 100 microns in diameter and have exceptional sample visualization systems capable of visualizing micron-sized crystals with extreme clarity. Large-area CCD-based ADSC Quantum 315 detectors at both beamlines not only provide the best diffraction data, but also make it possible to resolve large unit cell dimensions. Both beamlines are equipped with ALS style robotic sample mounting systems, thereby making screening of large numbers of crystals much faster and less effort intensive. A new software suite RAPD provides data collection strategies and quasi-real time data integration and scaling through 128 core computing cluster. A simple automated MR/SAD pipeline for rapid structure solution is implemented. Users of the beamlines are supported by experienced resident crystallographers and have access to a full suite of data processing and structure analysis. A fully equipped chemistry laboratory and cold-room are also available for users.

NE-CAT facility is used to focus on NE-CAT research on structural studies involving technically challenging crystallographic projects. In order to meet these needs several novel hardware and software ideas are implemented. A summary of beamline capabilities, technology, scientific highlights and details of availability will be presented.

NE-CAT maintains a website at http://necat.chem.cornell.edu/.

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Keywords: macromolecular crystallography, microdiffraction, synchrotron X-ray instrumentation

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Recent developments in modeling single molecule imaging by x-ray free electron lasers

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We study the possibility of imaging small cluster of atoms or single molecules [1] by intense and short x-ray free electron laser pulses. Lately, the first hard x-ray free electron laser (LCLS) came into operation. Experiments on this line have been started. In the first experiments 20-50 nm resolution is the best expectation, but ultimately atomic resolution is the goal. In the nm scale the radiation damage is not a problem within the time window of the probe pulse. However, going into the few Å resolution range, the motion of atoms in the samples during the x-ray pulse has to be taken into account. The other difficulty in single molecule imaging is that the 3D diffraction pattern has to be compiled from the measured 2D patterns with unknown orientation. However, the determination of the orientation of 2D patterns is hindered by the low statistics of individual measurements. This can be circumvented by sorting the patterns into classes, in which every particle has the same orientation. We studied both of the above problems. Using our special molecular dynamics tool we model the motion of atoms in biological specimens, and we give limits to pulse parameters [2,3]. Concerning the classification problem, we worked out a special quality threshold approach, which allows the classification of realistic large data sets within a practical time scale [4].

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Keywords: XFEL, imaging

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Bringing microfocus beam and improved sample environment to MX users at Diamond

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The phase I macromolecular cystallography (MX) beamlines at Diamond Light Source [1] are continually undergoing improvement. To bring together many of the developments by Diamonds scientific and technical staff a major upgrade project has been undertaken to incorporate the best of the original sample environment, goniometry and end-station alongside recent developments and to introduce microfocus optics to the phase I MX beamlines. To this end the end-station has been redesigned to accommodate all the new features and provide a stable, adaptable platform for the future.

One of the biggest changes to the beamlines is the addition of tools to facilitate mini- and micro-focus beams. An aperture based system has been incorporated which allows masking of the incoming beam to 5 - 20 microns. In addition, beam microfocusing at discrete energy ranges has been added by the use of compound refractive lenses. This gives a focussed beam of approximately 10 x 5 microns (h x v) with a flux density of ~5 x 10^{15} ph/mm^2/sec at 12.7 keV. These two upgrades individually and in combination bring a new dimension to the experiment types possible for users of Diamonds MX phase I beamlines.

For the sample environment we have retained the excellent goniometer and shutter which combined with the stable beam provided by the machine has to date given superb data quality yet added improved sample centering stages to give more accurate and quicker sample centering. In the near future *in-situ* plate screening and data collection will also be possible in this set-up. The goniometer and sample environment have been reconfigured and designed to accommodate the recently installed Pilatus 6M detector on I03 and the mini-kappa crystal positioning system with no collisions when fully open through full rotation when using standard SPINE pins. The end-station will continue to be combined with the fast and reliable ACTOR robot system with rapid sample pre-centering via an industrial vision system incorporated into the end-station. Sample visualisation is achieved with an improved on-axis viewing system which has a fast zoom, a stable mounting system and the possibility to upgrade cameras readily.

To assist investigations of sample environment on room temperature crystals a new support has been developed which allows the easy exchange by users from the cryojet, used for traditional low temperature data collection, to the humidity controller I (HCI) for investigations of crystal quality and data collection at room temperature and the effect of dehydration on diffraction quality.

First results from these advances on the recently commissioned set-up on I04 will be presented. Beamlines I03 and I02 will upgraded this year with the same developments.