

of plates with the period of 2.3 micron is induced. It is shown, that the scattering of the relativistic electrons on such a stacks with the period of dielectric permittivity about a few microns in amorphous quartz leads to formation of intense transition radiation. Radiated photons have the intensity $\sim 10^7$ photon/second and the energy 1.3 KeV in a solid angle ~ 30 angular seconds with the energy spread $\Delta E/E \sim 10^{-5}$ [3]. The peak values of the energy E are coincide with $\gamma \omega_{pt}$, where γ is the Lorentz factor, and ω_{pt} is the plasma frequency of the melted quartz [2]. The theoretical evaluation and its comparison with the experiment shows that the maximal number of plates, which gives contribution to the intensity of the transition radiation is order to 20. The problem under consideration is theoretically solved using Maxwell's equations. Corresponding numerical calculations are carried out and conditions are found which yields to formation of the maximum number of photons. The obtained results are in good accord with the experiment [3].

[1] G.M. Garibyan and C. Yang.// Sov. Phys. JETP 36, p.631, 1973.

[2] L.Sh. Grigorian, A.H. Mkrtchyan, A.A. Saharian.// Nuclear Instruments and Methods B, pp. 197-202, 1998.

[3] A.R. Mkrtchyan, et al. // Physics Letters A, vol. 152, No 5,6, pp. 297-299, 1991.

Keywords: X-rays, superlattices, ultrasonics

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A monochromatic station for macromolecular crystallography at diamond light source

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The fixed wavelength monochromatic beamline will be situated next to the Phase I I04 MX beamline. The photon beam will be produced by two undulators placed in a canted formation, allowing I04 and I04-1 photon beams to be separated by 1 mrad. The beamline will provide rapid and extensive access to synchrotron radiation for a growing user community composed by both academic and industrial research groups. I04-1 will be dedicated to high-throughput data collection for rapid structure solution using MR method. As more structures are available in databases, MR is the most used method for the structure solution of proteins. The wavelength of the I04-1 beamline will be fixed at 0.9163 Å (energy of 13530 eV). The beamline will also be fully automated with a sample changer robot, automated crystal alignment, data collection and processing. Optionally, single anomalous diffraction (SAD) experiments will be possible since anomalous signal of several heavy atoms can still be measured at this wavelength. Finally, an X-ray fluorescence detector will be available to establish the metal ions footprint of the sample. I04-1 is currently in the construction phase and is planned to be ready for operation in late 2009.

Keywords: macromolecular crystallography, high-throughput data collection, fixed-wavelength

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Experience from operation and commissioning of the phase 1 MX beamlines at diamond light source

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Diamond Light Source [1] is the new UK third generation synchrotron located south of Oxford. In January 2007 Diamond welcomed first users. In Phase 1 seven beamlines are funded which includes three beamlines for macromolecular crystallography (MX) [2]. These are currently in a commissioning phase aimed for optimisation of operation. The beamlines are similar in design and take radiation from an in-vacuum undulator. A double crystal monochromator and a Kirkpatrick-Baez mirror arrangement are the main optical components. First experience from operation and results of the commissioning of the MX beamlines will be presented. This will include discussion of the beam properties, status and performance of the optical components and diagnostics in the optics hutch as well as results from commissioning of the equipment in the experimental end station. The software environment and results from data collections will also be discussed.

[1] <http://www.diamond.ac.uk>

[2] <http://www.diamond.ac.uk/MX>

Keywords: diamond Light Source, beamline commissioning, synchrotron

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Installation of high throughput protein crystallography data collection at SPring-8 BL12B2

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The SPring-8 Taiwan Contract Bending Beamline (BL12B2) has been dedicated to studies related to macromolecular crystallography in order to facilitate biological communities to explore all aspects of structural molecular biology. High-throughput protein crystallography using industrial automation technologies have significantly reduced the time needed to conduct protein structure experiments at many facilities around the world. At SPring-8, we are in the process of installing the new instruments of equipment stage, crystal goniometer, sample auto-changer robot SPACE and Beamline Control Software (BSS). The BSS software controls the entire beamline machinery such as pulse motors, counter control, equipment stage, automated sample changing, crystal centering and automatic data collection through the graphical user interface (GUI) communication protocol. The facility serves experts and non-expert crystallographers, who benefit in structural analysis from protein purification to three-dimensional structure determination. The upgrade of protein end station at SPring-8 Taiwan Beamline (BL12B2)

facility will be available for structural biology researchers for routine use from October 2008. In the near future, we also have a plan to construct a micro focused beam at our BL12B2 beamline. To apply for beamtime or for more details about the NSRRC facilities, visit the General User program website: (<http://portal.nsrcc.org.tw/>). The details of the up-grade installation will be discussed.

Keywords: synchrotron X-ray instrumentation, data collection methods, technology

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Crystallography at MAX-lab

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MAX-lab, the synchrotron radiation facility in Lund, Sweden is focused on soft X-ray activities. However, on the largest of the three storage rings, the 1.5 GeV MAX II ring, there are three beamlines operating at energies suitable for crystallographic experiments. I711 is a multipurpose beamline and is presently running powder diffraction and SAXS experiments. It is a tunable wavelength station with a range of 0.8-1.55 Å and uses a single monochromator crystal. The material science beamline I811 is primarily used for EXAFS and surface diffraction experiments and is a tunable wavelength station between 0.6-5 Å. It is equipped with a large multiple axis goniometer capable of carrying heavy loads such as UHV chambers. I911 is the protein crystallography beamline a consist of 2 fixed wavelength stations (0.97 and 1.03 Å) and one tunable wavelength MAD station (0.7-2.1 Å). The MAD station is equipped with a kappa goniostat and a MAR 225 CCD and the fixed wavelength stations has MARdtb goniostats with MAR 165 CCDs. The Mar dtb on the 0.97 Å beamline has been redesigned to fit the MAR flatpanel. The three beamlines provide a very wide range of different setups and detectors ranging from the 430x350 mm² flatpanel detector to scanning point detectors. A comparison of the stations and setups using powder diffraction data will be presented.

Keywords: synchrotron radiation crystallography, synchrotron powder diffraction, crystallography instrumentation synchrotron radiat

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Macromolecular crystallography at Diamond Light Source: Automation and pathogenic sample environment

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At Diamond Light Source [1] the three phase I macromolecular crystallography (MX) beamlines [2] have experienced their first year of user experiments. The current user programme is interspersed

with commissioning and optimisation of the X-ray source (including automation of beam delivery) in conjunction with deployment and improvements in software and hardware to provide intuitive, state of the art MX beamlines. A large component of this work is to automate as many components and experimental processes as possible, from beam conditioning to user interaction. Aspects of automation of MX beamlines include tracking of information of protein crystal samples from before arriving on site, automounting and screening for crystal quality, collecting data and processing the results, and recording the results of all these steps. Of particular note, beamline I03, will provide biological containment category 3 facilities in the near future for work with pathogenic crystals at room temperature. Automation will be an essential component of this development, allowing tracking of crystals and the automounting of 1680 samples before decontamination of the working environment is required. Automation of the routine aspects of MX should aid both experienced and less experienced users and allow them to profit from their short time on the Diamond MX beamlines to maximise their scientific output. This suite of beamlines will provide an excellent environment for the collection of data from both cryogenic and room temperature crystals, using automation to guide the experiment rather than direct it. The current status of all aspects of automation on the phase I MX beamlines at Diamond Light Source will be presented.

[1] <http://www.diamond.ac.uk>

[2] <http://www.diamond.ac.uk/MX>

Keywords: crystallography, automation, synchrotron

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Approach for automated data collection at the photon factory protein crystallography beamlines

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Fully-automated X-ray diffraction data collection has been strongly demanded by structural biology researchers. The key technologies of the fully-automated data collection are automated sample exchange and automated sample centering. We have developed sample exchange robots named PAM (PF Automated Mounting) system and installed at the Photon Factory macromolecular crystallography beamlines; BL-5A, BL-17A and AR-NW12A, which are designed based on SAM system developed by SSRL macromolecular crystallography group. In order to reduce the time required for the sample exchange, we developed a double-tongs system, Gemini, which can hold two sample pins at the same time. The double-tonged PAM system can exchange samples without leaving the diffractometer area within 10 seconds successfully. Data collection experiments require alignment of the sample to the X-ray beam. We have developed and implemented an automated loop centering function onto our GUI software. It can be automatically executed after the PAM system mounts the sample. Moreover, we are developing an automated crystal centering function based on low-dose diffraction patterns for fully-automated X-ray diffraction data collection. For estimation of the best diffraction conditions, we are developing software, PROCESSOR, which evaluates the diffraction patterns. In order to monitor the X-ray diffraction experiments, we have developed REPORTER software and a PReMo (PF Remote Monitoring) system. The REPORTER collects the states and the results of present experiments, and stores them in a large-scale storage. The PReMo system permits users to access the information