

The concept of using a microfocus X-ray source in combination with X-ray optics for diffraction experiments was first pioneered by U. Arndt in the early 90's. Since then, there have been numerous research activities for finding suitable combinations of high-brilliant microfocusing sealed tube X-ray sources and X-ray optics (e.g. capillaries, TR mirrors). A major breakthrough was the development of graded multilayer mirrors by H. Goebel. Combining graded multilayer mirrors with a state-of-the-art high-brilliance microfocus sealed tube results in a new class of high-brilliant X-ray sources for the home lab. These sources are characterized by a high performance (high flux densities, high spatial resolution) and excellent beam stability together with low power consumption and low maintenance. Third generation microfocusing sealed tube sources, such as the I μ S (Incoatec Microfocus Source), are now well established and give a performance beyond that of typical traditional X-ray sources - at power settings far below 1 kW. However, the past research work was focused, almost exclusively, on sources using Cu radiation. We will present selected results from single crystal diffraction experiments with the I μ S for Mo radiation. The flux density obtained from this source is about 1.5 times the flux density of a 5 kW rotating anode plus graphite monochromator on a 100 μ m sample. In our experiments with very small crystals (< 50 μ m), we have achieved gain factors of up to 3. Our results show that this source-optics-combination is very well suited for the structure determination on small crystals, as well as on medium sized samples.

Keywords: multilayer thin films, X-ray optics, powder and single crystal instrumentation

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Optimizing signal-to-noise on a home X-ray source for the analysis of microcrystals

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Microfocus sources and multilayer optics have yielded enormous increases in flux for home X-ray sources. With these advances, optimization of signal to noise of the measured intensities has received little attention, despite the fundamental considerations being well understood and incorporated at synchrotron beamlines. We are developing a home X-ray system which allows easy experiment optimization in daily use. Some of the important considerations in this development include: A collimator assembly to allow real-time adjustable beam size and divergence which decreases noise by limiting exposure to the diffracting crystal; Minimize air scatter from the direct beam, but also allow measurement of very low resolution reflections through the use of collimator/beam stop/cold stream configurations; A noise-free photon counting detector (Axiom) to enable exposures required for tiny crystals with correspondingly tiny beam; High resolution imaging camera for accurate alignment and crystal quality assessment; Ice-free sample changer with semi-automated alignment protocols, to allow routine characterization of small crystals; Supporting software that exposes only true experimental considerations to the user, allowing even inexperienced users to routinely collect the best data possible. First versions of the system are intended to allow screening of extremely small crystals towards increasing efficiency of synchrotron beamtime. More ambitiously, we envisage that the system will allow routine collection of high quality datasets from small crystals that currently require synchrotrons. This is particularly pertinent in the context of Chemical

Biology at the SGC, which requires large numbers of protein-ligand datasets, even from marginally diffracting crystals

Keywords: microcrystal, homelab, microfocus

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Present status of energy recovery linac project in Japan

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The 5 GeV class ERL should be the most promising candidate to progress the new synchrotron radiation activities which are based on sub-pico second pulses and/or spatially coherence of the synchrotron radiation, as well as to support a large variety of user needs. The value of the emittance of the electron beam is the order of 10 pmrad, which corresponds to the value of the emittance of 10keV photon itself, so that the x-ray from the ERL is expect to have a good spatial coherence, and also the value of the bunch width is the order of the order of 100 femto-second to open the scientific field of the dynamics of the material science. To this end, the official organization of the ERL project office has started at KEK from 1st of April 2006. An R&D team for a compact ERL has been organized in collaboration with accelerator scientists from JAEA, ISSP, UVSOR, Spring-8 and AIST. Since there is no GeV-class ERL machine in a world now, it is necessary to construct the compact ERL with the energy of 60~200 MeV to develop several critical components. In 2006 and 2007, we concentrate the designing and development of the machine and key accelerator components. The compact ERL will bring us not only the opportunity as a test facility for several accelerator components but also characteristic scientific cases based by such as high intense THz radiation which is produced as a coherent synchrotron radiation (CSR) from short electron bunch and/or laser-inversed Compton X-ray source which will give us a scientific opportunities of femto-second X-ray or X-ray imaging. The present status of the ERL project including the scientific case, and the detail of R&D of the accelerator will be presented at the conference.

Keywords: synchrotron radiation, X-ray imaging, nanoanalysis

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Transition radiation of relativistic electron from the superlattice of dielectric permittivity

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The possibilities of formation of an intense source of monochromatic radiation in x-ray range [1], manageable in space and time are considered. It is based on the transition radiation of relativistic electrons from the superlattice of dielectric permittivity induced by electromagnetic field or double-walled nano-acoustic tube [2]. The experiments are carried out on the 20 MeV electron bunch. At the 1.2 GHz frequency of the electromagnetic field the superlattice - stack

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.

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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)