

**P01.01.01***Acta Cryst.* (2008). **A64**, C171**Two-dimensionally curved Ge for focusing crystals prepared by a hot plastic deformation**Hiroshi Okuda<sup>1</sup>, Kazuo Nakajima<sup>2</sup>, Kozo Fujiwara<sup>2</sup>, Kohei Morishita<sup>2</sup>, Shojiro Ochiai<sup>1</sup><sup>1</sup>Kyoto Univ., Mater.Sci. Engineering, Yoshida-Honmachi, Sakyo-ku, Kyoto, Kyoto, 606-8501, Japan, <sup>2</sup>IMR, Tohoku Univ. Katahira, Sendai 980-8577, Japan, E-mail: okuda@materials.mbox.media.kyoto-u.ac.jp

Hot plastic deformation was applied to Ge single crystal wafers to prepare monochromating crystals for X-rays with focusing functions. Deformation was made in one or two dimensions, corresponding to the functions required. Hot plastic deformation has a merit that the crystal does not require supporting materials, and large deformations. On the other side, naturally it results in introduction of lattice defects. Therefore, a balance between deformability and the crystal quality is required. It means that the present approach is a useful solution for conventional X-ray source and potentially for neutrons. In the present study, we demonstrate that Si and Ge wafers can be deformed into cylindrical or spherical shape with radius of curvature up to several cm with keeping mirror surface. The crystal quality of the deformed wafers were examined by a conventional X-ray source with channel-cut incident monochromator. For an example of point-focusing monochromating crystal, Ge (111) single crystal wafers were deformed just below the melting temperature. For Cu K $\alpha$  and 333 diffraction condition, a Johansson monochromator gives the condition that the crystal surface is spherical. X-ray diffraction with channel-cut monochromator showed that (111) lattice plane had a curvature 2R in the focusing plane and a curvature R perpendicular to it, with a hemispherical inner surface with a radius of R=600 mm. By using a Cu K $\alpha$  radiation, a diverging X-ray was focused to a small spot. Part of the present results was finally supported by JST and MEXT.

Keywords: hot plastic deformation, Johansson crystal, Ge

**P01.01.02***Acta Cryst.* (2008). **A64**, C171**New optics for molecular macromolecular crystallography**Joseph D Ferrara<sup>1</sup>, Adam Courville<sup>1</sup>, Angela R Criswell<sup>1</sup>, Licai Jiang<sup>2</sup>, Bret Simpson<sup>1</sup>, Kris F Tesh<sup>1</sup>, Boris Verman<sup>2</sup>, Cheng Yang<sup>1</sup><sup>1</sup>Rigaku Americas Corporation, 9009 New Trails Drive, The Woodlands, Texas, 77381, USA, <sup>2</sup>Rigaku Innovative Technologies, 1900 Taylor Road, Auburn Hills, MI, 48326, USA, E-mail: joseph.ferrara@rigaku.com

We have developed two new VariMax<sup>TM</sup> optics for macromolecular crystallography, one for screening very small samples and the other for easy switchover between Cr and Cu radiation. It is well known that automated crystallization methods produce smaller crystals. In order to provide for better screening of initial hits for further optimization of crystallization conditions, better screening for subsequent data collection at synchrotrons or even rapid data collection at home, we have developed a very high flux optic, the VariMax-VHF. This new optic provides a beam of 0.1 mm FWHM focused at the sample with up to 3.5 fold more flux at 0.1 mm than conventional optics when coupled to a microfocus rotating anode source. These enhanced properties of the beam provide for easier analysis of small crystals and faster screening of routine samples. Additionally, now that SAD techniques have surpassed MAD as the primary method for structure solution, we have developed the

VariMax-DW, a revolutionary dual-wavelength optic. This optic is designed to allow for easy switchover between chromium and copper radiation with only minor realignment of the optics path. It is accomplished by providing two sets of optical surfaces (one for each wavelength) and one slit to choose the desired wavelength. In this paper we will present results on the efficacy of both optics for macromolecular crystallography applications.

Keywords: X-ray focusing optical elements, X-ray monochromators, microbeam analysis

**P01.01.03***Acta Cryst.* (2008). **A64**, C171**X-ray diffractometry with a microfocus source**Carsten Michaelsen<sup>1</sup>, Joerg Wiesmann<sup>1</sup>, Bernd Hasse<sup>1</sup>, Uwe Preckwinkel<sup>2</sup>, Holger Cordes<sup>2</sup>, Ning Yang<sup>2</sup><sup>1</sup>Incoatec GmbH, Max-Planck-Strasse 2, Geesthacht, -, 21502, Germany, <sup>2</sup>Bruker AXS, 5465 East Cheryl Parkway, Madison, WI 53711-5373, U.S.A., E-mail: administration@incoatec.de

The increasing importance of X-ray diffractometry with 2-dimensional detectors has led to a rising demand for highly intense X-ray sources enabling the analysis of very small and weakly scattering samples in the home-lab within a reasonable time frame. Therefore, various microfocusing sealed tube X-ray sources with focal spot sizes below 100 $\mu$ m are now available. Results of the new low-maintenance high-brilliance Incoatec Microfocus Source I $\mu$ S will be presented. The source incorporates an optimized combination of an extremely bright and very durable stationary air-cooled 30 W microfocus source and the newest type of 2-dimensional beam shaping multilayer optics, the so called Quazar optics. We will present measurements with the I $\mu$ S equipped with different 2-dimensional beam shaping multilayer optics. The comparison of I $\mu$ S with typical sealed tube fine focus systems shows data of outstanding quality in diffractometry applications using a 2-dimensional detector. A great improvement in intensity and resolution by factors of about 15 was observed. I $\mu$ S delivers very promising results in particular with measurements of powders in transmission geometry. Better crystallite statistics and better resolution are achieved when focusing onto the detector enables. Depending on the applications intensity gain factors in the range of 100 can even be achieved. For small angle scattering a factor of 5 in comparison to a typical sealed tube instrument was observed when using an I $\mu$ S with optics for a parallel beam.

Keywords: microfocus source, multilayer optics, diffractometry

**P01.04.04***Acta Cryst.* (2008). **A64**, C171-172**Small X-ray beams for small crystals: Pushing the limits of home-lab X-ray sources**Juergen Graf<sup>1</sup>, Carsten Michaelsen<sup>1</sup>, Thomas Schulz<sup>2</sup>, Dietmar Stalke<sup>2</sup>, Christian Lehmann<sup>3</sup>, Michael Ruf<sup>4</sup><sup>1</sup>Incoatec GmbH, Max-Planck-Str. 2, Geesthacht, Schleswig-Holstein, 21502, Germany, <sup>2</sup>Institut fuer Anorganische Chemie, Universitaet Goettingen, Tammannstr. 4, 37077 Goettingen, Germany, <sup>3</sup>Max-Planck-Institut fuer Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Muelheim, Germany, <sup>4</sup>Bruker AXS Inc., 5465 East Cheryl Parkway, Madison, WI 53711-5373, U.S.A., E-mail: graf@incoatec.de

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 $\mu$ 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 $\mu$ 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  $\mu$ m sample. In our experiments with very small crystals (< 50  $\mu$ 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

### P01.04.05

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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