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Two-dimensionally curved Ge for focusing crystals prepared by a hot plastic deformation

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Hot plastic deformation was applied to Ge single crystal wafers to prepare monochromating crystals for X-rays with focuing 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 crylinderical 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 monochromater. For an example of point-focusing monochromating crystal, Ge (111) single crystal wafers were deformed just below the melting temperature. For Cu Kα and 333 diffraction condition, a Johansson monochromator gives the condition that the crystal surface is spherical. X-ray diffraction with channel-cut monochromater 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 Kα radiation, a diverging X-ray was focused to a small spot. Part of the present results was finatially supported by JST and MEXT.

Keywords: hot plastic deformation, Johansson crystal, Ge

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New optics for molecular macromolecular crystallography

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We have developed two new VariMax™ 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

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X-ray diffractometry with a microfocus source

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The increasing importance of X-ray diffractometry with 2-dimensional detectors has lead 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 100µm are now available. Results of the new low-maintenance high-brilliance Incoatec Microfocus Source IµS 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 IµS equipped with different 2-dimensional beam shaping multilayer optics. The comparison of IµS 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. IµS 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 IµS with optics for a parallel beam.

Keywords: microfocus source, multilayer optics, diffractometry

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Small X-ray beams for small crystals: Pushing the limits of home-lab X-ray sources

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