

performance as a microfocusing optics for synchrotron high energy x-rays in terms of efficiency, resolution and background suppression.

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PS-14.01.11 DETECTION OF ELLIPTICAL POLARIZATION BY MULTIPLE-BEAM DIFFRACTION by W.Schwegle*, K.Hümmel and E.Weckert. Institut für Kristallographie, Universität (TH) Karlsruhe. Germany

With the development of exotic insertion devices (wigglers and undulators), with new designs of sophisticated beam line optics and with an increasing interest in experiments requiring circularly polarized X-rays the complete determination of the state of polarization becomes more and more important. Recently, Shen and Finkelstein (*Phys. Rev.* **B45**, p. 5075, 1992) proposed a new method based on multiple-beam diffraction, which takes advantage of polarization-state mixing in a non-coplanar three-beam case.

The fundamental equations of dynamical theory contain phase-sensitive couplings between the excited wavefields due to the complex structure factors $F(\mathbf{n})$ with $\mathbf{n} = \pm \mathbf{h} \pm \mathbf{g} \pm (\mathbf{h}-\mathbf{g})$ as well as a geometrical coupling. For an appropriate choice of polarization vectors $\boldsymbol{\kappa}$ (parallel to primary scattering plane) and $\boldsymbol{\sigma}$ (perpendicular to this plane) the influence of any polarization can be illustrated by a perturbational approach (Bethe approximation). However, for quantitative results full dynamical theory for a parallel-sided slab of crystal has to be applied.

Systematic calculations as well as experimental results demonstrate, that sensitivity to any given polarization can be optimized by an appropriate choice of

- (i) moduli of the structure factors
- (ii) triplet phase $-\varphi(\mathbf{h}) + \varphi(\mathbf{g}) + \varphi(\mathbf{h}-\mathbf{g})$
- (iii) geometry of the three-beam case
- (iv) orientation of the three-beam geometry with respect to major axis of elliptical polarization.

Measurements have been performed with a (111)-oriented GaAs and a (001)-oriented SiO₂ (quartz) plate for wavelengths from 0.83 to 1.81 Å. Different states of left- and right-handed polarization were available at bending magnet beam line C at HASYLAB for radiation emitted above and below the plane of electron orbit selected by slits. A special 6-circle diffractometer allowed the realization of any desired diffraction geometry.

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PS-14.01.12 ABSORPTION, EXTINCTION AND DEAD-TIME CORRECTION FOR HIGH PRECISION IMAGING WITH SYNCHROTRON SOURCES. By D. du Boulay and E.N. Maslen*, Crystallography Centre, University of Western Australia, Nedlands, Western Australia 6009

High accuracy is not critical for strong reflections when determining crystal structures with X-ray structure factors. The least squares residuals for refinements of the atomic coordinates are dominated by high angle reflections which, on average, are less intense. When measuring vibration tensors it is sufficient to achieve comparable *relative* precision for low and high angle structure factors.

Different criteria apply to high precision diffraction imaging of the deformation density $\Delta\rho$. Small single crystals are used increasingly for those studies, to ensure that no extinction correction is far from unity, ensuring that the reliability of the extinction corrections is not limited by the uncertain validity of the underlying theory.

If the high order reflections are measured for very small crystals using a conventional X-ray tube source, the precision of $\Delta\rho$ images is often limited by counting statistics. Poisson statistics errors can be reduced dramatically by using synchrotron radiation. The smoothness of the $\Delta\rho$ maps for recent synchrotron radiation experiments indicates that precision is no longer limited by counting errors.

The reproducibility of synchrotron radiation $\Delta\rho$ maps does not yet approach estimates based on statistical errors alone. The accuracy of most $\Delta\rho$ images is limited by residual systematic error for the strong low order reflections. It is the absolute error in the structure factors, and not their relative precision, which limits the precision of diffraction images of the deformation density. The accuracy desired for the strong reflections imposes serious demands on how well the absorption, extinction and dead-time corrections are to be evaluated.

Precise absorption corrections require correctly indexed faces, measured with a precision which, for small crystals, taxes the power of optical microscopes. Care is required when evaluating absorption corrections by the analytical formula (N. W. Alcock, *Acta Cryst.*, 1974, B48, 639-644) to retain precision near points where the basic expression is indeterminate. The extinction correction formula of Zachariasen (*Acta Cryst.*, 1967, A23, 558-564) implies constraints on structure factor magnitudes which are not necessarily satisfied in practical cases. Dead-time corrections applied automatically by the circuitry are not necessarily precise enough for high precision studies.

Methods for attaining and checking the precision of absorption, extinction and dead-time corrections for standard diffraction experiments on small crystals will be described.