

16.2-5 NEW METHOD FOR INDEXING LAUE PATTERNS. By K. Ohsumi, K. Miyahara and M. Ohmasa<sup>\*</sup>, Photon Factory, National Laboratory for High Energy Physics, Japan, <sup>\*</sup>Institute of Materials Sciences, University of Tsukuba, Japan.

Synchrotron radiation (SR) makes it possible to obtain information of micro-size crystalline materials of less than 5  $\mu\text{m}$  on each edge. To deal with such a small specimen, special care should be paid to the measurement of diffraction intensities. The beam size of an incident X-ray should be made as fine as the crystal size in order to avoid high signal-noise ratio. Under such conditions, it seems impossible to maintain the specimen in the fine beam during data collection by a moving crystal method such as a four-circle diffractometer. Therefore, the Laue method combined with SR is employed for the microcrystallography.

In the course of obtaining observed structure amplitudes from the specimen, it is essential to know the index of each reflection. In the case of a micro-size crystal, it is difficult to decide the index from the outer face of the specimen even under a microscope. Accordingly it is impossible to set the crystal in symmetric orientation to an incident X-ray beam, depending on the outer form of the specimen. And it is also impossible to re-mount the specimen to adjust its orientation. This means that the usual way of assigning indices to diffraction spots cannot be used. A method of determining the indices of the diffraction spots on Laue photographs at arbitrary orientation needs to be available.

A new method for this purpose is developed, based on the comparison of inter-face angles obtained from pairs of diffraction spots with those calculated.

The method in principle is the same as the determination of axial ratio of the material from its morphology. In the case of an unknown material, the crystal data will be obtained, provided that the d-spacing of any reflection is determinable.

16.2-6 SINGLE-CRYSTAL ENERGY-DISPERSIVE LAUE-TYPE EXPERIMENTS. By K. F. Fischer and H.-G. Krane, Institute of Crystallography, University of Saarbrücken, Fed. Rep. of Germany (BRD).

Single-crystal Laue-type diffraction experiments are reported using conventional white radiation and employing a pure-Ge SSD with a multi-channel analyzer. Depending on  $d$ ,  $\theta$  and wavelength range of the x-ray source, a number of harmonic reflections can be observed separately at the same time (Knof, Spilker, Krane, Fischer, Z.Krist. 1986, 174, 117-120). A fixed crystal, fixed-counter technique permits measuring weak intensities in controlled environment, e. g. Bragg peaks disappearing under a phase transition (betaine phosphate) or the temperature dependence of "forbidden" reflections (Krane, Fischer, Z.Krist. 1986, 174, 121-123). Changing  $\omega$  and  $2\theta$ , anomalous dispersion effects were measured by scanning selected reflections across the absorption edge of anomalous scatterers (Fischer, Krane, Z.Phys.B. 1985, 61, 57-61).  $|F|^2$  of these reflections can thus be experimentally decomposed into 3 constituents (4 for non-centrosymmetric crystals) representing 3 different classes of interatomic vectors, in analogy to the vector-set separation in the "lambda-technique" (Fischer, A.Cryst. 1984, A40, C-398). First tests for direct analytical determination of the anomalous scatterers' coordinates from one of these  $|F|^2$ -constituents were successful (Knof, Ehses, Fischer, Z.Krist. 1987, in press).

We discuss examples for the above Laue-type measurements and for applications, together with experimental advantages (e. g. mechanically simple apparatus, little sensitivity to crystal alignment) and shortcomings of the technique (e. g. low resolution in reciprocal space, fluorescence effects).

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16.2-7 A NEW TYPE OF A FOCUSING X-RAY MONOCHROMATOR FOR SYNCHROTRON RADIATION  
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The monochromator was built for HASYLAB Hamburg at DORIS II. The wavelength can be varied in the range of 0.8 Å and 2.0 Å. The double crystal monochromator uses crystals cut with the same asymmetry angle. Looking downstream the first crystal is flat according to Fankuchen (Nature, Lond. (1937), 139, 193) and the second one is bent according to de Wolff (Appl. Sci. Res., (1950), B1, 119-126). The asymmetry angle is chosen in such a way that the divergence of the first crystal matches the acceptance of the second one. The asymmetry factor of each crystal reduces the beam height by a factor about 3. Furthermore the bending of the second crystal produces a focus. The height of the focal line is 1/3 of the unfocused parallel beam. Germanium crystals were used. In a powder diffraction pattern of  $\text{CaF}_2$  at 1.35 Å no higher harmonic wavelengths have been observed.

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16.2-8 QUID, QUEENSLAND UNIVERSITY INCLINATIONAL DIFFRACTOMETER, A LOW-COST COMPUTER-CONTROLLED DATA COLLECTION SYSTEM. By Nicholas J. Carlos and Colin H.L. Kennard, Department of Chemistry, University of Queensland, Brisbane, Q, 4067, Australia.

A commercial Stoe STADI-2 Weissenberg computer-controlled diffractometer has been modified by replacing the supplied obsolete and non-functioning computer with an Apple IIe. Although this type of diffractometer is limited in its capabilities compared to a four-circle device, the system shows promise beyond its original design. Because the controlling program has been written in Applesoft BASIC, and may be compiled, it is easily modified. Providing the crystal under investigation is mounted about a principal axis, its cell parameters, space group and the Miller indices for two reflection standards known, then the program will search for these standards and establish an orientation matrix for this particular layer. The program will also optimise scan parameters. Data collection is based on the ideas of Freeman et al. (1).

1. H.C. Freeman, J.M. Guss, C.E. Nockolds, R. Page & A. Webster, Acta Cryst., A26, 149-152 (1970).