16. APPARATUS AND TECHNIQUES

16.2-6 NEW METHOD FOR INDEXING LAUE PATTERNS. By K. Okumura, K. Miyahara and H. Ohmase**, Photon Factory, National Laboratory for High Energy Physics, J-PARC, 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 µm 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 microcrystalligraphy.

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 remount 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 morpholgy. In the case of an unknown material, the crystal data will be obtained, provided that the d-spacing of any reflection is determinable.


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 symmetry angle. Looking down stream 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), 81, 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 Co₂ 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 W.L. Renard, Department of Chemistry, University of Queensland, Brisbane, Q., 4067, Australia.

A commercial Stoel STADI-2 Weissenberg computer-controlled diffractometer has been modified by replacing the supplied obsolete and non-functioning computer with an Apple Ile. 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).