Reflections should be chosen so that those with the highest probability of containing large Miller indices have the highest \( n \) values; i.e. 10, 9, 8, etc.

Program improvements

At present, there is no incentive to improve the operating performance of the program since an overnight run is possible and, therefore, processing times are not a problem. Fig. 3 is an example of central processing times for the conditions shown. Obviously, processing times increase as the \((hkl)\) range, or the allowable angular error, is increased. There is a large incentive to choose reflections which have low indices (say \( h = k = l < 3 \)) and measure their positions as accurately as possible. For reference purposes, ten reflections with a 1° error and a range \((555) \leq (hkl) \leq (555)\) require 1580 s of processing time.

Computing times might be decreased by random access to a previously calculated array of interplanar angles; however, this is not certain nor is the technique straightforward. Also, once the number of schemes is small, it may be faster to 'zero find' a series of simultaneous equations using the given inter-reflection angles.

Lastly, similar to the method of Anazia et al. (1975), measuring errors could be decreased by using the \( x/y \) coordinates of the reflections rather than going through the intermediate step of a Greninger chart. As can be seen in Fig. 3, minimizing the error limit considerably decreases processing times.

Summary

The program LAUE has been used for several years at the author's laboratories with excellent results. At present, the program requires 170000 words of core memory, operates in Control Data Corporation (CDC), Fortran Extended Compiler, version 4.6 and in the NOS/BE system. Results refer to operation on a CDC Cyber 175 computer. The program is available upon written request and is currently being used by another institute on a CDC 6600.

References


Laboratory Notes


Optical adjustment of bent-crystal monochromators

A simple device is described for making preliminary adjustment of the bending radius of a focusing monochromator with visible light, prior to final alignment with X-rays. It is applicable to the variable-radius presses used in low-angle work (Huxley & Brown, 1967) and incorporated in the Searle small-angle scattering camera (Elliott Neutron Division, Marconi Avionics Ltd., Borehamwood, Herts WD6 1RX, UK).

When a variable-radius camera is set up in the X-ray beam there is sometimes a risk of passing through the point of focus and fracturing an expensive crystal by over-tightening. The chance of such a mishap will be increased if forthcoming safety regulations (Blow, 1978) restrict the close approach of an operator.

The apparatus (Fig. 1) consists of a horizontal semicircular table (1) with a rotatable mount (2) at the centre of the circle; on this is placed the crystal press with its direct-beam stop withdrawn to give maximum aperture. An adjustable vertical slit (3) is illuminated by a lamp and lens combination (4). The crystal surface is arranged to pass through the centre of rotation by making the crystal tangential to the incident light and moving the press until a shadow of the crystal lies at the origin (5) of a vertical scale. The mount is then rotated until a focused image of the slit (6) appears on the scale. Adjustment of bending radius changes the position of focus, which is determined by the approximate formula

\[ X = D \sin^{-1} \left( \frac{D}{2R} \right), \]

where \( X \) = length of arc from origin to focus, \( D \) = diameter of semicircular table and \( R \) = bending radius of crystal. (The derivation of this formula is similar to that used in the case of focused X-rays.) The apparatus used in this laboratory has \( D = 250 \text{ mm} \) and a scale calibrated from \( R = 200 \text{ mm} \) to \( R = 2 \text{ m} \). By examining the image with a magnifier the radius can be set to within ±2% at \( R = 500 \text{ mm} \).

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