Elimination of film shrinkage error in Weissenberg photographs.

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The unit-cell dimensions of a crystal are usually determined from Weissenberg photographs. For obtaining accurate values, it is essential to correct the values of Bragg angles of different reflexions for the errors arising due to 'film shrinkage' and uncertainty in the radius of the film due to its finite thickness.

These errors can be eliminated by the method of Bradley & Jay (1932), by casting on the film shadows of two knife edges at known angular separation. The second method, most commonly employed in this laboratory is to sprinkle pure aluminium dust on the crystal, so that powder photograph of aluminum is superimposed on the Weissenberg photograph of the crystal. Since the angles for the powder lines of aluminum are known, the film may be completely calibrated.

A method given in this note requires neither the sharp edges nor the standard substance for correcting the film of zero-layer Weissenberg photographs.

Consider the zero-layer Weissenberg photographs with b as the rotation axis. Let $h0l$ and $\bar{h}0\bar{l}$ reflections be separated by a distance p along the translation of the film. Let us take the direction of motion of the film as the X axis and perpendicular to that as Y axis. It is easy to see that the distance p along the X axis corresponds to the distance of translation of the film, during which the crystal has rotated by 180°, since the two reflections are due to the $h0l$ and $\bar{h}0\bar{l}$ planes. In zero-layer photographs, Bragg planes are parallel to the rotation axis, which

therefore will give straight streaks of white radiation in Weissenberg photographs. Taking the angle of inclination of these streaks to the X axis as ψ, we can easily see that $p \tan \psi$ in Y-direction will also correspond to 180° of rotation of the crystal. Thus a knowledge of the Y coordinates only of the reflections will yield the Bragg angles θ in degrees of reflections by the following relation

$$\theta = 180Y/(p \tan \psi)$$

$\tan \psi$ may be determined from the coordinates of any two points on a very prominent white-radiation streak. Substituting this value of $\tan \psi$ to the above relation, all the quantities are known absolutely, and hence the film shrinkage errors are eliminated automatically without any extra standard line.

The Bragg angles which differed by even more than 3° on different films for Anthrone crystal, before this correction is applied, were found to agree within 0·5° (which corresponds to 0·5 mm. for the camera used by us).

Reference

BRADLEY, A. J. & JAY, A. H. (1932). *Proc. Phys. Soc. Lond.* **44**, 563.

On an analytic approximation to the atomic scattering factor.

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In a recent paper by Vand, Eiland & Pepinsky (1957) it was shown that the atomic scattering factor, f, can be approximated as a function of $\sin \theta = x$, as far as $\theta = 90°$ for Cu $K\alpha$ by an expression of the form

$$f(x) = A \exp(-ax^2) + B \exp(-bx^2)$$

and it was suggested that a better fit as far as $\theta = 90°$ for Mo $K\alpha$ could be obtained by an expression

$$f(x) = A \exp(-ax^2) + B \exp(-bx^2) + C .$$

We have calculated values of the parameters A, a, B, b and C using the following modifications to the method of Vand, Eiland & Pepinsky (1957):

(1) We have chosen as our reciprocal-space variable $s = \sin \theta/\lambda$ rather than $x = \sin \theta$; the values of a and b are then independent of the value of λ.

(2) We have relaxed the condition that

$$A + B + C = N$$

where N is the number of electrons in the atom or ion; the enforcement of this condition is equivalent to giving the point for $s = 0$ a weight equal to the sum of the weights of all the other points fitted, and we feel that its relaxation allows an improved fit over the more useful range of s values.

(3) Since most of the data used in crystallographic work occur around $s = 0·5$, we have applied a weighting factor of the form $\exp\{-(s-0·5)^2\}$ to the least-squares fitting procedure so that the 'middle' of the curve has the best agreement with the tabulated data.

The least-squares fitting was performed on EDSAC II using as an initial approximation the values given by Vand, Eiland & Pepinsky (1957) after suitable conversion of the values of a and b; the results obtained are given in Table 1 together with the value of

$$\varepsilon = \frac{100}{f_0} \left(\frac{\Sigma \omega_i \delta_i^2}{\Sigma \omega_i} \right)^{\frac{1}{2}}$$