principles to an accuracy comparable with that already achieved for the spherical term.

References

BANYARD, K. E. & MARCH, N. H. (1956). *Acta Cryst.* **9**, 385.

BANYARD, K. E. & MARCH, N. H. (1957). *J. Chem. Phys.* **26**, 1416.

BANYARD, K. E. (1960). *J. Chem. Phys.* **33**, 832.

BERGHUIS, J., HAANAPPEL, IJ. M., POTTERS, M., LOOPSTRA, B. O., MACGILLAVRY, C. H. & VEENENDAAL, A. L. (1955). *Acta Cryst.* **8**, 478.

BERNAL, M. J. M. (1953). *Proc. Phys. Soc.* A, **66**, 514.

BERNAL, M. J. M. & MASSEY, H. S. W. (1954). *M. Notices Roy. Ast. Soc.* **114**, 172.

BUCKINGHAM, R. A., MASSEY, H. S. W. & TIBBS, S. R. (1941). *Proc. Roy. Soc.* A, **178**, 119.

CARTER, C., MARCH, N. H. & VINCENT, D. (1958). *Proc. Phys. Soc.* A, **71**, 2.

HARTREE, D. R. & HARTREE, W. (1948). *Proc. Roy. Soc.* A, **193**, 299.

MCDONALD, T. R. R. (1960). *Acta Cryst.* **13**, 113.

MILLS, I. (1958). *Molecular Phys.* **1**, 99.

Acta Cryst. (1961). **14**, 360

Estimation of a Crystallographic Orientation Relationship

BY HENRY M. OTTE

RIAS (Research Institute for Advanced Study) 7212 Bellona Avenue, Baltimore 12, Maryland, U.S.A.

(*Received 24 March 1960 and in revised form 27 June 1960*)

Two alternative procedures for obtaining the orientation relationship using the stereographic net and numerical methods are described. Their principal advantage over Mackenzie's method is the greatly increased speed achievable; the accuracy is commensurate with that of standard Laue photographs.

In a recent article, Mackenzie (1957) described a very elegant and precise method of determining the orientation relationship between the axes of two systems (structures) given the correspondence for an arbitrary set of two or more directions in the respective systems. However, the method which requires at least a desk calculator, is exceedingly lengthy.

Mackenzie points out that the conventional procedures using stereographic manipulations have limited accuracy and if high precision is required numerical methods are necessary at least in the final stages. No references were given to any such methods and no specific discussions of this topic could be found in the literature. In view of this, two methods (*A* and *B* below), employed successfully by the writer, (1960), are worth recording here. They are based on the well-known theorems of Euler & Rodrigues (Coe, 1938; Gibbs, 1943, 1948; Whittaker, 1944). The methods are a great deal faster than Mackenzie's, especially when a large number of directions such as are available from a Laue photograph have to be taken into consideration; in the one method no numerical computations need be made. The precision of the methods is in keeping with that obtainable from a standard Laue photograph, and compares favourably with Mackenzie's.

Method *A*

In manipulations with the stereographic net, any rotation not about the [001] axis (in the standard projection) or about an axis perpendicular to it can always be decomposed into two rotations θ_1 and θ_2, one of which is about the axis $[001]=\hat{\mathbf{n}}_1$ and the other about an axis $[x, y, 0]=\hat{\mathbf{n}}_2$ perpendicular to $\hat{\mathbf{n}}_1$. The procedure involves superimposing two pieces of tracing paper on a stereographic net, with the standard orientation (say) plotted on the one piece and the 'unknown' orientation on the other. The two tracing papers are then adjusted individually about the center point of the net until trial checks show that the correct position for $\hat{\mathbf{n}}_2$ and the correct values for θ_1, θ_2 have been found. Numerical substitution, in one of the equations below, to determine the axis $\hat{\mathbf{n}}_0$ and angle θ_0 of the equivalent single rotation is made at this stage. The value of $\hat{\mathbf{n}}_0$ may then be plotted on the original stereogram for a graphical presentation.

In general a rotation θ about the direction with unit vector $\hat{\mathbf{n}}=[n_1n_2n_3]$ (where n_i is a direction cosine) can be expressed by the 3×3 rotation matrix R with elements

$$r_{ii}=n_i^2(1-\cos\theta)+\cos\theta$$
$$r_{ij}=n_in_j(1-\cos\theta)-\delta n_k\sin\theta \quad (i\neq j)$$

(δ is $+1$ when the permutation is cyclic and -1 when anticyclic). $R_0=R_2R_1$ then gives the single rotation matrix necessary to bring one orientation into coincidence with the other, i.e. the orientation relationship.

The axis $\hat{\mathbf{n}}_0$ and angle θ_0 of the rotation can be extracted from R_0 by using the relationship

$$\theta = \cos^{-1} \tfrac{1}{2}(\Sigma r_{ii} - 1)$$
$$n_i = [(r_{ii} - \cos\theta)/(1 - \cos\theta)]^{\frac{1}{2}},$$

where the correct sign for n_i is determined from the condition that

$$n_i = -(r_{jk} - r_{kj})/2 \sin\theta \; .$$

Alternately, $\hat{\mathbf{n}}_0$ and θ_0 may be obtained from the vector relation

$$\hat{\mathbf{n}}_0 \tan \tfrac{1}{2}\theta_0 = \frac{\hat{\mathbf{n}}_1 \tan \frac{1}{2}\theta_1 + \hat{\mathbf{n}}_2 \tan \frac{1}{2}\theta_2 - (\hat{\mathbf{n}}_1 \times \hat{\mathbf{n}}_2) \tan \frac{1}{2}\theta_1 \tan \frac{1}{2}\theta_2}{1 - \hat{\mathbf{n}}_1 . \hat{\mathbf{n}}_2 \tan \frac{1}{2}\theta_1 \tan \frac{1}{2}\theta_2}$$

provided none of the rotations is through 180°. In the present case $\hat{\mathbf{n}}_1 . \hat{\mathbf{n}}_2 = 0$, so that the denominator on the right hand side reduces to unity.

If the observations are subject to experimental error, then the two rotations must be selected so that the best fit with the data is obtained. This may be estimated visually on the stereographic net and is equivalent to choosing arbitrary weighting factors ω in Mackenzie's analysis.

Method *B*

If the direction of two normals $\mathbf{A}'$ and $\mathbf{B}'$ is known with respect to their direction $\mathbf{A}$ and $\mathbf{B}$ in the standard orientation, then the axis $\hat{\mathbf{n}}$ and angle θ of rotation can be found by applying directly on the stereographic net the theorems of Euler & Rodrigue. They are expressed (in vector notation) for the general case, by the formula

$$\frac{(\mathbf{B}' - \mathbf{B}) \times (\mathbf{A}' - \mathbf{A})}{(\mathbf{B}' - \mathbf{B}) \; . \; (\mathbf{A}' + \mathbf{A})} = \hat{n} \tan \tfrac{1}{2}\theta \; .$$

The unit vector parallel to $(\mathbf{A}' + \mathbf{A})$ is located midway between $\mathbf{A}'$ and $\mathbf{A}$ on the zone (or great circle) passing through these poles and the unit vector parallel to $(\mathbf{A}' - \mathbf{A})$ is on the same zone, at 90° from $(\mathbf{A}' + \mathbf{A})$. Similarly for $\mathbf{B}'$ and $\mathbf{B}$. The pole of the zone joining $(\mathbf{A}' - \mathbf{A})$ and $(\mathbf{B}' - \mathbf{B})$ provided these are not coincident then gives $\hat{\mathbf{n}}$. In the special case when $(\mathbf{A}' - \mathbf{A})$ and $(\mathbf{B}' - \mathbf{B})$ coincide, the above formula is not applicable. The rotation axis $\hat{\mathbf{n}}$ is then the intersection of the great circles through $\mathbf{AB}$ and $\mathbf{A}'\mathbf{B}'$. θ is obtained by determining the amount of rotation about $\hat{\mathbf{n}}$ required to bring $\mathbf{A}$ into coincidence with $\mathbf{A}'$ (or $\mathbf{B}$ into coincidence with $\mathbf{B}'$). This can be done by standard stereographic manipulation. For the purposes of this method the denominator is treated as being unity, since θ is determined graphically. When $\theta =$ 180°, $\hat{\mathbf{n}}$ coincides with $\mathbf{A} \times \mathbf{B}$ or $\mathbf{A} + \mathbf{A}'$, as the case may be.

If the direction of a number of normals $\mathbf{C}$, $\mathbf{D}$, etc. is known, then this process can be repeated for any combination of the two. The values of $\hat{\mathbf{n}}$ and θ will always be the same within the accuracy of the stereographic net except for any experimental error greater than this. If the experimental error is detectable, then a cluster of poles about some true value is obtained. A weighting procedure may then be adopted to calculate the true value or simply a visual estimation made on the stereographic net.

Either of the above methods is well suited to the accuracy attainable with the standard Laue techniques (Barrett, 1952; Cullity, 1956). Method *B* has been used by Donnay and others (1956, 1959) in the special case of twinning; it is also sometimes mentioned in older textbooks (Friedel, 1926) on crystallography in connection with this particular problem. Method *A*, though somewhat longer than method *B*, is more useful when rotations are to be translated onto a two-circle goniometer. A method, actually an approximate form of method *B* has been used by Cahn *et al.* (1953), to determine tilt axes in deformed zinc. No particular short-cut or increase in speed is obtained as a result of the approximations, and of course the method is only valid for small angles of rotation.

The author is grateful to J. D. Eshelby & J. D. H. Donnay for discussions and a referee for a number of useful comments.

References

Barrett, C. S. (1952). *Structure of Metals*. New York: McGraw-Hill.

Cahn, R. W., Bear, I. J. & Bell, R. L. (1953–54). *J. Inst. Metals*, **82**, 481. (Appendix, p. 488.)

Coe, C. J. (1938). *Theoretical Mechanics*, pp. 159–170. New York: McMillan.

Cullity, B. D. (1956). *X-ray Diffraction*. New York: Addison-Wesley.

Donnay, J. D. H. & Donnay, G. (1959). *International Tables for X-ray Crystallography*, vol. II, p. 104. Birmingham: Kynoch Press.

Friedel, G. (1926). *Leçons de Cristallographie*, p. 245. Paris: Berger-Levrault.

Gibbs, J. W. (1948). *Collected Works*, vol. II (pt. II), ch. III. Yale: Univ. Press.

Gibbs, J. W. & Wilson, E. B. (1943). *Vector Analysis*, ch. VI. Yale: Univ. Press.

Hurst, V. J., Donnay, J. D. H. & Donnay, G. (1956). *Miner. Mag.* **31**, 145.

Mackenzie, J. K. (1957). *Acta Cryst.* **10**, 61.

Otte, H. M. (1960). *Acta Met.* (In press.)

Whittaker, E. T. (1944). *Analytical Dynamics*, ch. I. Dover.