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The Estimation of an Orientation Relationship from Traces of Known Planes

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A least-squares method is given for the refinement of an approximate orientation relationship determined from measurements of the positions of traces of known crystallographic planes on the surfaces of a specimen.

Introduction

The orientation relationship between crystallographic axes and axes fixed with respect to a specimen is often determined from measurements of the positions of traces of crystallographic planes of known type on one or more surfaces of a specimen. These traces are commonly those arising from twins, slip or thermal etching. Barrett (1952) describes methods for determining this orientation relationships using a stereographic net and points out that the result is not necessarily unique. In this paper it is assumed that one of these approximate orientation relationships has been found (e.g. by one of Barrett's methods) and the method set out below provides a least-squares type of refinement for improving it. The method is numerical and should be used only when both the data and the need justify an accuracy of a few tenths of a degree or better.

The method is not limited in accuracy by graphical manipulations and uses all the observational data simultaneously. Furthermore, it leads to quantitative statistical estimates of the (non-systematic) errors. These advantages are, of course, achieved only at the cost of the labour of the numerical computations. The present method complements a previous paper (Mackenzie, 1957*a*) where a similar type of method was described for the determination of an orientation relationship from observations of normals to known planes; Otte (1961) has described alternative graphical (and numerical) methods for this case.

Before proceeding, two points need to be made clear. In the first place, although the original information gives only the type of crystal plane associated with a particular trace on the specimen surface, the specific indices of this plane will, in fact, be known from the preliminary approximate orientation relationship. Thus, these specific indices will be assumed known. The second point is important although it may appear pedantic at this stage. It concerns the axes of reference with respect to which all measurements are made. These axes are, clearly, fixed with respect to the measuring instrument and not with respect to the specimen. Thus, it is the orientation of the crystal axes with respect to the instrument axes which is primarily determined below. The specification of the result relative to the specimen axes requires, in principle, another independent determination of the orientation of the specimen axes with respect to the instrument axes. However, in practice, the latter determination is unnecessary provided the specimen is appropriately located. The specimen is usually set so that the specimen axes are as nearly parallel as possible to the instrument axes and, furthermore, the measurements are usually made in such a way that any setting errors lead to negligible differences between the actual observations and those that would have been obtained if the setting-up had been exact. Thus, the difference between the orientation of the crystal axes with respect to the instrument axes and that with respect to the specimen axes can usually be neglected in practice. On the other hand, a matter of principle is involved and the estimates of the errors are affected by the point of view adopted.

The equations of condition

The components of a vector relative to an orthonormal basis* can be written as the elements of a 3×1 column matrix. Thus, let t_r be the (unit) column matrix representing the direction of the rth $(1 \leq r \leq N)$ measured trace relative to the (orthonormal) basis I fixed relative to the measuring instrument, and let n_r be the column matrix representing the (unit) normal to the known crystal plane nominally containing t_r; this normal is given relative to the (orthonormal) basis C fixed relative to the crystal axes and its components are known exactly from the preliminary approximate result. The problem is to determine the relation between the components of a vector referred to the (crystal) basis C and the components of the same vector referred to the (instrument) basis I. This relation can be specified by means of the 3×3 orthogonal (rotation) matrix

$$\mathsf{R} = (\mathrm{I}\mathsf{T}\mathrm{C}) , \qquad (1)$$

* i.e. the base vectors are mutually perpendicular unit vectors.

which is such that if y represents the vector y relative to the basis C, Ry represents it relative to the basis I. Then, of course, $RR'=I$, where the prime denotes transposition and I is the identity matrix. The matrix R is here regarded as defining a change of basis. However, it can also be interpreted as the matrix representation, referred to I, of the rotation which carries vectors parallel to the base vectors of I into vectors parallel to those of C.

The angle θ_r between the observed trace t_r and the plane with normal n_r is given by

$$\sin\theta_r = n_r' R' t_r \,. \tag{2}$$

If the N observations were ideal and not subject to error all the angles θ_r would be zero for the correct choice of R. However, in practice, this is not so and an adjustment procedure such as the method of least-squares is necessary. This procedure involves minimizing the quadratic form

$$S = \sum_{i,j=1}^{N} w_{ij} \sin\theta_i \sin\theta_j \,, \tag{3}$$

where the w_{ij} are the elements of an $N\times N$ positive definite matrix W. The best possible choice for this weight matrix is known to be (see Plackett, 1949)

$$W = V^{-1}, \tag{4}$$

where V is the $N\times N$ covariance matrix of the quantities $\sin\theta_r$. This procedure, rather than minimizing a simple sum of squares, takes account of correlated values of $\sin\theta_r$. In fact, as will become clearer below, observations of more than one trace in a given specimen surface can lead to such correlations and there is not much increase in numerical complexity to take account of them.

In the following calculations the approximation $\sin\theta=\theta$ is made and the choice of W is modified slightly.

Suppose that R_0 is an approximation to R derived, say, from preliminary graphical manipulations. Put

$$R=[I+(hh'-I)(1-\cos\varphi)-\{h\}\sin\varphi]R_0 \,, \tag{5}$$

where

$$\{h\} = \begin{pmatrix} 0, & -h_3, & h_2 \\ h_3, & 0, & -h_1 \\ -h_2, & h_1, & 0 \end{pmatrix} \tag{6}$$

is a skew symmetric matrix such that $\{h\}y$ is a column matrix with elements equal to the components of the vector product $\mathbf{h}\times\mathbf{y}$. The factor in square brackets on the right of equation (5) represents a right-handed rotation about an axis in the direction of the unit vector **h** through a (small) angle $-\varphi$. Then, writing

$$m_r = R_0 n_r \,, \tag{7}$$

$$\{h\}\varphi = \{x\} \,, \tag{8}$$

it follows from equations (2) and (5), on neglecting terms of order φ^2 and higher, that

$$\sin\theta_r \simeq m_r' t_r - m_r'\{t_r\}x \,. \tag{9}$$

The components of the matrix m_r are approximately equal to the components of the normal $\mathbf{n}_r$ referred to the instrument basis I, the approximation being that in which $R=R_0$.

Thus, changing to the perhaps clearer vector notation, the equations of condition which are to be solved for x by minimizing S in equation (3) are

$$(\mathbf{m}_r\times\mathbf{t}_r).\mathbf{x} = \mathbf{m}_r.\mathbf{t}_r - \delta_r \,, \tag{10}$$

where δ_r is the (unknown) error term equal to $\sin\theta_r$. Note that when expressed in matrix notation the components of the vector product $\mathbf{m}_r\times\mathbf{t}_r$ are written out as a row and those of **x** as a column.

In practice, the numerical procedure is first to calculate m_r from the given n_r by means of equation (7) and then compute the coefficients required in equation (10). With the choice of W given in the next section, an estimate of x can be derived from these equations by the method of least-squares described in the last section. Finally, back substitution through equations (8) and (5) gives R. In this last step a term $(hh'-1)\varphi^2/2$ may need to be included to make R an orthogonal matrix within the accuracy of the calculations. The number of significant figures carried will depend on the accuracy required but initial observations to within 0·1° (3 figures) may well justify more figures in the final result and so 5–6 figures should be kept in the intermediate steps leading to equation (10) (including R_0). The least-squares solution requires care and the retention of an even greater number of figures.

The choice of W

In equations (10) the errors arise from the errors in the measurements of the t_r so that the coefficients on both the left- and the right-hand sides are subject to error. Therefore, the standard least-squares theory does not immediately apply. Equations of this type have been discussed by Mackenzie (1957*b*) who has shown that in a first approximation the standard theory can be applied provided the matrix of weights W is suitably modified and the estimate of x corrected for bias. However, in the present case where both x and the errors in the t_r are small both the bias and the modification to W can be safely neglected. Thus, W^{-1} can be taken proportional to the covariance matrix V of the right-hand sides of equations (10). This covariance matrix will depend on the particular way in which the observations are made. Thus, it is necessary to specify a suitable method in some detail and each method of observation will require a separate analysis. The analysis for a common method of observation is set out below.

Suppose that traces can be measured on two surfaces of the specimen. Further, suppose that the specimen is set up relative to the instrument basis I (with base vectors i_1, i_2, i_3) so that the edge at which the two specimen surfaces meet is as nearly parallel as possible to i_1, and the outward normal to one of the specimen

surfaces is as nearly parallel as possible to i_3. This specimen surface will be called the primary surface and the other the secondary surface; i_2 then lies (approximately) in the primary surface perpendicular to the common edge. When the specimen is set up in this way the outward normal to either surface can be specified by the angle β that it makes with i_3, with β increasing positively for a right-handed rotation about i_1. Similarly, the position of a trace in either surface can be specified by the angle α that it makes with the common edge parallel to i_1. This specification is illustrated in Fig. 1 (for the primary surface $\beta=0$).

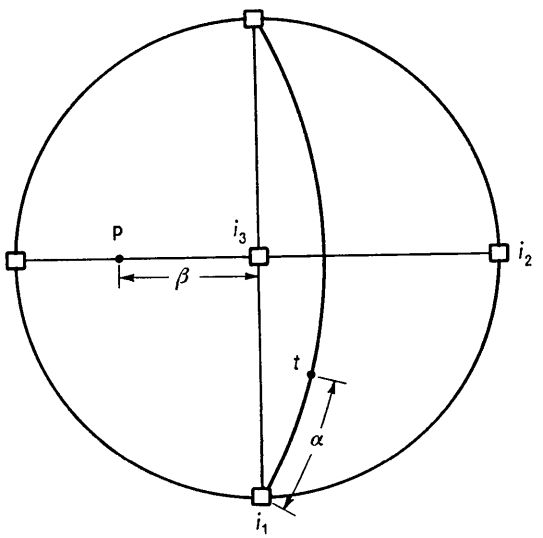

Fig. 1. Stereographic projection showing the specification, relative to the instrument axes, of a trace t on a specimen surface with normal p. The base vector i_1 is approximately parallel to the edge of the specimen common to the two surfaces on which observations are made and the base vector i_3 is approximately parallel to the normal to one of these surfaces.

It will be assumed that the measurements are made in such a way that all the α readings corresponding to traces on one surface are made with a *fixed* setting of β on the instrument. This is common practice and results in correlated errors since, although the errors in successive measurements of α will be independent, the *same* error in β will be associated with all measurements on the one specimen surface. On the other hand, the values of β for the two different surfaces will be independent. In any given surface the value of α for a particular trace is found as the difference between readings obtained by a setting on the specimen edge and one on the trace. The variance (square of the standard deviation) of an α value obtained in this way is the sum of the variances of the results for the two settings; these variances may be quite different due to the short length or lack of definition in the direction of the trace. Since, in the procedure below, the results for the primary (or secondary) surface will be reduced as a group before finally combining them, the appropriate variance for β is that corresponding to the errors in β for the group in question.

When the observations are obtained in the above manner, the differences between the values of α and β which are actually obtained and those which would have been obtained if the specimen had been set up exactly are proportional to the squares of the angles which define the deviation from exact setting. For example, if these deviations are less than $2\frac{1}{2}°$, the actual and ideal values of α and β differ by less than $0{\cdot}1°$. Thus, even with a relatively crude setting of the specimen the values of α and β obtained are for all practical purposes those for the specimen set up exactly. Thus, the value of R obtained is the same whether referred to either instrument axes or specimen axes.

The reason for the pedantic distinction made earlier now becomes clear. On the present view that all measurements are referred to axes fixed in the instrument, there are errors in β associated with each specimen surface independently and the two surfaces are treated on the same basis. On the other hand, if the measurements were regarded as referred to axes fixed in the specimen, there is an error associated with the β value for the secondary surface but, by definition, none for that associated with the primary surface. This asymmetry can lead to (slightly) different values of both R and the confidence limits for it, depending on which of the surfaces is regarded as the primary one: this is an undesirable situation which I believe to be wrong in principle.

The covariance matrix V and hence W can now be derived for the method specified above. Since the values of α and β are all statistically independent, the set of measurements on the primary surface is independent of the set made on the secondary surface. Therefore, it is convenient to divide the equations (10) into two sets, each containing only measurements on one surface, and to treat each set separately. The contributions to the normal equations from each set are then simply added before solving for x. A typical set is treated below.

For a typical trace

$$\mathbf{t}=[\cos\alpha,\ \sin\alpha\cos\beta,\ \sin\alpha\sin\beta]_{\mathrm{I}}\,, \qquad (11)$$

and it is easily shown that

$$\delta\mathbf{t}=(\mathbf{p}\times\mathbf{t})\delta\alpha+(\mathbf{i}_1\times\mathbf{t})\delta\beta\,, \qquad (12)$$

where $\mathbf{p}$ is the normal to the specimen surface for the set being considered ($\mathbf{p}=\mathbf{i}_3$ and $\beta=0$ for the primary surface). Thus, the corresponding error in the right-hand side of an equation (10) is

$$\mathbf{m}.\delta\mathbf{t}=-(\mathbf{m}\times\mathbf{t}).\mathbf{p}\delta\alpha-(\mathbf{m}\times\mathbf{t}).\mathbf{i}_1\delta\beta\,. \qquad (13)$$

It is convenient to divide each of the equations (10) through by a divisor such that errors in the resulting equations of condition arising from errors in α_r all

have the same, but unknown, variance σ^2. To do this the relative values of the variances of the α_r must be assumed known and then the variance of α_r can be written in the form $\sigma^2[\sigma(\alpha_r)]^2$, with σ^2 unknown but the $\sigma(\alpha_r)$ known. Therefore, the appropriate divisor for each of the equations (10) is $(\mathbf{m}_r \times \mathbf{t}_r).\mathbf{p}\,\sigma(\alpha_r)$. Thus, defining

$$\mathbf{m}_r^* = \mathbf{m}_r/[(\mathbf{m}_r \times \mathbf{t}_r).\mathbf{p}]\sigma(\alpha_r)\,, \tag{14}$$

equations (10) become

$$(\mathbf{m}_r^* \times \mathbf{t}_r).\mathbf{x} = \mathbf{m}_r^*.\mathbf{t}_r - \delta\alpha_r/\sigma(\alpha_r) - (\mathbf{m}_r^* \times \mathbf{t}_r).\mathbf{i}_1\delta\beta\,, \tag{15}$$

the error terms being given explicitly.

Since $\mathbf{m}_r$ is approximately the same as the normal to the crystal plane containing the trace $\mathbf{t}_r$ and is not parallel to $\mathbf{p}$, the factors $(\mathbf{m}_r \times \mathbf{t}_r).\mathbf{p}$ in the above divisors are not zero. For the primary plane the factor $(\mathbf{m}_r \times \mathbf{t}_r).\mathbf{p}$ is just the coefficient of x_3 appearing on the left-hand side of the corresponding equation (10). For the common case where the secondary plane is approximately perpendicular to the primary plane ($\beta = 90°$) the factor is just the coefficient of x_2 and even if β deviates from 90° by 10° or so, this coefficient can be used as the factor without affecting the results appreciably; only a small change in the set of weights used is involved.

The s equations of type (15) in a set with the same β can be compactly written in matrix notation as

$$\mathsf{A}\mathsf{x} = \mathsf{b} - \delta\boldsymbol{\alpha}^* - \mathsf{a}_1\delta\beta\,, \tag{16}$$

where A is the $s \times 3$ matrix of coefficients with rows $(\mathbf{m}_r^* \times \mathbf{t}_r)$, b and $\delta\boldsymbol{\alpha}^*$ are the $s \times 1$ column matrices with elements $\mathbf{m}_r^*.\mathbf{t}_r$ and $\delta\alpha_r/\sigma(\alpha_r)$, and a_1 is the first column of A. Now the covariance matrix V is the mean value of $(\delta\boldsymbol{\alpha}^* + \mathsf{a}_1\delta\beta)(\delta\boldsymbol{\alpha}^* + \mathsf{a}_1\delta\beta)'$ so that after discarding the irrelevant factor σ^2

$$\mathsf{W} = \mathsf{I} - k\mathsf{a}_1\mathsf{a}_1'/(1 + k\mathsf{a}_1'\mathsf{a}_1)\,, \tag{17}$$

where $k\sigma^2$ is the variance of β. Note that $\mathsf{a}_1\mathsf{a}_1'$ is an $s \times s$ matrix.

The normal equations

The normal equations corresponding to equations (16), but with $\mathsf{W} = \mathsf{I}$, are well known (Whittaker & Robinson, 1946). In matrix notation they are

$$\mathsf{A}'\mathsf{A}\mathsf{x} = \mathsf{A}'\mathsf{b}\,, \tag{18}$$

which, for convenience, will be written

$$\mathsf{B}\mathsf{x} = \mathsf{c}\,. \tag{19}$$

For a general W the normal equations become

$$\mathsf{A}'\mathsf{W}\mathsf{A}\mathsf{x} = \mathsf{A}'\mathsf{W}\mathsf{b}\,, \tag{20}$$

and when W is given by (17) it is easily shown that these reduce to

$$\mathsf{C}\mathsf{x} = \mathsf{d}\,, \tag{21}$$

where

$$\mathsf{C} = \mathsf{B} - r\mathsf{b}_1\mathsf{b}_1'\,, \tag{22}$$

$$\mathsf{d} = \mathsf{c} - rc_1\mathsf{b}_1\,, \tag{23}$$

$$r = k/(1 + kb_{11})\,, \tag{24}$$

and b_1 is the first column of B, and c_1 is the first element of c, and b_{11} is the element of B in the upper left-hand corner. Thus, the correct normal equations are very simply derived from the usual ones given in equation (18). Note that $\mathsf{b}_1\mathsf{b}_1'$ is a 3×3 matrix. Further, the contribution to the 'sum of squares', S_0, which is used in calculating $S_{\min}$ is

$$S_0 = \mathsf{b}'\mathsf{b} - rc_1^2\,. \tag{25}$$

Finally, using subscripts 1 and 2 to denote the primary and secondary sets, the normal equations to be solved for x are

$$(\mathsf{C}_1 + \mathsf{C}_2)\mathsf{x} = \mathsf{d}_1 + \mathsf{d}_2\,, \tag{26}$$

and

$$S_{\min} = (S_0)_1 + (S_0)_2 - \mathsf{x}'(\mathsf{d}_1 + \mathsf{d}_2)\,. \tag{27}$$

The significance tests and confidence limits which can now be derived will not be discussed here. Reference can be made to any standard text on statistics, for example, Cramer (1946). A brief summary is given in Mackenzie (1957*b*). However, one overall result can be stated. For no direction can the p% confidence limit differ from the direction predicted from the above calculated R by more than $t_p\lambda_{\max}[S_{\min}/(N-3)]^{\frac{1}{2}}$ radians (approximately), where $\lambda_{\max}^2$ is the largest characteristic root of the matrix, $(\mathsf{C}_1 + \mathsf{C}_2)^{-1}$, and t_p is the value derived from tables of the t-distribution for $N-3$ degrees of freedom.

If observations are made of traces on only one surface, equations (21) are derived from equations (19) on premultiplication by the matrix $\mathsf{I} - r\mathsf{b}_1\mathsf{i}_1'$. Thus, equations (19) and (21) have the same solution, and, of course, lead to the same value of $S_{\min}$. This is as it should be since, in this case, any error in β is in the nature of a systematic error and can neither be detected nor determined by any statistical analysis: the observations are effectively independent.

The author will be happy to furnish upon request, an illustrative numerical example, worked out in detail.

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