SOME STATISTICS ASSOCIATED WITH THE RANDOM DISORIENTATION OF CUBES

BY J. K. MACKENZIE AND M. J. THOMSON

Division of Tribophysics, Commonwealth Scientific Industrial Research Organization, University of Melbourne, Australia

ABSTRACT. A Monte Carlo method is used to estimate the frequency functions of various angles in a random aggregate of cubic crystals. Estimates are made of the frequency function for the angle of disorientation, i.e. the least angle of rotation required to rotate a crystal into the same orientation as a neighbouring crystal, and for the angles Min ⟨100⟩, Min ⟨110⟩, Min ⟨112⟩, Min ⟨123⟩ and Min [⟨110⟩, ⟨112⟩, ⟨123⟩], where Min ⟨100⟩ is defined as the least of the nine acute angles between ⟨100⟩ directions in neighbouring crystals and similar definitions apply for the other angles.

1. INTRODUCTION

This paper is concerned with the estimation, by means of random sampling, of some probability distributions which arise from a class of problems in three-dimensional geometrical probability. The results obtained are of interest to metallurgists in particular and perhaps to crystallographers in general. They are presented here in the hope that some statistician may be sufficiently interested to try to obtain the exact distributions in a more or less explicit form.

Before stating the specific problems it is desirable in the interests of the general reader to describe the standard crystallographic notation for directions and planes. A particular direction can be specified by the components u, v, w of a vector (in this direction) relative to an orthonormal basis and the symbol $[uvw]$, in square brackets, is used to denote this direction. Thus, [100] is the direction of the x-axis. A cube with its centre at the origin and edges parallel to the base vectors (axes) is invariant under the 48 symmetry operations of the cubic group consisting of 24 proper rotations and 24 improper rotations which are proper rotations together with an inversion or reflexion. Starting with a given direction $[uvw]$, 47 other equivalent directions (24 lines in all) can be derived by the use of the symmetry operations and are called variants of $[uvw]$. These are simply derived from the given direction by permuting the indices u, v, w in sign and in order in all possible ways. This set of 48 equivalent directions is denoted by $\langle uvw \rangle$, in carets, and not all the 48 directions need be distinct, e.g. the set ⟨100⟩ consists of the set of 6 directions [100], $[\bar{1}00]$, [010], $[0\bar{1}0]$, [001], $[00\bar{1}]$, the bar over an index being used instead of a minus sign. Similarly, if h, k, l are the components of a normal to a particular plane, this plane is denoted by the symbol (hkl), in brackets. While the set of all planes equivalent to the plane (hkl) is derived in the same way and denoted by $\{hkl\}$, in braces. These symbols for planes are not used in the present paper.

The simplest of all the problems under consideration can be stated as follows. Given a single fixed reference line (defined by one of two opposite directions) and another single line defined by a random direction, uniformly distributed on a sphere, what is the probability distribution of the least angle between these two lines or of the least angle of rotation required to make the random line coincide with the reference line? It is known that the cosine of both these angles is uniformly distributed in the range (0, 1), but what is the answer if instead of two single lines there are two congruent (i.e. superposable) sets of lines, the lines of each set being fixed relative to one another? The present paper gives practical answers to some problems of this latter type when the lines of each set are invariant under the rotations of the cubic group.

2. Statement of problems

Consider two cubes, A and B, and imagine A to be a fixed reference cube and B to be initially coincident with A but free to rotate in any manner about the common centre of A and B. If B is rotated through an arbitrary angle about some arbitrary axis there are 24 definite rotations which will restore B into coincidence with A. These rotations are just the reverse of the original rotation taken together with the 24 proper symmetry operations associated with a cube having indistinguishable faces. Further, each of these 24 rotations can be represented as a single rotation about some definite axis and through some definite angle. Then, of the 24 angles of rotation so defined, there is one (or more) which is least in magnitude and this least angle may be taken as a measure of the disorientation of the two cubes and will be called the angle of disorientation.

In 1949, F. C. Frank proposed over morning coffee the problem of determining the greatest possible angle of disorientation of two cubes. The answer to the analogous problem for squares in two dimensions is of course 45°, but in three dimensions the answer is not at all obvious. However, by a tedious consideration of all possibilities it can be shown that the maximum value of the angle of disorientation is $2 \arccos \frac{1}{4}(2+\sqrt{2}) = 62{\cdot}80°$, and that the rotation which achieves this maximum disorientation is most simply described as a rotation of 90° about any of the axes $\langle 110 \rangle$, i.e. axes parallel to a face diagonal. A more difficult problem is to determine the probability distribution of the angle of disorientation when the cube B takes all orientations with equal probability. An estimate of this probability distribution is made in the present paper.

Another problem which has arisen in the course of experimental work (Ogilvie, 1952) can be described in simplified form as follows. In an aggregate of cubic crystals a particular event may occur only when one of the directions, $\langle 100 \rangle$ say, in one crystal is within, say, 5° of one of the $\langle 100 \rangle$ directions in a neighbouring crystal. Then it may be asked what proportion of pairs of crystals in a random aggregate would comply with this last requirement. The problem can be formulated as follows. Imagine a set of three fixed wires passing through the centre and parallel to the directions $\langle 100 \rangle$ of cube A and a similar set of three wires parallel to the directions $\langle 100 \rangle$ of cube B. Then, if B is given a random rotation there are nine definite acute angles between pairs of wires (taking one from each set) and the least of these angles will be called Min $\langle 100 \rangle$. The probability distributions of Min $\langle 100 \rangle$, and the analogous Min $\langle 110 \rangle$, Min $\langle 112 \rangle$, Min $\langle 123 \rangle$ and Min $[\langle 110 \rangle, \langle 112 \rangle, \langle 123 \rangle]$ are also estimated in the present paper.

The method of calculation is described in § 3 and the results are given in § 4. The method of constructing 150 random orthogonal matrices and their testing for randomness is set out in § 5.

3. Method of calculation

The calculations were performed by the method of random sampling. Since any rotation can be represented by a 3×3 orthogonal matrix (Jeffreys & Jeffreys, 1946, p. 114), 150 random orthogonal 3×3 matrices were constructed as described in § 4. Then with each matrix the following calculations were made.

If a given matrix represents a rotation through an angle θ about some axis, then the trace of the matrix (i.e. the sum of the elements in the leading diagonal) is equal to $1+2\cos\theta$. Thus, to determine the angle of disorientation it is necessary, in principle, to calculate the trace of each of the 24 matrices found by combining the given matrix with the 24 symmetry operations of a cube and to choose the greatest of these 24 values. However, this greatest trace can be found easily from the following rule. Taking into account only the magnitude of each element, add to the largest element the greater of the two diagonal sums of the four elements not lying in the same row or column as the largest element. This rule can be derived by straightforward but tedious consideration of all the possibilities.

Since the elements of the given matrix are just the cosines of the 9 angles between the new and the old $\langle 100\rangle$ directions, Min $\langle 100\rangle$ is determined by the element of largest magnitude in the matrix.

The remaining calculations are all similar and only the determination of Min $\langle 123\rangle$ will be described. First the matrix is used to calculate the new directions corresponding to each of the 24 (proper) variants of [123] (the remaining 24 are obtained by changing all signs). If a particular member of the set $\langle 123\rangle$ is transformed into $[u_1 u_2 u_3]$ then the cosine of the angle between this direction and the nearest direction of the set $\langle 123\rangle$ is

$$\tfrac{1}{14}(|u_s|+2|u_m|+3|u_l|),$$

where u_s, u_m and u_l are the numerically smallest, middle and largest of u_1, u_2 and u_3. The greatest of the 24 cosines so calculated determines Min $\langle 123\rangle$. A table showing the bounds for $|u_s|$, $|u_m|$ and $|u_l|$ consistent with a series of different angular deviations from [123] was used to reject most of the 24 possibilities by visual inspection; the cosines were only computed accurately for the few remaining cases.

Finally, when the results of the calculations had been accumulated for the 150 matrices, the number of cases in which the various angles lay in suitably chosen ranges were counted and the numbers so obtained used as estimates of the corresponding frequencies.

4. RESULTS AND DISCUSSION

The results are presented in the form of a series of histograms in Fig. 1. The ordinates have been normalized to represent probability densities when the unit of measurement along the abscissa is 1°, and the figures along the top of each histogram are the actual number of cases counted in the indicated range. If p is the estimated probability of an angle lying in a particular range, then an estimate of the standard error of p based on a sample of 150 is $[p(1-p)/150]^{\frac{1}{2}}$, and horizontal dotted lines have been drawn one standard error above and below the top of each rectangle of the histograms. The mean $\bar{x}$ and the standard deviation s of the estimated distribution are given on each histogram and are also indicated by means of the arrow and range at the bottom of each histogram.

The dotted curves superposed on each histogram give an indication of the form of each frequency function. These have been adjusted so that the area under each curve is unity. Except for Min $\langle 110\rangle$ each frequency function appears to have a single maximum, and even in the case of Min $\langle 110\rangle$ the existence of a double hump is by no means certain. However, there are, for finer subdivisions of the ranges, indications of more than one hump in some of the other frequency functions and the nature of the problem suggests that the true frequency functions may consist of a number of continuous arcs which join at sharp corners.

As was mentioned in the introduction, a tedious argument shows that the greatest possible value for the angle of disorientation is 62·80°. A similar argument shows that the greatest possible value of Min ⟨100⟩ is $\arccos \frac{2}{3} = 48{\cdot}19°$ and that the rotation which achieves the corresponding disorientation is most simply described as a rotation of 60° about an axis ⟨111⟩. Although no further results of this type are known to the authors it is easily

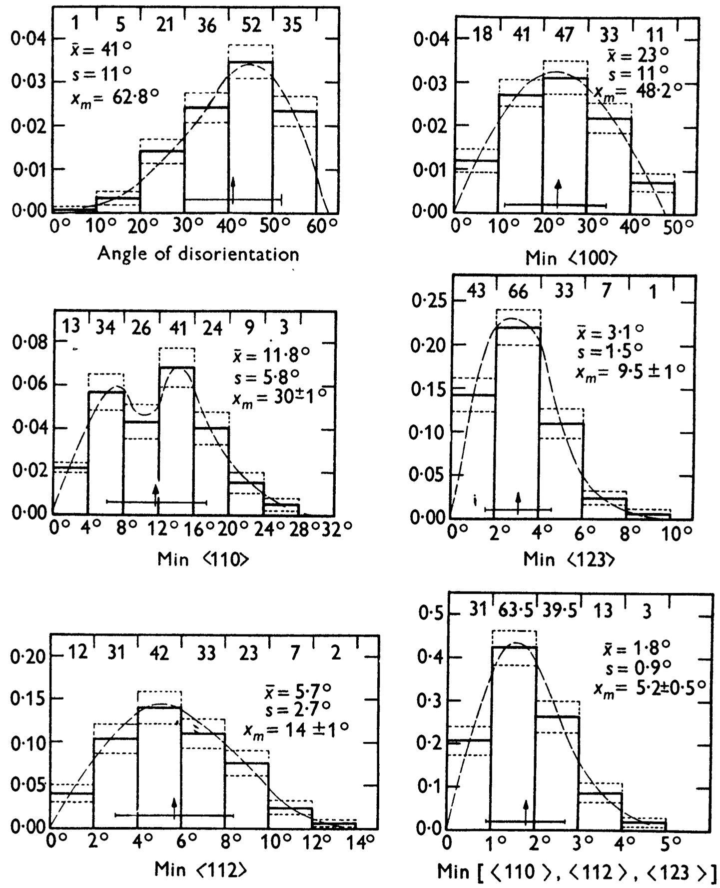

Fig. 1. Histograms derived from a random sample of 150. The ordinate is probability density when the angles are measured in degrees. The figures at the top are the number of cases counted in each range while the horizontal dotted lines indicate limits corresponding to one standard error from the estimated total probability for each range. The mean $\bar{x}$ and the standard deviation s of the estimated distribution are indicated by the arrow and range at the bottom. An estimate of the maximum value x_m of each variable is also given. The dotted curves indicate the general shape of each frequency function.

shown that a rotation of 45° about an axis ⟨100⟩ gives Min ⟨110⟩ $= \arccos \frac{1}{4}(2+\sqrt{2}) = 31{\cdot}40°$, and the results given in Fig. 1 suggest that this is probably its greatest possible value. The values, x_m, of the greatest possible values of each variable are given in Fig. 1 and where the value is associated with limits of error it has been estimated as follows.

A rotation is uniquely defined by three suitable independent variables (e.g. the Eulerian angles) so that the variation of Min ⟨110⟩, say, can be represented by means of a four-dimensional hypersurface. Now experience obtained in the calculation of the maximum values of the angle of disorientation and Min ⟨100⟩ suggests that in all cases the appropriate hypersurface can be approximated in the neighbourhood of $x = x_m$ by a number of hyperplanes all intersecting at a common point. Thus, when x is sufficiently near x_m the probability density would be expected to be proportional to $(x_m - x)^2$. Except for the angle of disorientation and Min $\langle 100\rangle$ this expected behaviour can be roughly verified from Fig. 1 and x_m has been estimated by plotting $p^{\frac{1}{2}}$ against the mean value of x for the range concerned. The limits of error stated in Fig. 1 are no more than reasonable guesses and the maximum $30 \pm 1°$ given for Min $\langle 110\rangle$ is to be compared with the known result that the maximum is probably 31·40°.

A simple argument accounts for the initial linear rise of the frequency functions for all the Min $\langle uvw\rangle$ in Fig. 1. If the set $\langle uvw\rangle$ has $2n$ members defining n distinct lines Min $\langle uvw\rangle$ is the least of the n^2 angles θ_i between pairs of lines and $\cos\theta_i$ is uniformly distributed on the range (0, 1). Now the method of inclusion and exclusion shows that $\Pr\{\text{Min}\,\langle uvw\rangle < \theta\}$ lies between the limits* $\sum_i \Pr\{\theta_i < \theta\}$ and $\sum_i \Pr\{\theta_i < \theta\} - \sum_{i<j} \Pr\{\theta_i < \theta, \theta_j < \theta\}$. Thus, for θ sufficiently small

$$\Pr\{\text{Min}\,\langle uvw\rangle < \theta\} \simeq n^2 \Pr\{\theta_i < \theta\} = n^2(1 - \cos\theta).$$

The corresponding density function is $n^2 \sin\theta$, and the estimated frequency functions in Fig. 1 are in substantial agreement with this prediction up to an angle of about $24/n$ degrees.

5. CALCULATION OF RANDOM ORTHOGONAL MATRICES

Since the elements in successive columns of an orthogonal 3×3 matrix can be regarded as the components of three orthogonal unit vectors, a random orthogonal matrix can be constructed as follows. Choose a random unit vector $\mathbf{x}$ and write its components as the first column. Choose a second random vector $\mathbf{y}'$ which is independent of $\mathbf{x}$. These two vectors define a random plane and in this plane there is a unit vector $\mathbf{y}$ perpendicular to $\mathbf{x}$. The components of $\mathbf{y}$ form the second column while the third column consists of the components of $\mathbf{x} \times \mathbf{y} = \mathbf{z}$ which is normal to the random plane. Thus, the problem is reduced to that of computing the components of a random unit vector.

Let x_1, x_2, x_3 be three independent unit normal deviates with joint probability density

$$(2\pi)^{-\frac{3}{2}} \exp\left(-\tfrac{1}{2}\Sigma x_r^2\right).$$

This density is constant on the surface of the sphere $\Sigma x_r^2 = \text{constant}$, so that given the value of $S = \Sigma x_r^2$ the probability that the point (x_1, x_2, x_3) lies in any area of the surface of the sphere is simply proportional to that area. Thus, the direction of the vector $[x_1, x_2, x_3]$ is distributed uniformly and

$$\mathbf{x} = [x_1, x_2, x_3]/S^{\frac{1}{2}}$$

is a random unit vector.

Similarly, we can find another independent random unit vector

$$\mathbf{y}' = [y_1, y_2, y_3]/T^{\frac{1}{2}},$$

where $T = \Sigma y_r^2$. Then, if $P = \mathbf{x}\,.\,\mathbf{y}'$,

$$\mathbf{y} = [Sy_1 - Px_1, Sy_2 - Px_2, Sy_3 - Px_3]/[S(ST - P^2)]^{\frac{1}{2}}.$$

Finally, the remaining column of the required matrix follows by computing $\mathbf{z} = \mathbf{x} \times \mathbf{y}$. The values of the random normal deviates were taken from the tables of Mahalanobis,

* This remark is due to Dr H. A. David of the Department of Statistics, University of Melbourne.

Bose, Ray & Banerji (1934) and as a check on the overall accuracy of the calculations the column sums c_1, c_2 and c_3 were formed and it was verified that

$$c_1^2+c_2^2+c_3^2 = 3.$$

The standard deviation of divergences from this equality due to rounding off errors is about 2 units in the last figure retained in the matrix elements.

The distributions of $x_r/S^{\frac{1}{2}}$ and of the column sums c are closely related to the t-distribution and in three dimensions are both distributed uniformly* (Cramer, 1946, pp. 240, 387). Thus, although they are not independent, all nine elements of a random orthogonal matrix are uniformly distributed on the range $(-1, 1)$ while the column sums are uniformly distributed on the range $(-\sqrt{3}, \sqrt{3})$.

The 150 matrices were tested for deviations from these predictions by dividing the range of each variable into 10 equal parts and testing for uniformity of distribution by means of a χ^2-test with 9 degrees of freedom. The greatest value of χ^2 obtained from the elements was 15·7 and for the column sums 22·6, while the corresponding mean values of χ^2 were 9·4 and 16·9. However, after permuting the columns in all the six possible ways,† these maxima dropped to 13·1 and 15·9 respectively while the corresponding means were 9·7 and 12·4. Thus there was then no significant deviation from uniformity of distribution at the 5% level ($\chi^2 = 16{\cdot}9$).

The following four rotation matrices are typical of those computed by the above method:

0·8527	0·4846	0·1953	0·2294	−0·6454	−0·7286
0·2780	−0·7374	0·6155	0·9035	0·4196	−0·0872
0·4423	−0·4705	−0·7636	0·3620	−0·6383	0·6794
0·0443	−0·9973	0·0584	−0·3763	0·5764	0·7254
0·9773	0·0554	0·2045	0·7487	0·6504	−0·1285
−0·2072	0·0480	0·9771	−0·5458	0·4947	−0·6763

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REFERENCES

Cramer, H. (1946). *Methods of Mathematical Statistics.* Princeton University Press.

Jeffreys, H. & Jeffreys, B. S. (1946). *Methods of Mathematical Physics.* Cambridge University Press.

Mahalanobis, P. C., Bose, S. S., Ray, P. R. & Banerji, S. K. (1934). *Sankhya*, **1**, 289.

Ogilvie, G. J. (1952). *J. Inst. Met.* **81**, 491.

* Thus, the cosine of the angle between a fixed direction and a random direction is uniformly distributed on the range $(-1, 1)$. Hence, if ξ the cosine of the co-latitude is chosen at random in the range $(-1, 1)$ and the longitude ϕ at random in the range $(-\pi, \pi)$

$$[(1-\xi^2)^{\frac{1}{2}} \cos \phi,\ (1-\xi^2)^{\frac{1}{2}} \sin \phi,\ \xi],$$

is a random unit vector; the sign of the square root is taken positively and negatively at random. This method of calculation of a random unit vector is suitable for high speed computers.

† This removes any bias due to calculating the successive columns in a definite order.