

Finite strain estimation using 'anti-clustered' distributions of points

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(Received 30 June 1982; accepted 20 December 1982)

Abstract—A new method for the estimation of finite strain using spatially 'anti-clustered' distributions of points is described. Besides having been empirically validated via simulation, it is also evaluated by means of analysing a deformed spilite containing calcitic amygdules, which have retained their originally spheroidal shape, as well as elliptical chloritic amygdules with the same ductility as the matrix in which they are embedded. There is complete agreement between the results obtained using the R/ϕ method on the chloritic amygdules, and those provided by the method now proposed when applied to the centres of the calcitic amygdules.

INTRODUCTION

THE CORPUS of techniques for the determination of finite strain in rocks has undergone a sizeable growth during the last fifteen years (for a survey see Ramsay 1976). However, two conditions have been restraining the range of application of those methods. Firstly, objects of spherical or ellipsoidal shape do not occur as often as one might wish throughout deformed regions, and secondly, the proposed methods do not take into account the ductility contrast between the marker objects and the matrix in which they are embedded.

To overcome these difficulties, the centres of objects may be considered, following the centre-to-centre method of Ramsay (1967, pp 195–197). Strain is then studied by means of configurations of points. A general theory is required for the deformation of spatial distributions of points in geological materials. This is the object of the present paper.

SOME THEORETICAL CONSIDERATIONS

We wish to use the concept of a spatial distribution of points as a model for the naturally occurring distributions of particles or points in space. Accordingly, and restricting our attention to the two-dimensional case, let us define a spatial distribution of points in the Euclidean plane as a set of points such that every circle of finite radius contains only a finite number of them.

We are not particularly interested in regular patterns (those that are determined by the position of one particle and by some 'law' defining the geometry of the pattern). The distributions of points relevant to us are those which can be regarded as the outcome or realization of some random mechanism (which we may describe as a stochastic point process). Although we shall have to consider in practice a wealth of different models for such random-

ness, we will be mainly concerned with point processes whose statistical properties are shift-invariant (homogeneous or stationary) and rotation-invariant (isotropic).

That the natural diversity requires different stochastic models for its description becomes apparent from the analysis of very simple cases. Consider, for instance, the distribution of pyrite crystals scattered in an argillaceous matrix, and suppose that at the scale of observation they may be regarded as points. It being reasonable to assume 'complete' independence between the law of nucleation of different crystals (in the sense that the numbers of crystals in disjoint regions of the rock are independent random variables), we are led to regard the Poisson process as a likely model for such a situation. However, if the distribution of points corresponds, say, to the centres of oolites, then no two centres can lie arbitrarily close to each other (the distance between pairs of centres must be larger than twice the minimum oolite radius if there is no pressure solution). In these circumstances a Poisson model is no longer appropriate. Spatial distributions of the latter type are referred to by Fry (1979) as 'anti-clustered'; probabilists usually call them 'processes with exclusion' (e.g. Murmann 1978).

Both Ramsay (1976) and Fry (1979) have shown that the state of finite strain cannot be estimated using realizations of Poisson point processes. Indeed, any method of strain estimation from spatial distributions of points will have to use as raw material the relative positions of the points; since the linear transformation of a Poisson process yields a Poisson process (the ratio of the intensity measure of the strained process to that of the unstrained one being equal to the determinant of the transformation), the strained configuration will always still enjoy the same 'extreme independence property' which characterizes the Poisson process in general (Miles 1970).

Fry's (1979) 'all object separations' method seems to

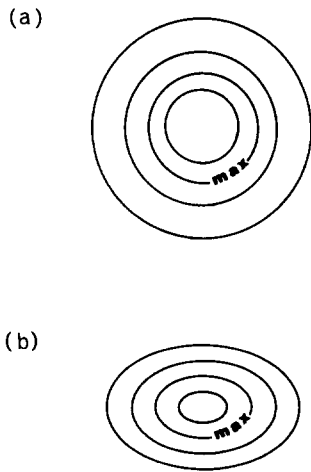


Fig. 1. Level curves of the density of the conditional spatial distribution of points around a given point ('max' denotes the highest level). (a) Initial configuration; (b) deformed configuration.

be applicable to the estimation of strain suffered by initially homogeneous isotropic point processes such that the conditional spatial distribution of points in the neighbourhood of a given point has a density of the type outlined in Fig. 1. There exist, however, certain special models for which other techniques are adequate. One such is Thomas's (1949) double Poisson process, whose realizations consist of clusters or galaxies of points, so that the 'centres' of the clusters are determined by a Poisson process (with intensity λ_1 , say), and the number of points for cluster is a Poisson random variable (with mean λ_2 , say).

If the bivariate probability distribution which determines the allocation of points in a cluster around its centre has finite and equal variances and null covariance (hence, circular dispersion matrix), then we have the following simple result:

Let Σ_0 be the circular dispersion matrix of the probability distribution determining the spatial allocation of points within a cluster. Let T be a linear transformation with $\det T > 0$. Then, the ratio of the eigenvalues of $\Sigma_1 = T\Sigma_0T'$ (which is the dispersion matrix of the strained cluster) is equal to the square of the axial ratio of the strain ellipse, and the eigenvectors of Σ_1 define the orientation of the axes of the strain ellipse.

To show that this is true let

$$T = \begin{bmatrix} a & b \\ c & d \end{bmatrix},$$

and

$$\Sigma_0 = \begin{bmatrix} \sigma_0^2 & 0 \\ 0 & \sigma_0^2 \end{bmatrix},$$

so that

$$\Sigma_1 = \begin{bmatrix} a^2 + b^2 & ac + bd \\ ac + bd & c^2 + d^2 \end{bmatrix} \sigma_0^2.$$

This has the same eigenvalues as

$$\begin{bmatrix} c^2 + d^2 & -(ac + bd) \\ -(ac + bd) & a^2 + b^2 \end{bmatrix} \sigma_0^2.$$

But

$$\begin{bmatrix} c^2 + d^2 & -(ac + bd) \\ -(ac + bd) & a^2 + b^2 \end{bmatrix} (\det T)^{-2}$$

is Cauchy's strain tensor, whose eigenvalues are λ_2^{-1} and λ_1^{-1} , where λ_1 and λ_2 denote the principal quadratic elongations. Thus, if σ_1^2 and σ_2^2 denote the eigenvalues of Σ_1 , then (Possolo 1977)

$$\begin{aligned} \sigma_1^2/\sigma_2^2 &= (\lambda_2^{-1}(\det T)^2\sigma_0^2)/(\lambda_1^{-1}(\det T)^2\sigma_0^2) \\ &= \lambda_1/\lambda_2. \end{aligned}$$

Moreover, the orientation of the eigenvectors of Σ_1 is given by

$$\tan 2\alpha = 2(ac + bd)/(a^2 + b^2 - c^2 - d^2)$$

(α being the angle between one of them and the Ox axis), which is a well known result from finite strain theory for the direction of the axes of the strain ellipse (Jaeger 1969).

Although this is directly applicable only when the original process consists of galaxies of points and the whole of one of them is observable, Kullberg (1980) has used it as the starting point for developing a method based on variance-covariance calculations which can be used to estimate the state of finite strain in more general spatial distributions of points.

INFLATING ELLIPSE METHOD

It is in the very nature of variances and covariances (of the coordinates) of a finite set of points in the plane that they be very sensitive to the location of the outermost points, hence sensitive to the shape of their convex hull.

In particular, consider a homogeneous, isotropic, 'anti-clustered' point process in the plane whose realizations are sets of points fairly uniformly scattered, so that whenever a bounded region is given, the dispersion matrix of the (finite number of) points that lie within it will depend essentially on the shape and size of that region. Furthermore, consider a circle in the plane, which, upon deformation, will become an ellipse (the points inside the latter are exactly those which had originally lain inside the former). The result presented in the previous section now shows that the positive square root of the ratio of the eigenvalues of the dispersion matrix of these points is an estimator of the axial ratio (Rs) of the strain ellipse.

Any method based on variance-covariance computations will have to be able to determine a set of points in the deformed configuration whose dispersion matrix is 'equivalent' to the matrix defining the irrotational component of strain.

The method we now describe relies on the assumption that the direction of maximum elongation is known.

Inflating ellipse: algorithm

- (1) Determine the centre (C) of the largest rectangle

(with one side parallel to the direction of maximum elongation) included in the section to be analysed.

(2) Define a lower bound (R_{min}), and an upper bound (R_{max}) for R_s (clearly, we can always put $R_{min} = 1$; the value of R_{max} is not critical, and only has to be large enough, cf. below).

(3) Define a positive increment ϵ , less than or equal to the precision one wishes to achieve in the determination of R_s .

(4) Initialize R as R_{min} .

Outer loop: Increment R by ϵ , while $R \leq R_{max}$, and for each value of R ;

Inner loop: Consider a sequence of inflating elliptical domains, all centred at C , with axial ratio R , and with the major axis parallel to the direction of maximum elongation. The increase in b (minor semi-axis of the elliptical domains) proceeds in discrete steps, and terminates whenever an ellipse is no longer (wholly) contained within the rectangle mentioned in (1). For each elliptical domain determine its minor semi-axis (b), the variance-covariance matrix of the coordinates of the points lying inside it, compute the positive square root of its eigenvalues (R_d), and plot a point with Cartesian coordinates (b , R_d).

(5) The outer loop in (4) yields a set of curves (each one corresponding to elliptical domains all with the same shape), which typically behave in an oscillatory fashion (Fig. 2).

However, the one corresponding to a value of R closest to the value of R_s will tend to become horizontal and flat from some value of b onwards, thus losing the sinusoidal behaviour. This R will be our estimate of R_s .

The amplitude of the oscillation may decrease (with increasing b) for other values of R , but this will only happen for values of b larger than the one corresponding to the value of R we have chosen as our estimate of R_s .

The sinusoidal aspect of each curve is due to the way in which the elliptical domain captures new points as it grows. The point processes we have been considering allow the estimation of strain; hence neighbouring points tend to be furthest away in the direction of maximum elongation, and closest to each other in an orthogonal direction. Under a constant inflation rate, the elliptical domain will acquire points more often along the latter direction than along the former. This means that while points are being acquired in the direction of minimum elongation, the ratio of the eigenvalues of the dispersion matrix will decrease, and then increase somewhat abruptly whenever points in the direction of maximum elongation are incorporated.

This effect can be very clearly appreciated when the method is applied to a rectangular lattice of points, which also provides additional insight into the rationale of the method (Fig. 3).

The shape of the curves corresponding to real data may thus be regarded as having a deterministic component as in the case of a deformed lattice, and a random component with stochastic fluctuation around the line $R = R_s$ (Fig. 2).

It should be noticed that other scales of measurement

might have been adopted for the abscissae; e.g. area of the elliptical domain would be a natural choice. We have tried various of these. However it turns out that in the R_d/b plots the behaviour of the curves in the critical region (when one of them becomes flat) is depicted in a particularly clear fashion.

If the deformed, anti-clustered distribution of Fig. 2 is progressively 'unstrained', and after each 'unstraining' increment the anisotropy of the points lying inside a circle is computed, then the minimal value 1.0 (which means a 'circular' distribution) shall be attained when the applied axial ratio reaches R_s (Fig. 4).

THE CASÉVEL SPILITE: A CASE STUDY

In order to evaluate the applicability of the inflating ellipse method to analyse the state of strain of a natural tectonite, it would be most appropriate to use a rock containing objects with some ductility contrast with respect to the matrix in which they are immersed; e.g. oolites of dolomite and calcite in a calcitic matrix.

If some technique like R_f/ϕ were applied separately to each of those classes of objects, different estimates of R_s would be obtained for calcitic oolites and dolomitic oolites. However, we would expect the inflating ellipse method, under the same conditions, to yield identical estimates for each of the classes of objects.

The existence, in the Casével region (135 km SE of Lisboa, Portugal), of deformed spilites with calcitic and chloritic amygdales in a chloritic matrix, has led us to regard them as good raw material on which to test the method.

Microscopic examination shows that the chloritic amygdales are clearly ellipsoidal while the calcitic ones retain their original spherical shape and, generally, there is no interaction between particles. The R_f/ϕ analysis of the chloritic vesicles would thus yield an estimate of R_s , against which we should compare the value obtained through use of our method on the centres of the calcitic amygdales.

Geology and petrography

For a general description of the volcanism and its facies in the region see Schermerhorn (1970, 1979) and Munhá & Kerrich (1980). Structurally, the southern tract of Portugal is an imbricate thrust belt. The main structures are arcuate (the general strike is N-S in the western portion, and E-W in the eastern part). Vergence is towards the SW.

In the Iberian Pyrite Belt (located in the inner region of the arc) the slaty cleavage dips at high angles to the NE, is axial planar to the folds but locally transects them. Stretching is in a . For further details see Ribeiro *et al.* (1979).

The spilites near Casével display a fragmental fabric, with angular pieces of amygdaloidal spilite together with a variety of rock types and sometimes hematite pellets set in a tuffaceous spilite matrix. Some slates and jaspers

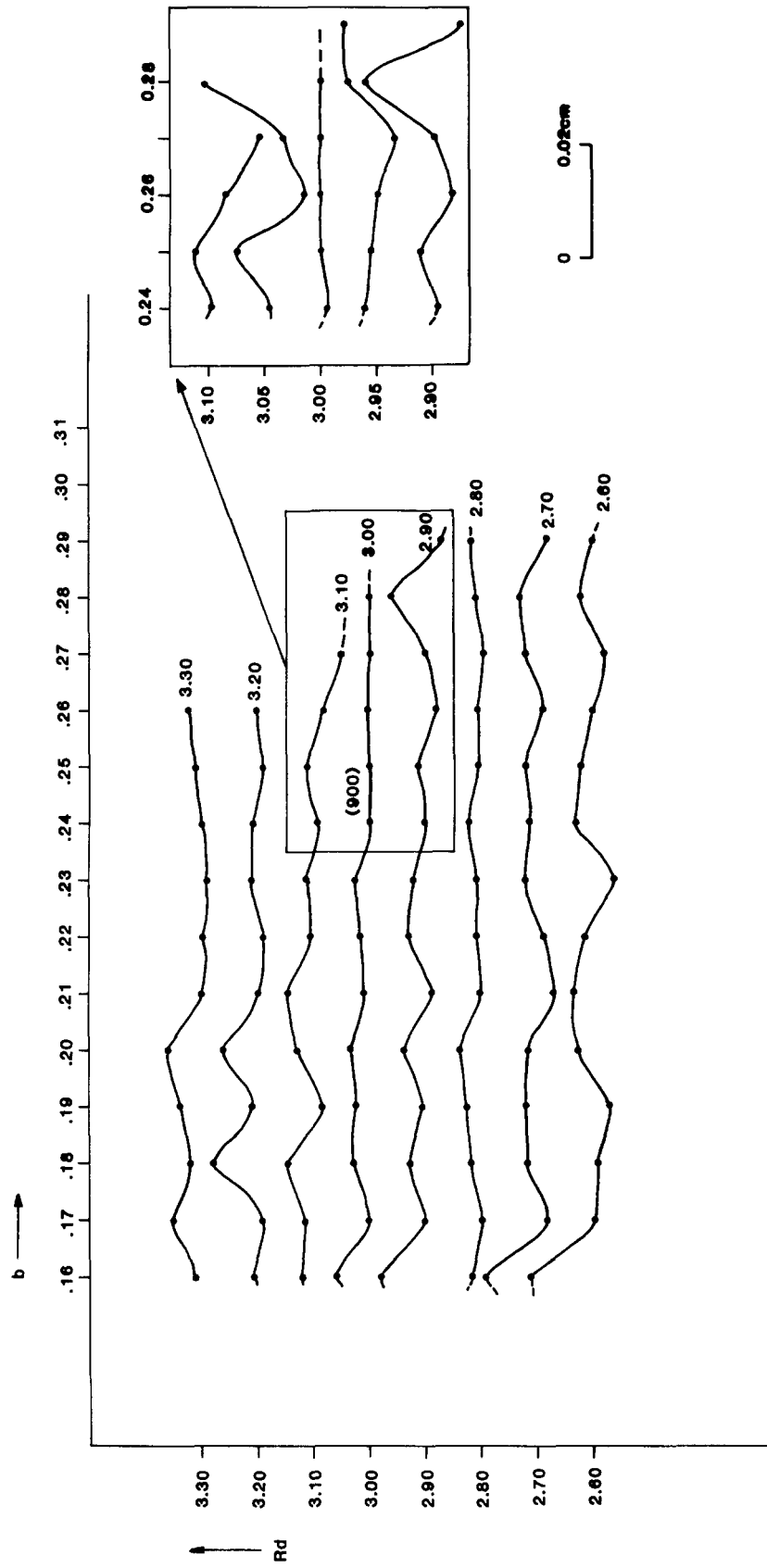


Fig. 2. Inflating ellipse method applied to a strained ($R_s = 3$) distribution of points which in the undeformed configuration corresponded to the centres of 1552 hard-discs packed in the unit square; plot of axial ratio (R_d) of the sample anisotropy ellipse, vs the length (b) of the minor semi-axis of the elliptical domain (whose axial ratio ranges from $R_{min} = 2.7$ to $R_{max} = 3.2$).

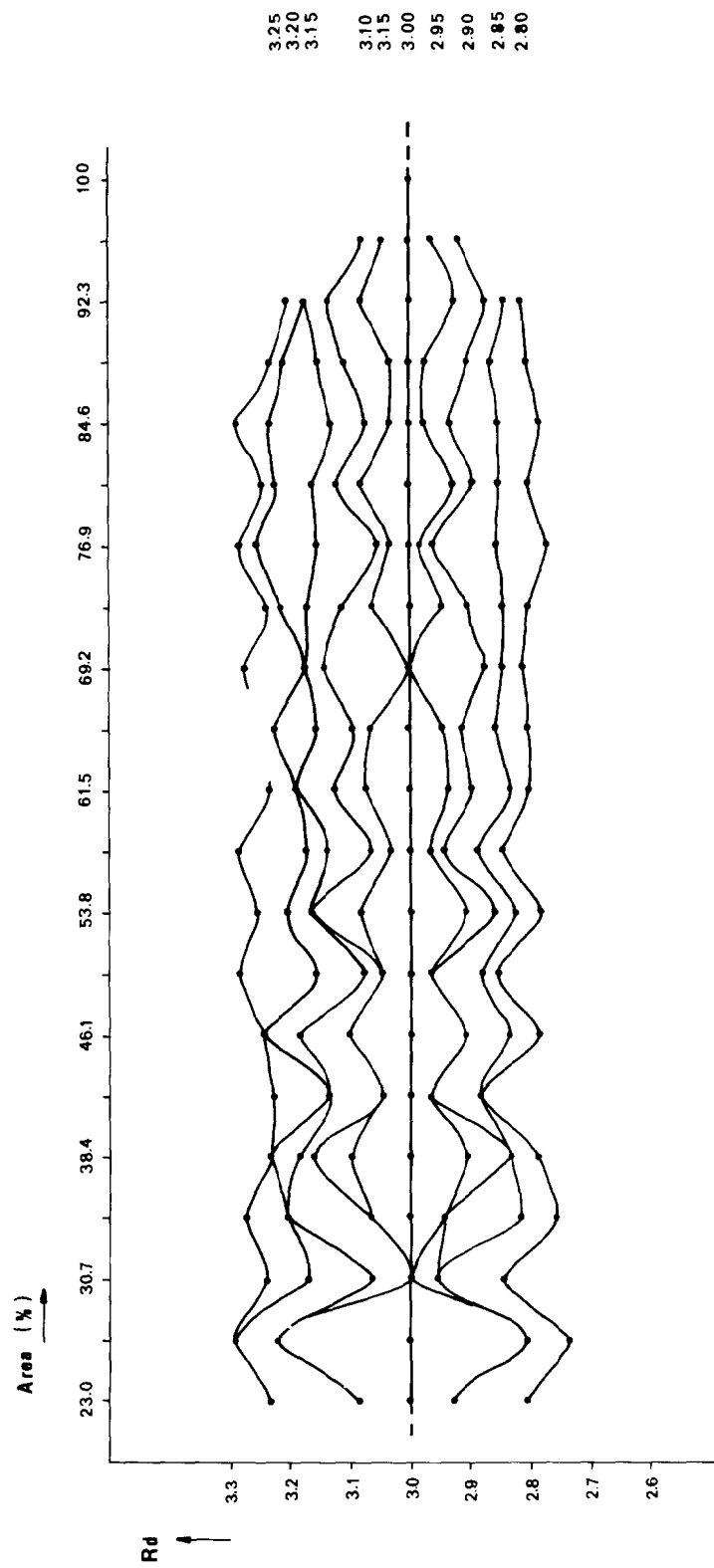


Fig. 3. Inflating ellipse method applied to a rectangular lattice of points (rectangle has length/width = 3) with 4332 points in the unit square. Plot of measured axial ratio of anisotropy ellipse (Rd) vs proportion of area of the deformed domain with axial ratio varying from 2.80 (Rmin) to 3.25 (Rmax).

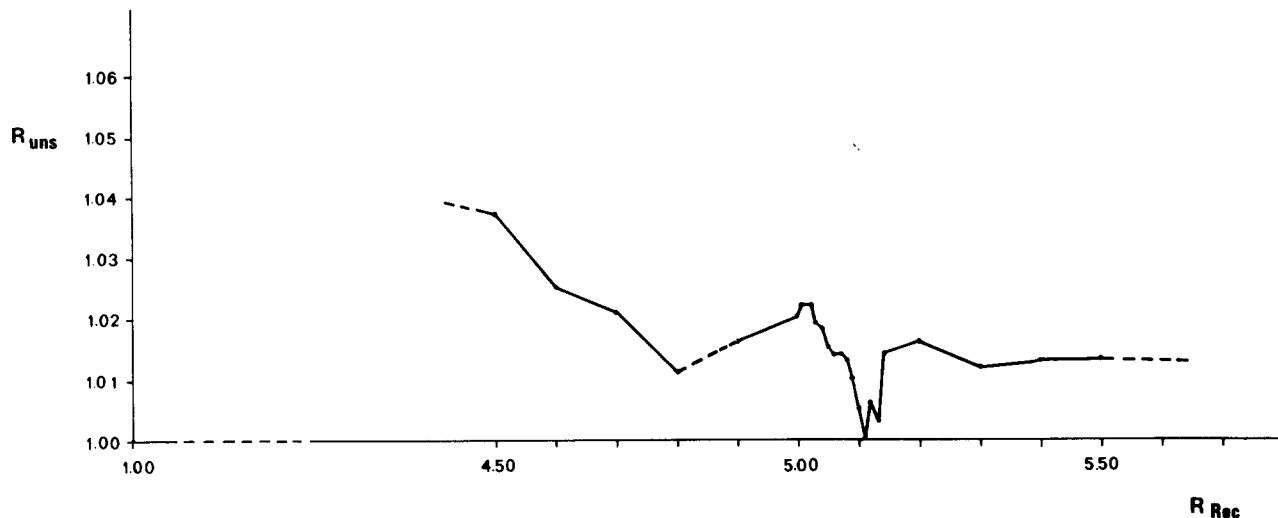


Fig. 4. 'Unstraining' method applied to the deformed distribution of Fig. 2. R_{Rec} is the axial ratio of the reciprocal strain ellipse and R_{uns} is the axial ratio of the anisotropy ellipse of the distribution of points lying inside a circle of maximum radius.

are interbedded with spilites and these are overlain by slates and acid tuffites. The bedding is not well defined in the massive spilites but is clearly seen in the slates. The top of the spilites is marked by an increase in the density of calcitic vesicles.

In the spilites the cleavage is stronger in the matrix, moulding itself to the flattened fragments. There is cleavage refraction at the contact of slates to spilites, showing that the latter are less deformed than the slates.

Our object of study is an XZ -section of an amygdaloidal microlitic spilite (Fig. 5) ($X > Y > Z$ are principal axes of the strain ellipsoid). The matrix is microcrystalline, very finely grained, containing chlorite, albite, opaque minerals and somewhat rare calcite. There are approximately 15 times more calcitic amygdaloids than chloritic ones.

The radii of the calcitic amygdaloids range between 200 μm and 2 mm. The results of intracrystalline deformation are bent cleavage planes and increased twinning. The regions around Z are affected by pressure solution, and those around X exhibit pressure shadows consisting of slightly bent syntaxial calcite fibres. The smallest axis of the chloritic vesicles is generally less than 200 μm long. The chlorite inside the amygdaloids has blue polarization tones, and is generally surrounded by a thin, discontinuous envelope, whose nature we have been unable to identify under the microscope; it exhibits undulatory extinction. When this film is continuous, both the internal and external boundaries are elliptical with the same axial ratio, which shows that there is no significant ductility contrast between the chloritic nucleus and that envelope.

Since there is no deflexion of the cleavage trace around the chloritic amygdaloids, we may conclude that no ductility contrast between these vesicles and the matrix exists.

Strain analysis

The following methods have been applied to the Casével spilite (Kullberg 1980).

(i) 'All object separations' method (Fry 1979). Only the centres of 566 calcitic amygdaloids have been used, and the corresponding plot is shown in Fig. 6. The estimate of R_s is 2.6. However, due to an unclear definition of the central ellipse, this cannot be a precise estimate.

(ii) *Method RF/ϕ* . It has been applied only to the chloritic amygdaloids, since the others are practically spherical. The variant due to Dunnet (1969) and Dunnet & Siddans (1971) yields 2.65 as the estimate of R_s (Fig. 7).

The corresponding plot is symmetrical with respect to the cleavage trace, which suggests a random initial fabric. This has been confirmed by means of removing estimated strain, and plotting the initial axial ratios (R_i) and orientation of the major axis with respect to the cleavage trace (θ) in polar coordinates (Fig. 8).

The analysis of this plots shows that the density of

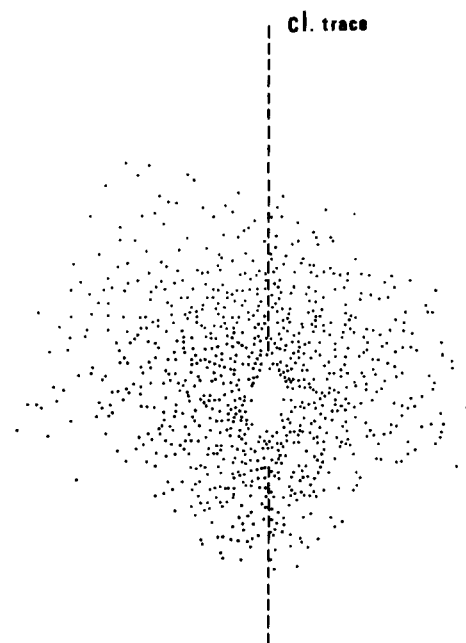


Fig. 6. Casével spilite. 'All object separations' using the centres of 566 calcite amygdaloids.

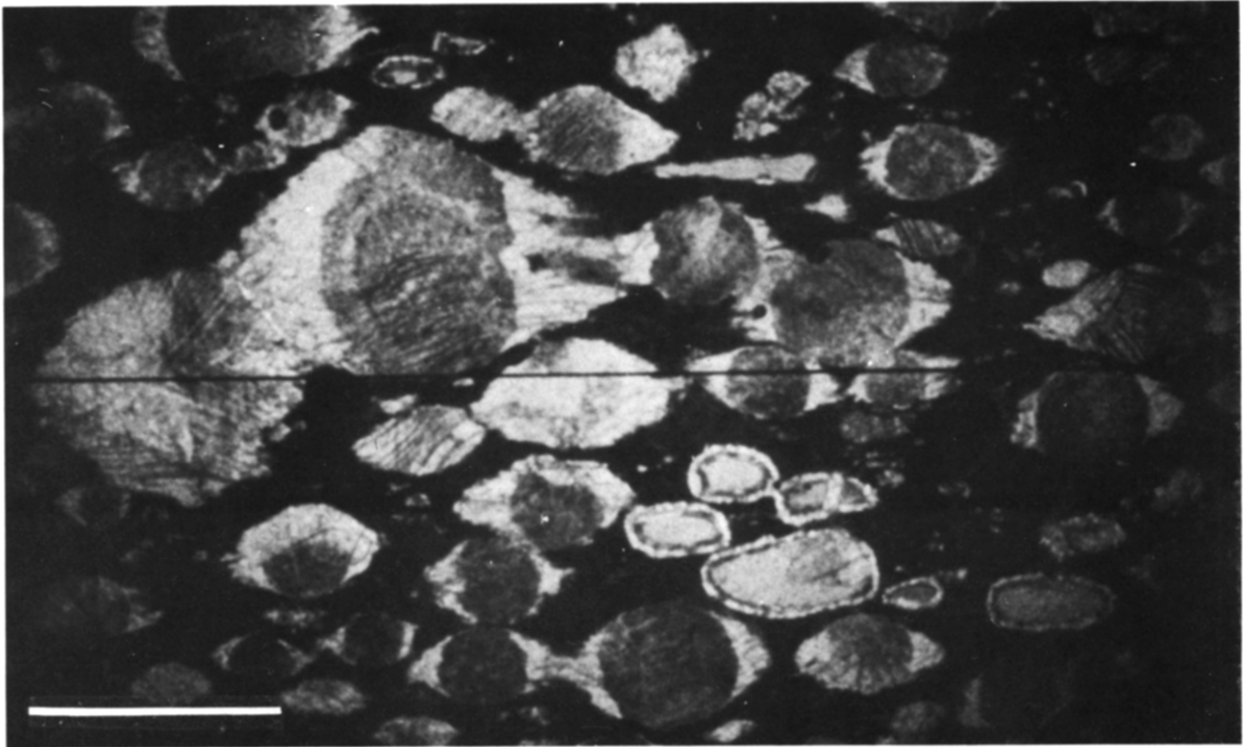


Fig. 5. Photomicrograph of the XZ section of Casével spilite. Scale bar is 1 mm long.

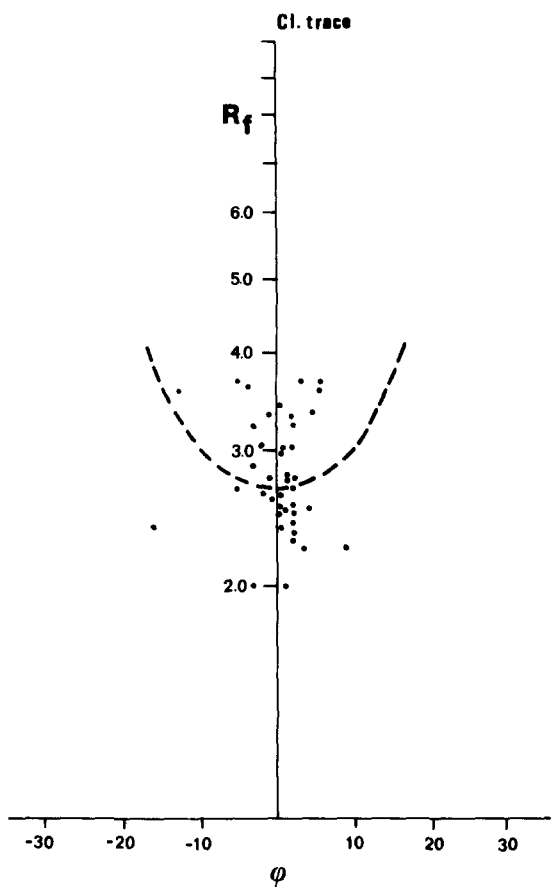


Fig. 7. Casével spilite. R_f/ϕ applied to the chlorite vesicles.

points decreases rapidly as we move away from the region corresponding to values of R_i close to 1, hence suggesting only slight fluctuation around an initially circular shape. Also, a chi-square test to the distribution of θ yields a statistic whose value (5.6 in a χ^2_5) by no means leads to the rejection of the null hypothesis of uniformity in the range $[-90^\circ, +90^\circ]$.

The numerical variant of the method, as proposed by Shimamoto & Ikeda (1976), yields an estimate of 2.68 for R_s .

(iii) *'Inflating ellipse' method.* The spatial distribution of points used was the same as in (i), and the subjects analysed contained between 222 (for the largest domain with $R = 2.80$) and 246 ($R = 2.50$) points. The corresponding diagram (Fig. 9) shows that the curve pertaining to the sequence of elliptical domains with axial ratio 2.65 is the one which becomes flat and horizontal, and assumes such a trend for domains including approximately 180 or more points. The perfect agreement with the estimate obtained in (ii) is very suggestive.

(iv) *'Unstraining' method.* The 'unstraining' method yielded poor estimates for the state of strain of the Casével spilite. This is probably due to the small number of points lying inside the circular domain used for the anisotropy calculations. As a general rule, since deformation usually reduces the variability of quantities of interest (e.g. the orientation of the major axes of pebbles), a method based on a Eulerian description (as 'inflipse') should be preferred to one following a Lagrangian approach (as 'unstraining').

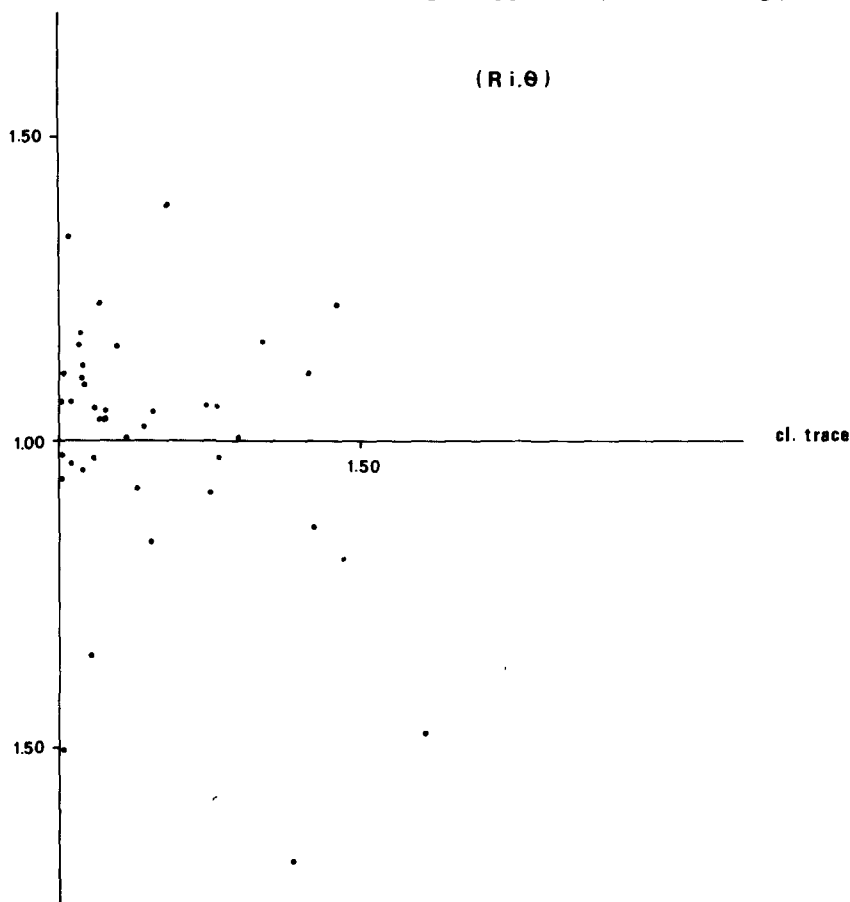


Fig. 8. Polar diagram (R_i, θ): analysis of the initial fabric of the chlorite vesicles in the Casével spilite (unstrained using $R_s = 2.65$).

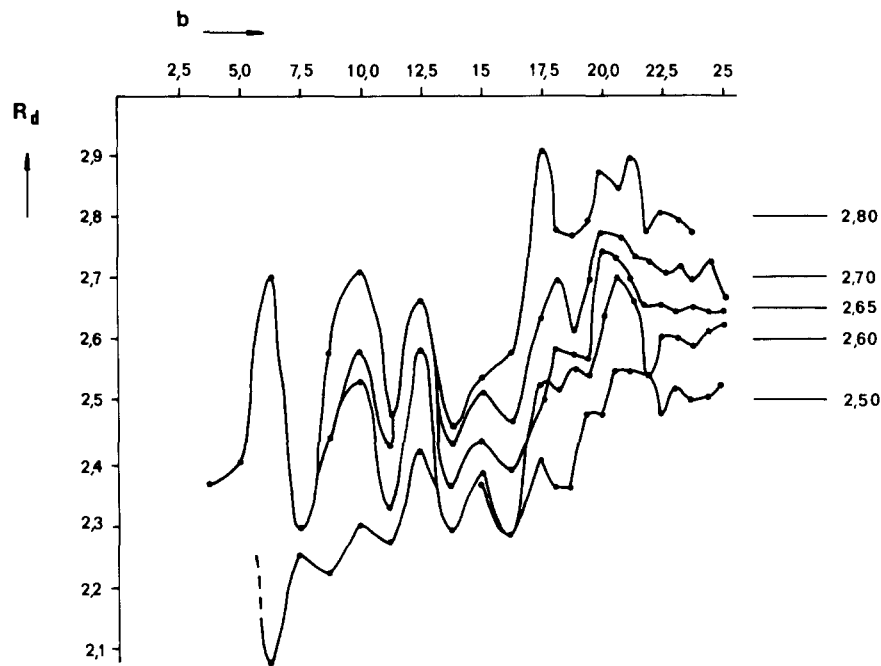


Fig. 9. Casével spilite. Inflating ellipse using the centres of the calcite amygdales: cf. Fig. 2 for fuller explanation.

SUGGESTIONS FOR FURTHER STUDY

Ranking of methods

The study of the Casével spilite suggests a general approach to the estimation of finite strain using spatially 'anti-clustered' distributions of points. First, Fry's method should be applied to the population of points available. If this method is unable to produce any estimate, the material cannot be used for the purpose under discussion. Otherwise, it will yield a first approximation to the value of R_s , and so the values of R_{min} and R_{max} (cf. inflating ellipse algorithm) can be chosen so that the estimate lies between them and their difference is small, thus speeding up the process of refining the aforementioned estimate via the 'inflating ellipse' method.

Limitations of the method

Hanna & Fry (1979) discussed various situations in which Fry's method could not be used: realizations of point processes for which a Poisson process constitutes a good approximation, and deformation by sliding at object boundaries. The method also fails whenever strain leads to the disruption of objects, and so does the 'inflating ellipse' method; this is so because a one-to-one correspondence between points in the unstrained and strained configurations is a necessary condition for estimability. The domain of cataclastic deformation is thus beyond the reach of these methods (Mukhopadhyay 1980).

It should be stressed that the assumption of homogeneity is indeed crucial, as experience has shown in various analyses of natural materials.

From two to three dimensions

The transition from two to three dimensions cannot be carried out along the lines usually followed in strain analysis.

Indeed, in the plane the problem of the existence of some ductility contrast between particles and matrix is circumvented since the rigid body rotation induced by such contrast is around the centroid of each object. In three-dimensional Euclidean space, a section through an object does not allow the determination of the point invariant for the rotation which the object has undergone due to the ductility contrast, and so the problem does not seem to be easy to overcome.

In the case of the Casével spilite, a three-dimensional analysis will not change the results obtained via the two-dimensional study. Since the calcite vesicles have had a rheologic behaviour close to rigidity, we may think of what happens in a section as if the circle, defined by the intersection of a sphere with the plane of the section, had undergone a rigid body rotation, which will necessarily have as centre the centroid of such a circular section.

Future work

The method here described may be regarded as a general tool for the analysis of the fabric of any rock: sedimentary, igneous or metamorphic. It allows a quantitative characterization of the anisotropy of any fabric. One particle can be replaced by its centroid, which depends only on its shape and not on the process which has originated it. In particular, some preliminary results of an ongoing study of layered fabrics seem promising (Kullberg 1980).

It is the generality of the method that makes it useful in structural analysis, since it sizeably broadens the scope of materials in which the state of finite strain can be estimated. We no longer require that the objects be ellipsoidal, but only that the rigid body rotation due to the ductility contrast between them and the matrix, be around axes through the objects' centroids.

Finally, the comparison between the results obtained via the Rf/ϕ method and these obtained using the 'inflating ellipse' method will allow the computation of ductility contrasts between objects and the matrix in which they are immersed. This will be an important contribution for the palaeo-rheology of deformed rocks.

Acknowledgements—The study has been carried out under the research project 'Statistical methods for the analysis of finite strain' of the Geological Survey of Portugal. It has received some support from the 'Sociedade Portuguesa de Empreendimentos', through M. Bernardo Reis.

We would like to thank Paula Lena, Xavier Leca, Luisa Ribeiro, Fernando Barriga and José Brandão Silva for their cooperation in the project, and Andrew Siddans for his comments on the manuscript.

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