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ANALYSIS OF POLAR PLOTS FORMED BY CIRCLES OR SPHERES

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ABSTRACT

Polar plots formed by circles or spheres appear in different contexts, such as in the stereology of oriented structures and in simple calculations of the surface energy of crystals. They represent functions, f(**n**), of the orientation, **n**, of a particular type, when f is proportional to the sum of the normal projections onto **n** of a set of given vectors, {**v**}. New graphical methods of analysis of these f-polar plots are developed with which the {**v**} set can be determined. The methods are based on the concept of principal vectors which can be determined graphically from the f-plot and from which, by another graphical method, the v-vectors are obtained as the edges of a convex polygon (2D) or polyhedron (3D). The method can also be applied to continuous distributions of **v**-vectors.

Three-dimensional f-plots are usually displayed in planar sections. The information on the v-vectors that can be derived from these sections is discussed. Cusps in f-plots are analysed and it is shown how their sharpness can be related to the principal vectors.

KEY WORDS: oriented distributions, rose of directions, polar plots, cusps, polyhedra.

INTRODUCTION

There are various problems in stereology and in other disciplines in which a scalar quantity f(**n**) is defined as a function of the orientation **n** in space, through the relation

$$f(\mathbf{n}) = \sum_i |\mathbf{v}_i \cdot \mathbf{n}| \qquad (1)$$

where the $\mathbf{v}_i$ are a (finite) set of given vectors. f(**n**) is therefore the sum of the normal projections of the $\mathbf{v}_i$ onto **n**.

Equations of this type occur in the field of stereology of oriented distributions of surfaces or curves (e.g. Hilliard, 1962; Underwood, 1970). Table 1 summarizes the relevant problems. The orientation of surfaces is defined by the unit normal, **e**, and the orientation of curves by the unit tangent, which we also denote by **e**. We assume for the moment that the distributions are discrete, each orientation, i, being defined by a vector $\mathbf{e}_i$. The area of surfaces and the length of curves of orientation i, per unit volume of a 3D distribution, are denoted by S_{V_i} and L_{V_i}, respectively; and the length of lines of orientation i, per unit area of a 2D distribution, is L_{A_i}.

Table 1. Intersection of oriented structures

	Oriented features	Intersected by
3D	Surfaces: normal e_i ; S_{V_i}	Lines: direction n ; P_L
3D	Curves: direction e_i ; L_{V_i}	Planes: normal n ; P_A
2D	Curves: direction e_i ; L_{A_i}	Lines: normal n ; P_L

An oriented distribution is intersected by parallel test planes of unit normal $\mathbf{n}$ or by parallel test (straight) lines, with orientation defined by the unit normal $\mathbf{n}$ in 2D problems or by a unit vector, $\mathbf{n}$, parallel to their direction, in 3D problems, as indicated in Table 1. In all cases listed , a distribution of intersection points on the test planes or test lines results, with average densities P_A (per unit area) and P_L (per unit length), respectively.

Both P_A and P_L depend on $\mathbf{n}$ and, obviously, on the intersected distribution. The relevant equations were first derived by Hilliard (1962). For a discrete set of orientations, $\mathbf{e}_i$, they can be written in the form

$$P_L(\mathbf{n}) = \sum_i S_{V_i} \left| \mathbf{e}_i \cdot \mathbf{n} \right| \tag{2}$$

$$P_A(\mathbf{n}) = \sum_i L_{V_i} \left| \mathbf{e}_i \cdot \mathbf{n} \right| \tag{3}$$

$$P_L(\mathbf{n}) = \sum_i L_{A_i} \left| \mathbf{e}_i \cdot \mathbf{n} \right| \tag{4}$$

respectively for surfaces intersected by test lines (3D), curves intersected by test planes (3D) and curves intersected by test lines (2D)*. It is apparent that eqs. 2-4 are of the type of eq. (1), with $\mathbf{v}_i$ vectors defined by $S_{V_i}\,\mathbf{e}_i$, $L_{V_i}\,\mathbf{e}_i$ and $L_{A_i}\,\mathbf{e}_i$, respectively.

Another example of a problem that leads to an equation of type (1) appears in the calculation of the surface energy of a crystal with one atom per lattice point, when the atoms interact by a pairwise central potential, $\epsilon(r)$. The equation for the (unrelaxed) surface energy, γ, for an orientation of the surface with unit normal $\mathbf{n}$, is given by the lattice sum (Herring, 1951; Correia and Fortes, 1985)

$$\gamma(\mathbf{n}) = -\frac{1}{2v} \sum_i \epsilon\,(\ell_i) \left| \ell_i \cdot \mathbf{n} \right| \tag{5}$$

where the ℓ_i define the atomic positions relative to a reference atom, and v is the volume per atom. For each ℓ_i there is a $-\ell_i$, but only one should be taken in the

* The intersection of surfaces by test planes does not lead to an equation of type (1): the scalar product is replaced by a vector product.

sum of eq.(5). Defining v_i - vectors by

$$v_i = -\frac{1}{2v}\,\epsilon(\ell_i)\,\ell_i \qquad (6)$$

and noting that $\epsilon(r)$ is negative for all interactions in the crystal, we conclude that (5) is also of the type of eq. (1).

Let us now consider a continuous distribution of vectors, defined by a density function v(e), where e is a unit vector defining a direction in space and v is parallel to e. In 2D, v(e) is the sum of vectors per unit angular interval of orientations in the neighbourhood of e. In 3D, n(e) is the sum of vectors per unit solid angle centred at e. The equations that replace eq. (1) are

$$f(\mathbf{n}) = \int |\mathbf{v}(\mathbf{e}) \cdot \mathbf{n}|\, d\theta_e \qquad (7)$$

$$f(\mathbf{n}) = \int |\mathbf{v}(\mathbf{e}) \cdot \mathbf{n}|\, d\Omega_e \qquad (8)$$

where $d\theta_e$ and $d\Omega_e$, respectively, represent an elementary angle or solid angle in the neighbourhood of e. For example, if e is defined by cylindrical angles θ, ϕ, then $d\Omega_e = \sin\theta \, d\theta \, d\phi$.

The function f(n) is frequently displayed in a polar plot, or f-plot, in which the distance to the pole, 0, in each direction n, is proportional to f(n). The plot, frequently termed the rose of directions (Saltikov, 1958), is a closed curve or surface, respectively, in 2D and 3D. When the distribution of v-vectors is discrete (eq.1), the polar plot is known (e.g. Underwood, 1970) to be formed by portions of circles (2D) or spheres (3D).

Experimentally it is possible, at least in principle, to obtain f(n) or the corresponding plot. The central question that we address in this paper is the following: how can one obtain the v-vectors (i.e. the individual vectors of a discrete set or the density function v(e)) from the f-plot?

Graphical methods will be developed with which this problem can be solved. To do this we introduce the concept of principal vectors which can be obtained from the f-plot and with which the v-vectors can be determined, either analytically or graphically. The singularities (cusps) in the polar plot of f(n) will also be studied and their sharpness will be related to the principal vectors. Finally, the information on the v-vectors that can be obtained from planar sections of a 3D f-plot will be discussed.

Previous attempts at solving equations of type (1), (7) and (8) to obtain the v-vectors were made by Hilliard (1962), using methods based on Fourier and spherical harmonics expansions and also a second differences method. These are relatively complicated analytical methods. A simple method to solve eq. (7) is described by Serra (1982), in which the equation is first transformed into a second order differential equation in v(e). Another approach to the solution of the integral equations was recently developed by the present author (to be published), which is based on the linearization of the equations that relate f(n) to the v-vectors. This method is quite general, but in each case requires a separate calculation of the coefficients in the linear relation. The graphical methods to be developed are simple, exact and of general applicability. Being graphical methods they give the results in a graphical form, which is usually easier to visualize.

PRINCIPAL VECTORS, DISCRETE DISTRIBUTIONS

Consider a finite set of vectors, v_i, with no two parallel vectors. If a set of vectors is given with two or more parallel vectors, a vector v_i is constructed, parallel to those vectors, the modulus of which is the sum of the moduli of the parallel vectors. This set is termed a reduced set of v_i -vectors. For example, the set of vectors (6) is not a reduced set. The direction of the vectors is irrelevant, i.e., v_i can be replaced by $-v_i$.

For a given direction, **n**, in space, we define the principal vector (P--vector), P(**n**), associated with **n**, as the linear combination of the v_i, with coefficients ± 1, that has the largest normal projection on **n**:

$$P(\mathbf{n}) = \sum_i (\pm\, v_i) \qquad ; \qquad |P \,.\, \mathbf{n}| \text{ largest} \tag{9}$$

Clearly

$$P(\mathbf{n}) = -P(-\mathbf{n}) \tag{10}$$

meaning that for each P-vector, P, there is a P-vector, -P. Note also that the P-vectors are not affected if v_i is replaced by $-v_i$. Equation (1) can be written as

$$f(\mathbf{n}) = P(\mathbf{n}) \,.\, \mathbf{n} \tag{11}$$

If the P-vectors are placed at a common origin, we obtain the P-plot. When the distribution of v-vectors is discrete, as we are presently assuming, there are intervals or domains of **n** (i.e. regions in space) which have the same P. The vector P that corresponds to a domain may not be within the domain (see example below, Fig. 1c).

The domains are separated by planes (3D) or lines (2D) perpendicular to the v_i-vectors. The P-vectors of two domains adjacent at a plane (3D) or line (2D) are termed adjacent P-vectors. Their difference is, from the definition (9), a $2v_i$-vector.

There are two problems that we shall address in this section. The first is the determination of the P-vectors of a given discrete set, v_i. The second is the reverse problem of determining the v-distribution from the P-vectors.

The first problem can in general be solved by the following method, based on the definition of the P-vectors: a combination of the v_i with coefficients ± 1 is a principal vector if there is a direction **n** (in the plane for 2D problems; in space for 3D problems) for which P . **n** is larger than P'. **n**, where P' is any other ± 1 combination of the v_i.

There is a simple construction that can be used to find the P-vectors in 2D. The v_i-vectors are placed at a common origin, starting with an arbitrary v_i; the direction of the other vectors is chosen such that their angles with v_i, measured anticlockwise, are smaller than 180° (Fig.1a). The successive vectors are v_1, v_2, v_3 ... and their orientation is taken as positive (+). The sum of these vectors will be represented by +++ ··· ++ and is the principal vector in the direction perpendicular to v_1. The other principal vectors are the sums obtained from this one by replacing successive + signs by – signs, as in the following example for 4 vectors (Fig.1b):

\+ + + +
\+ + + –
\+ + – –
\+ – – –

These sums and their symmetrics are the P-vectors. For example, (+ + + –) means $v_1 + v_2 + v_3 - v_4$. Other $\pm$ combinations do not give principal vectors. The number of P-vectors is then twice the number, n, of v_i-vectors. The domain of each vector P is bounded by two straight lines in the P-plot, through the pole, and perpendicular to the v_i-vectors by which P differs from the two adjacent P's (dotted lines in Fig.1c). Conversely, if the 2D P-plot is given, we can obtain the

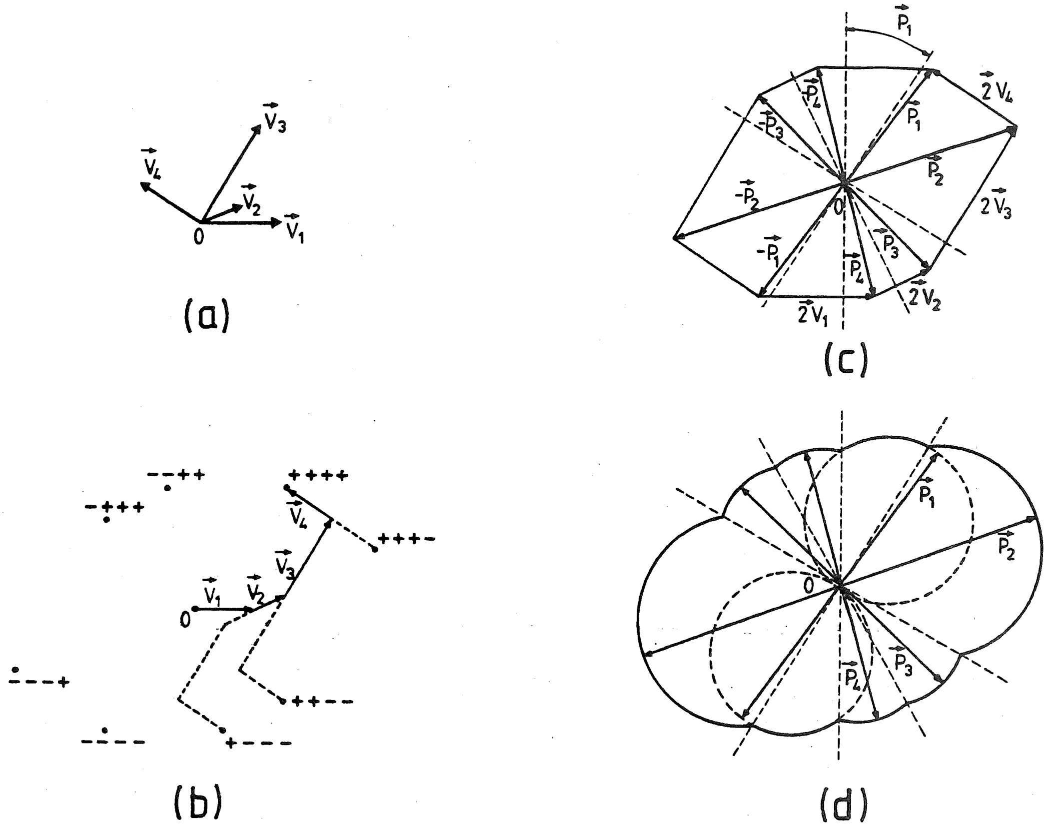

Fig.1 - a) Four vectors are arranged in order of increasing angle with one of them, $\mathbf{v}_1$. This defines the + orientation of the vectors and their order. b) Construction to obtain the principal vectors: they are the vectors between the origin, or pole, 0, and the points ++++, +++-, ++--, etc.. c) The P-plot and the v-polygon; note that P_1 is outside its own domain. d) The f-plot of the v-vectors is formed by arcs of circles each with a P-vector as a diameter; each circle appears in the corresponding domain, and intersects other circles at point cusps.

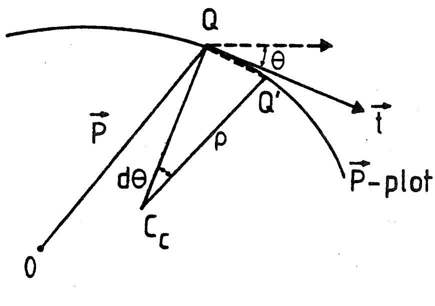

Fig.2 - Determination of a 2D continuous distribution of v-vectors from the P-plot. The vector density $\mathbf{v}(\theta)$ is tangent to the P-plot and its modulus is $\rho/2$, where ρ is the radius of curvature of the P-plot.

$2v_i$-set by simply joining the extremities of the successive P-vectors. We obtain a convex, centro-symmetric polygon (the v_i-polygon), the edges of which are the $2v_i$-vectors (Fig.1c).

For 3D discrete distributions there is no simple algorithm to determine the P-vectors. They have to be obtained by the general method described above. However, their total number can be calculated by a simple equation (eq.26) that we shall derive later and which depends on how the v_i-vectors are distributed in planes.

Adjacent P-vectors in 3D can be identified with the help of the f-plot. Two P-vectors are adjacent if their spheres in the f-plot intersect along a line (cusp). This line lies in a plane perpendicular to the $2v_i$-vector by which the adjacent P-vectors differ. From the P-plot it is possible to construct a polyhedron having the $2v_i$-vectors as edges and the extremities of the P-vectors as vertices. This will be discussed later in more detail. Therefore, if the P-vectors are known and their adjacencies have been identified, it is possible to obtain the set of v_i-vectors. As an alternative (which can also be applied to 2D problems), the v_i-vectors can be obtained by subtracting all pairs of P-vectors. The resulting set has the $2v_i$-vectors as a vector base, with coefficients ± 1.

PRINCIPAL VECTORS, CONTINUOUS DISTRIBUTIONS

When the distribution of v-vectors is continuous, the P-plot is a closed curve (2D) or surface (3D) with no singularities. It is easily concluded from the previous discussion that the direction, **n**, associated with each P coincides with the normal to the P-plot at the point corresponding to that P. We assume that the P-plot is known or has been determined from the f-plot (see below) and discuss how the distribution of v-vectors can be obtained from the P-plot using a construction similar to the one described for discrete distributions.

Consider first a 2D P-plot (Fig.2) an a point Q at which the unit tangent is t. This vector t can be identified by the angle, θ, with a reference direction in the plane. The tangent at a point Q' in the neighbourhood of Q is defined by $\theta + d\theta$. The vector between Q and Q' is 2dv, in the direction of t, where dv is the v-vector for the interval θ, $\theta + d\theta$.

The modulus of 2 dv is the arc length, $\rho\, d\theta$, between Q and Q', ρ being the radius of curvature of the P-plot at Q. Therefore, the density function $v(\theta)$ is given by

$$v(\theta) = \frac{\rho}{2}\, t \tag{12}$$

which completely defines the distribution of v-vectors.

A similar method to obtain, from the P-plot, the density of v-vectors in 3D distributions is as follows. Consider a point Q in the P-plot (Fig. 3a) where the normal is **n**. As already stated, **n** is in the direction associated with P = OQ. Consider all points, Q', in the P-plot for which the normal is at an angle $d\psi$ with **n**. A pair of P-vectors corresponding to two Q' points on each side of the normal **n** (i.e. the normals at the two points and at point Q are coplanar) differ by two times a principal vector of the v-vectors in the plane perpendicular to **n**. We refer to these principal vectors as **p**-vectors. The length of each of these vectors is $2Rd\psi$, where R is the radius of curvature of the corresponding normal section of the P-plot. Let R_1 and R_2 be the principal radii of curvature at Q, and α the angle between a normal section and the principal section of radius of curvature R_1. Then

$$\frac{1}{R} = \frac{\cos^2\alpha}{R_1} + \frac{\sin^2\alpha}{R_2} \tag{13}$$

The planar plot of the **p**-vectors (**p**-plot) parallel to the tangent plane at Q and within the range $d\psi$ is then defined by this equation and is shown in Fig. 3b for $R_1/R_2 = 2$. This plot can be analysed by the graphical method previously described for 2D distributions to find the **v**-vectors in the tangent plane. The tangent to the p-plot at S defines the direction of a **v**-vector, of orientation θ relative to the principal direction of radius R_1; the modulus of this vector is $\rho d\theta d\psi$, where ρ is the radius of curvature of the **p**-plot at S (a factor 1/2 cancelled with the factor 2 in $2Rd\psi$). The density of **v**-vectors is then ρ, defined per unit interval of ψ and unit interval of θ. Simple calculations lead to the following equations for the orientation θ as a function of α and for ρ/R_1

$$tg\theta = tg\alpha \; \frac{(\lambda - 1)\cos^2\alpha + \lambda}{(\lambda - 1)\cos^2\alpha + 2 - \lambda} \tag{14}$$

$$\frac{R_1}{\rho} = \left[2 - \lambda + 3(\lambda - 1)\cos^2\alpha\right]\cos^3(\theta - \alpha) \tag{15}$$

where

$$\lambda = R_1/R_2 \tag{16}$$

POLAR PLOT OF f(**n**): DETERMINATION OF P-VECTORS

The polar plot of f(f-plot) is formed by circles (in 2D) or spheres (in 3D) each associated with a P-vector and passing through the origin and the extremity of the P-vector placed at the origin. The f-plot is formed by the portions of the circles or spheres that are, in each direction, further away from the pole. For continuous distributions, the f-plot is the external envelope of the circles or spheres. Examples of 2D f-plots are shown in Figs. 1d and 4, respectively, for 2D discrete and continuous distributions. The f-plots are centro-symmetric in virtue of (9). Each circle or sphere appears in the domain of each P-vector, and has that P-vector as a diameter. In 2D, adjacent circles are associated with adjacent P-vectors; in 3D, adjacent spheres, which intersect along a line, are associated with adjacent P-vectors.

The P-vectors can be obtained from the f-plot by the following construction, which is, to a certain extent, the reverse of the construction method to obtain the f-plot from the P-vectors. At a point F of the f-plot in the direction **n** (Fig.5), draw the normal ν to the f-plot and locate a point C in it equidistant from F and the pole 0. The vector OC is the vector P/2 for the direction **n**. This construction can be applied to 2D and 3D discrete or continuous distributions, and is schematically shown in Fig. 5. Its validity for 2D distributions can be proved quite easily. It will be shown later that the angle β, between **n** and ν is equal to the angle between P and **n**. Since the angle between OC and **n** is also β (see Fig. 5), it follows that P is in the direction of OC. But the projection of OC in the direction **n** is $\frac{1}{2}$ P . **n**, implying that OC = $\frac{1}{2}$ P.

In the case of discrete distributions, the points C are the centres of the circles or spheres of the f-plot. This is also true for continuous distributions (Fig. 4) when the f-plot is the external envelope of circles or spheres through the pole and the extremities of the P-vectors.

PLANAR SECTIONS OF 3D f-PLOTS

A 3D f-plot is usually displayed in planar sections through the pole, each giving f(**n**) for orientations **n** in the plane of the section, of unit normal N.

The information on the principal vectors that can be drawn from the section concerns exclusively the subset of P-vectors that are principal vectors for the

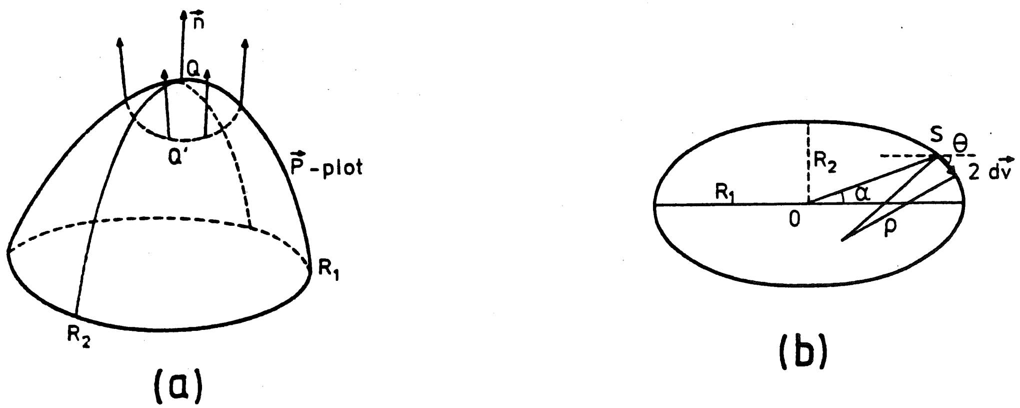

Fig.3 - Determination of a 3D continuous distribution of **v**-vectors from the P-plot. a) At the points in the dotted curve, the normals to the P-plot are at a constant angle, $d\psi$, with the normal, **n**, at point Q. b) The curve (eq. 13, for $R_2/R_1=2$) gives the radii of curvature of the normal sections at Q; it is the P-plot of the **v**-vectors in the tangent plane at Q, from which the vector density function $v(\theta,\psi)$ can be determined by the method of Fig. 2.

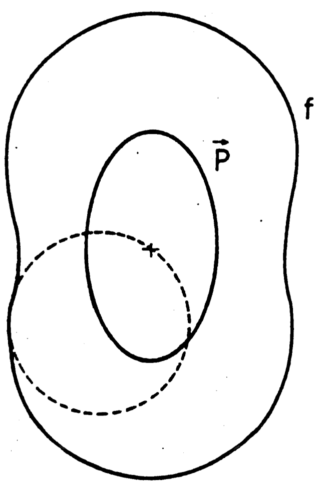

Fig.4 - An arbitrary P-plot (internal curve) of a continuous distribution of vectors and the corresponding f-plot (external line), obtained as the external envelope of circles each having a P-vector as a diameter. The distances to the pole in the f-plot have been multiplied by 2, for the sake of clarity.

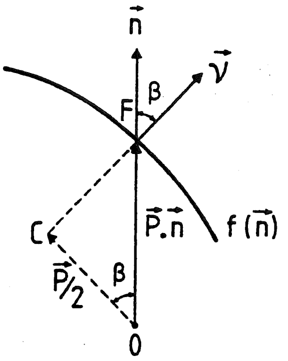

Fig.5 - Determination of the P-vectors from a 2D f-plot. The P-vector associated with the direction n is obtained by drawing the normal ν to the P-plot and locating the point C in it, equidistant from the pole and F. Then OC=P/2.

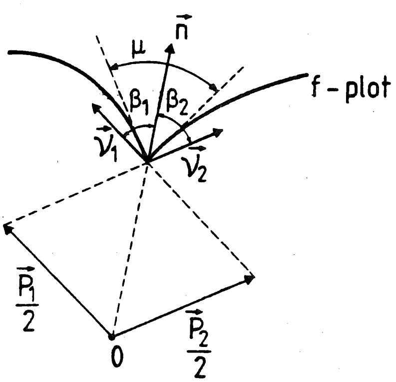

Fig.6 - The sharpness of a cusp in a 2D f-plot, at the orientation **n**, is associated with a discontinuity in the principal vector, which changes from P_1 to P_2 . The sharpness of the cusp is the angle μ between the tangents to the f-plot at the cusp: $\mu=\pi-\beta_1-\beta_2$; the normals to the f-plot at the cusp are ν_1 and ν_2, their angles with **n** being β_1 and β_2, respectively.

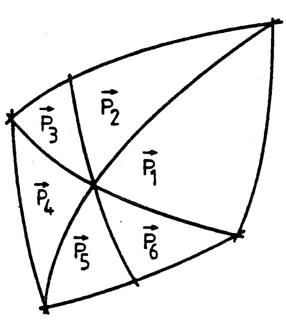

Fig.7 - Graph obtained by projection from the pole of the f-plot onto a sphere surrounding the f-plot. Each region is associated with a principal vector. Two regions are separated by a line cusp. The vertices of the graph are the projections of the point cusps. Note that each line cusp is continuous, with, for example, $P_2 - P_3 = P_5 - P_6$.

directions, **n**, perpendicular to N. More precisely, the section of the f-plot is related to the vectors P_p that are the normal projections on the plane N of that subset of principal vectors. One can write

$$P = P_n \ N + P_p \tag{17}$$

and therefore

$$f(\mathbf{n}) = P \cdot \mathbf{n} = P_p \cdot \mathbf{n} \tag{18}$$

This shows that the P_p-vectors can be obtained from the f-section by the construction previously described for planar distributions. The difference between adjacent P_p vectors is $2v_p$, where v_p is the sum of the projections of the v_i--vectors in the same plane perpendicular to the plane N. That is, various v_i may contribute to the difference between two adjacent P_p.

In general, the reconstruction of the complete set of P- or v-vectors requires various planar sections of the f-plot, since each contains information on the projections of a subset of P- and v-vectors. The complete determination of the P-vectors, and, therefore, of the v-vectors, can in principle be achieved from a finite number of sections, if the distribution is discrete with a finite number of v_i-vectors. A continuous distribution of v-vectors can only be determined from the complete, 3D, f-plot. Suppose that the set of P-vectors is known. In order to obtain the section of the f-plot by a plane N we first project all P-vectors on the plane and place them at a common origin. Circles are drawn in the usual way, each having a projected P-vector as a diameter. The section of the f-plot is the external envelope of these circles and includes only some of them, which correspond to the P_p-vectors of the spheres in the 3D-plot that are intersected by the plane N.

CUSPS IN f-PLOTS

A singularity (cusp) occurs in the f-plot at the boundary between two regions dominated by adjacent principal vectors that differ by a finite v_i-vector.

In 2D, point singularities occur for the directions, **n**, perpendicular to each of the v_i-vectors. The number of cusps in 2D is then 2n, where n is the number of v_i-vectors (or the number of singularities in the 2D distribution of v-vectors).

In 3D, the basic singularity is a (planar) line cusp in the plane perpendicular to a v_i-vector. Two or more line cusps may intersect at a point originating a point singularity. These point cusps occur for directions, **n**, perpendicular to planes containing a number, $i(i \geq 2)$, of v_i-vectors and are the intersection of i line cusps. This implies that in general a line cusp will contain point cusps, and that isolated point cusps cannot occur. A line cusp is a closed planar curve, containing point cusps; at a point cusp, the principal vectors associated with the line cusp change, but the difference between them is unchanged.

The number of line and point cusps in 3D f-plots will be discussed in the following section.

The sharpness of a point cusp in 2D or of a line cusp in 3D is related to the derivatives of f(**n**) on either side of the cusp. Let us consider a point F in the direction **n** in a region of the f-plot with no singularities, and find the variation of f when **n** is rotated by an angle $d\theta$ in a direction **t**, i.e. for **dn** given by

$$d\mathbf{n} = d\theta \cdot \mathbf{t} \tag{19}$$

Since n is a unit vector, the unit vector t is perpendicular to n. The differential of $f = P . n$ is

$$df = P . dn + n . dP \tag{20}$$

But dP is perpendicular to n, as previously shown. Therefore

$$\frac{df}{d\theta} = P . t \tag{21}$$

Consider a 2D f-plot. The angle, β, between n and the normal ν to the f-plot is, from simple differential geometry, given by

$$tg\beta = \frac{1}{f}\frac{df}{d\theta} \tag{22}$$

Combining eqs. (11) and (21) it is easily concluded that β is equal to the angle between n and the principal vector P(n) (Fig.5).

The sharpness of a point cusp in a 2D f-plot can be defined by the angle, μ, between the tangents to the plot on either side of the cusp. Sharp cusps correspond to small values of μ. The angle μ is given by (Fig.6)

$$\mu = \pi - (\beta_1 + \beta_2) \tag{23}$$

where β_1 and β_2 are the β angles on either side of the cusp. The angle μ is therefore complementary to the angle between the two (adjacent) principal vectors associated with the cusp (Fig.6). Since two adjacent P-vectors differ by a $2v_i$--vector, it is clear that large v_i favour sharper cusps, although the sharpness depends on all v-vectors.

Consider now a 3D line cusp associated with two (adjacent) P-vectors, P_1 and P_2 , which differ by $2v_i$. The line cusp is in a plane perpendicular to v_i. For each orientation, n, along the cusp we take a section of the f-plot by a plane containing n and perpendicular to the plane of the line cusp. The sharpness of the cusp in this section is measured by the angle, μ, such that $(\pi - \mu)$ is the angle between the projections of P_1 and P_2 on the plane of the section. When the plane of the section coincides with the plane of P_1 and P_2 (and also of v_i), and is therefore perpendicular to the plane of the cusp, the angle μ is a minimum and equal to the angle between the tangent planes on either side of the cusp. This angle measures the sharpness of the line cusp and is, again, complementary to the angle between the principal vectors associated with the cusp. The sharpness of a line cusp will in general change at a point cusp.

A point cusp in a 3D plot occurs at the intersection of two or more line cusps. The sharpness of the point cusp can be measured by the solid angle, Ω, defined by tangent planes to each sphere meeting at the cusp; Ω is equal to 2π minus the solid angle subentended by the P-vectors associated with the point cusp.

THE v_i - POLYHEDRON AND THE NUMBER OF PRINCIPAL VECTORS

Consider the P-plot of a 3D discrete distribution of v_i-vectors and the associated f-plot. We recall that adjacent (spherical) regions in the f-plot, i.e., regions intersecting at a line cusp, are associated with adjacent P-vectors and these differ by the v_i-vector perpendicular to the plane of the line cusp. The number of line cusps is then twice the number of v_i-vectors.

Suppose we place the f-plot inside a sphere and project from the pole onto it the various regions (spheres associated with each P-vector) and their intersections. Part of this projection is schematically shown in Fig.7. The complete projection is the graph of a polyhedron with faces (the regions), edges (the line cusps) and vertices (the point cusps). The number of faces, F, equals n_P, the number of principal vectors. The number of vertices, V, is twice the number of π-planes that can be defined with the v_i-vectors, a π-plane containing two or more v_i-vectors. Let n_i be the number of π-planes containing i vectors v_i. Then

$$V = 2 \sum_i n_i \tag{24}$$

This is also the number of point cusps.

The degree of a vertex (i.e. the number of edges that meet at the vertex) associated with a π-plane containing i vectors is 2i (i line cusps go across the point cusp). Since each edge is connected to two vertices, the number E of edges is

$$2E = 4 \sum_i i\, n_i \tag{25}$$

Finally, using Euler's relation, F + V - E = 2, we obtain for the number of principal vectors

$$n_P = 2 \sum_i (i - 1)\, n_i + 2 \tag{26}$$

We can also define a polyhedron (the v_i-polyhedron), the vertices of which are the extremities of the P-vectors and the edges of which are obtained by joining adjacent P-vectors (they are therefore the $2v_i$-vectors). The faces of this polyhedron are planar, each face corresponding to a π-plane. In fact, two faces appear in the polyhedron for each π-plane and the faces are centro-symmetric polygons. This polyhedron is obviously the dual of the polyhedron previously defined, based on the f-plot. We then conclude that it is always possible to construct a polyhedron, the edges of which are the vectors v_i of a given set of vectors (no two parallel vectors). The numbers of faces, edges and vertices in the v_i-polyhedron are, respectively,

$$\begin{aligned} F &= 2 \sum_i n_i \\ E &= 2 \sum_i i\, n_i \\ V &= 2 \sum_i (i - 1)\, n_i + 2 \end{aligned} \tag{27}$$

A few examples follow. The v_i-polyhedron of three non-coplanar vectors ($n_2 = 3$) is a parallelipiped. For n vectors, with no three in the same plane, the number of faces in the v_i-polyhedron is n(n-1) and the number of vertices (number of principal vectors) is n^2-n+1. If the v_i-vectors are the edges of a regular tetrahedron ($n_3 = 4$, $n_2 = 3$), the v_i-polyhedron is the regular Kelvin's polyhedron with 14 faces (8 hexagonal and 6 square faces). Polyhedra with edges of equal lengths can be constructed as v_i-polyhedra of a set of v_i-vectors of the same length; in particular, there are polyhedra of this type with n(n-1) four sided faces, for any n.

SUMMARY

A detailed analysis of polar plots formed by portions of circles (2D) or spheres (3D) was undertaken. These are polar plots of functions f(n) defined by eqs. (1) or (7), (8) and are based on a distribution of vectors, v. Examples of functions of this type can be found in problems of stereology of oriented structures and in the calculation of the surface energy of a crystal, when the

atoms interact by a pairwise central potential.

The analysis undertaken was based on the concept of principal vectors. The principal vector P(n) for a direction **n** is the sum of the v-vectors that has the largest normal projection on **n**. A graphical construction was developed which allows the determination of the P-vectors (or of the P-plot) from the f-plot. It was then shown how the v-vectors can be obtained from the P-plot by another graphical construction. In conclusion, the distribution of v-vectors can be obtained graphically from the f-plot. The v-vectors obtained in this way form a reduced set, i.e. a set with no two parallel vectors. When sections of the 3D-plot are available, instead of the complete f-plot, information can be derived by these methods on the projections of the v-vectors on the plane of the section.

If the distribution of v_i-vectors is discrete or has singularities, cusps appear in the f-plot: point cusps in 2D plots and line cusps in 3D plots, each being associated with a v_i-vector or with a singularity of the v-distribution. In 3D f-plots, line cusps in general intersect producing a point cusp. The sharpness of the cusps was shown to be directly related to the angle between the principal vectors associated with the cusp.

The extremities of the principal vectors in the P-plot define a (convex) polygon in 2D or a (presumably convex) polyhedron in 3D, the edges of which are the v_i-vectors of a discrete and finite set of vectors. It was shown how the v_i--polygon or the v_i-polyhedron can be constructed. The concept of principal vectors leads to simple methods for constructing polyhedra, the edges of which are the vectors of a given set of vectors.

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