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Rodrigues Parameterization for Orientation and Misorientation Distributions

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Abstract

The Rodrigues parameterization of rotations offers an intuitively simple space which enables visualization of the geometric configuration of orientations and misorientations. Recent efforts have concentrated on promoting the use of Rodrigues vectors for orientation parameterization. In the present work a procedure for determining the boundaries of the asymmetric domains for orientations and misorientations in Rodrigues space is given for all crystal symmetries, and the complete description of these zones is presented. Geometric properties of Rodrigues space are described in detail and important relations useful in crystallographic texture analysis are derived. It is demonstrated that the special properties and geometry of the Rodrigues space facilitate analysis of texture function reproduction from pole figures and of texture evolution in plastic deformation of polycrystals.

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§1. Introduction

Since the work of Frank (1988) there has grown considerable interest in representing orientations of crystallites, and especially relative orientations, or misorientations, using Rodrigues parameters (*cf* Randle 1990, 1992). Rotations by an angle ω about an axis given by vector $\mathbf{n}$ with Cartesian components n^i can be parameterized by $r^i := n^i \tan(\omega/2)$. The advantage of such a parameterization lies in its intuitive nature. Considering the Miller index convention, an orientation defined by a rotation about an $[h\,k\,l]$ axis can be easily visualized. A set of Rodrigues parameters can be treated as a vector lying in a Cartesian coordinate system with the axes chosen to coincide with the sample (laboratory) reference coordinate system. In this way, the Rodrigues parameterization can take advantage of Miller indices in that $\mathbf{n}$ may be thought of as the normalized $[h\,k\,l]$ vector of a reference orientation aligned with the sample coordinate system. The magnitude of this vector is scaled by the rotation angle. The resulting orientation map obtained using Rodrigues parameters is conceptually simple and can be interpreted by intuition alone. Similarly, for the parameterization of misorientations the vector $\mathbf{r}$ lies along an $[h\,k\,l]$ axis which is common to the two crystallites and has a magnitude related to the angle of misorientation about that axis. In this way, the mapping of the misorientation to Rodrigues space is sufficient to allow direct interpretation of the geometrical relationship between the two lattices. Such an intuitive approach is difficult when other parameterizations, such as Euler angles, are used. Rodrigues space is also convenient for derivation of various properties of orientations and misorientations. For example, recent work has demonstrated the utility of this space in deriving misorientation angle distributions and distributions of the corresponding rotation axes (Morawiec 1995).

The purpose of the present work is to offer a review of the Rodrigues space parameterization and to describe some of its inherent advantages in relation to alternative measures. Asymmetric domains important for unique description of orientations and misorientations are given for all proper symmetries. Some useful properties of Rodrigues vectors are described as related to crystallographic texture evolution and to reproduction of orientation distribution function from pole figures. Some more detailed calculations are included in appendices.

§2. Rodrigues parameters and their relation to other parameters

As was mentioned in the introduction, a rotation (and hence orientation or misorientation) is parameterized by three quantities. The Rodrigues parameters are defined by

$$r^i = n^i \tan(\omega/2) \ ,$$

where $\omega \in [0, \pi]$ is the rotation angle and n^i $(i = 1, 2, 3)$ are components of the rotation axis described in a Cartesian coordinate system. The three numbers $\{r^1, r^2, r^3\}$ can be treated as elements of R^3 and denoted by $\mathbf{r}$. The identity rotation is represented by vector

0, and the rotation inverse to **r**, by vector $-\mathbf{r}$. Points corresponding to all rotations fill the infinite three dimensional space. Each of those with the rotation angle equal to π, is represented by two opposite points in infinity. Although this last feature is a drawback in numerical calculations, in theoretical considerations the points at infinity can be treated as any other points because they have specified direction and concrete (infinite) distance from **0**.

The Rodrigues vector **r** can be expressed with components of the orthogonal matrix g representing the same rotation by

$$r^i = -\frac{\varepsilon_{ijk} g_{jk}}{1 + g_{ll}} \ . \tag{1}$$

The inverse relation has the form

$$g_{ij} = \frac{1}{1 + r^2} \left((1 - r^2)\delta_{ij} + 2 r^i r^j - 2 \varepsilon_{ijk} r^k \right) \ , \tag{2}$$

where $r^2 := r^k r^k$. Using these formulae one can deduce a method to compose rotations represented by $\mathbf{r}_1$ and $\mathbf{r}_2$. Let matrices g_1 and g_2 and Rodrigues vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ correspond to two successive rotations. The composition of these rotations corresponds to the matrix $g_2\, g_1$. Using Eq.(2) this product matrix can be expressed through $\mathbf{r}_2$ and $\mathbf{r}_1$. And then applying Eq.(1) one gets the Rodrigues vector $\mathbf{r}_2 \circ \mathbf{r}_1$ corresponding to the composition of two successive rotations $\mathbf{r}_1$ and $\mathbf{r}_2$

$$\mathbf{r}_2 \circ \mathbf{r}_1 = (\mathbf{r}_1 + \mathbf{r}_2 - \mathbf{r}_1 \times \mathbf{r}_2)/(1 - \mathbf{r}_1 \cdot \mathbf{r}_2) \ . \tag{3}$$

The derivation of basic relations (1–2) is reminded in Appendix A.

Rodrigues vectors are related to quaternion components $q^0 = \cos(\omega/2)$ and $q^i = n^i \sin(\omega/2)$ by

$$q^0\, r^i = q^i \ .$$

Since only unit quaternions are considered, one has $1 = (q^0)^2 + q^k q^k = (q^0)^2(1 + r^k r^k)$ and thus there occurs

$$q^0 = \frac{1}{\sqrt{1 + r^2}} \ , \quad q^i = \frac{r^i}{\sqrt{1 + r^2}} \ .$$

Because rotations of π cannot be parameterized by $\{r^1, r^2, r^3\}$, it is desirable to use quaternions in numerical calculations, and to use Rodrigues vectors in displaying the final results. Eqs (1) allow one to easily obtain the relation between components of a Rodrigues vector and the commonly used Euler angles; see e.g., Becker and Panchanadeeswaran (1989) or Morawiec and Pospiech (1989). One should also mention here that the sign in Eq.(1) distinguishes between active and passive approaches (Appendix A).

§3. Geometry of the Rodrigues space

Some geometric features of the space are useful in texture analysis. Let us begin with finding the 'difference' rotation $\delta\mathbf{r}$ separating two infinitesimally close orientations. Let

$\delta\mathbf{r}$ be parameters of the rotation leading from orientation $\mathbf{r}$ to the point $\mathbf{r}+\mathrm{d}\mathbf{r}$, i.e., $\delta\mathbf{r}=(\mathbf{r}+\mathrm{d}\mathbf{r})\circ(-\mathbf{r})$. Omitting terms of order higher than $\mathrm{d}r^i$ the components of $\delta\mathbf{r}$ are

$$\delta r^i=\frac{\delta_{ij}+\varepsilon_{ijk}r^k}{1+r^2}\,\mathrm{d}r^j\ . \tag{4}$$

This expression can be used directly to get components of the metric tensor d.

Metric tensor and invariant volume Let the distance between two close orientations be proportional to the angle of rotation leading from one orientation to the other, i.e., in terms of components of metric tensor d_{ij} one has $d_{ij}\mathrm{d}r^i\mathrm{d}r^j=c(\mathrm{d}\omega)^2$, with $c=\mathrm{const}>0$ to be set below. The rotation angle $\mathrm{d}\omega$ corresponding to $\delta\mathbf{r}$, due to $(\mathrm{d}\omega/2)^2\approx\tan^2(\mathrm{d}\omega/2)$, is given by

$$(\mathrm{d}\omega)^2=4\delta r^i\delta r^i\ ,$$

with terms of higher order omitted. On the other hand, from Eq.(4), one has

$$\delta r^i\delta r^i=\left((1+r^2)\delta_{ij}-r^ir^j\right)\mathrm{d}r^i\mathrm{d}r^j/\left(1+r^2\right)^2\ .$$

Thus, because of the initial assumption ($c(\mathrm{d}\omega)^2=d_{ij}\mathrm{d}r^i\mathrm{d}r^j$), the components of the metric tensor are

$$d_{ij}=4c\left((1+r^2)\delta_{ij}-r^ir^j\right)/\left(1+r^2\right)^2\ .$$

The invariant volume can be found by calculating the determinant of the metric tensor $\{d_{ij}\}$. From the previous formula, the invariant volume in Rodrigues space is $dV=\det\{d_{ij}\}\mathrm{d}r^1\mathrm{d}r^2\mathrm{d}r^3$, with

$$\det\{d_{ij}\}=1/\left(\pi(1+r^2)\right)^2\ .$$

The coefficient c is set at $1/(4\pi^{2/3})$ so the total volume of the space is normalized to 1.

Christoffel symbols and geodesic lines It is worth mentioning that the Christoffel symbols (defined by $\Gamma^i_{jk}=d^{im}(d_{jm,k}+d_{mk,j}-d_{jk,m})/2$ with d^{ij} being the inverse of d_{ij}, $d^{ij}d_{jk}=\delta^i_k$) have the form

$$\Gamma^i_{jk}=-\frac{\delta_{ij}r^k+\delta_{ik}r^j}{1+r^2} \tag{5}$$

and hence the equation of geodesic lines is (Appendix B)

$$\frac{\mathrm{d}}{\mathrm{d}\omega}\left(\frac{1}{1+r^2}\,\frac{\mathrm{d}r^i}{\mathrm{d}\omega}\right)=0\ .$$

Solving this equation one finds that the solution can be written in the form $r^i=a^i\tan(\omega/2)+b^i$ (Appendix B). With ω changing from $-\pi$ to π the geodesic in Rodrigues space is represented by a straight line.

It is obvious that for established $\mathbf{n}$ and changing ω points $\mathbf{r}=\tan(\omega/2)\mathbf{n}$ represent rotations about the same axis determined by $\mathbf{n}$, and lie on a straight line through $\mathbf{0}$. Although not so obvious, it is also true that every straight line represents rotations about

an established axis. Each line which does not contain the origin corresponds to a rotated reference frame and could be mapped back through $\mathbf{0}$. In other words, the lines representing rotations with established axis and changing rotation angle (geodesic lines in SO(3)) are straight lines in Rodrigues space and, moreover, every straight line represents a set of rotations of this type. Geodesic remains geodesic even if the reference frame is changed. Thus rotations applied to the whole set transform a line to another line. The obvious conclusion is that a plane is transformed to a plane (Frank 1988).

§4. Space tessellation due to symmetry

Let us notice here that the relation $\mathbf{c} \circ \mathbf{r}$ can be understood as a transformation $\mathbf{c}$ of orientation $\mathbf{r}$ to orientation $\mathbf{c}(\mathbf{r}) := \mathbf{c} \circ \mathbf{r}$. As can be seen from the previous paragraph these transformations have interesting properties in Rodrigues space. Some additional features will be exploited below. We concentrate first, however, on the so-called fundamental zone (Frank 1988) and other zones symmetrically equivalent to it.

4.1 *Fundamental zones*

At the beginning let us find all points $\mathbf{x}$ which are at the same angular distance from a given point $\mathbf{r} = \mathbf{n}\tan(\omega/2)$ as from point $\mathbf{0}$. The vectors representing orientation differences between $\mathbf{0}$ and $\mathbf{x}$ and between $\mathbf{r}$ and $\mathbf{x}$ are given by $(-\mathbf{x}) \circ \mathbf{0} = -\mathbf{x}$ and $(-\mathbf{x}) \circ \mathbf{r}$, respectively. The equality of angular distances means that $(-\mathbf{x}) \cdot (-\mathbf{x}) = ((-\mathbf{x}) \circ \mathbf{r}) \cdot ((-\mathbf{x}) \circ \mathbf{r})$. This is the equation for $\mathbf{x}$. Using Eq.(3) it can be transformed to $(\mathbf{r} \cdot \mathbf{x})^2 + 2(\mathbf{r} \cdot \mathbf{x}) - (\mathbf{r} \cdot \mathbf{r}) = 0$. Its only solution has the form $\mathbf{x} = h\mathbf{r} + \mathbf{y}$ where $\mathbf{y}$ is an arbitrary vector perpendicular to $\mathbf{r}$ and $h = (-1 \pm \sqrt{1 + \mathbf{r} \cdot \mathbf{r}})/(\mathbf{r} \cdot \mathbf{r})$. Thus, the points at the same angular distance from $\mathbf{0}$ and from $\mathbf{r}$ lie on two planes, each perpendicular to vector $\mathbf{r}$, and located on both sides of the origin at the (Euclidean) distances

$$\sqrt{h^2 \mathbf{r} \cdot \mathbf{r}} = (\tan(\omega/4))^{\mp 1} \ .$$

At the same time these planes separate points which are closer to $\mathbf{0}$ than to $\mathbf{r}$ from those points which are not. For angles ω being in the range $[0, \pi)$, the distance $\tan(\omega/4)$ is smaller than the distance $1/\tan(\omega/4)$.

An orientation $\mathbf{r}$, due to crystal symmetry $\mathbf{c}$, is equivalent to $\mathbf{c} \circ \mathbf{r}$. To make the representation unique, one can confine the admissible orientations to those with the smallest rotation angle. This part of the space was called by Frank (1988) the fundamental zone. In other words, the fundamental zone is a polyhedron filled with points which have smaller angular distance to $\mathbf{0}$ than to any other point symmetrically equivalent to $\mathbf{0}$. It can be described formally as

$$\bigcap_{i=2}^{N} \{ \ \mathbf{r} \ ; \ \ \tan(\omega_i/4) \pm \mathbf{r} \cdot \mathbf{l}_i \geq 0 \ \} \ .$$

Here $\omega_i \in [0, \pi]$ and $\mathbf{l}_i$ are the rotation angle and the unit vector of the rotation axis of the i-th element of the rotation symmetry group, respectively. N is the order of the group

and the identity is assumed to correspond to $i = 1$. The fact is ignored that some points on the boundary of this zone may correspond to physically indistinguishable orientations.

Fundamental zones for individual symmetries are as follows:

Cyclic symmetries For C_1 the fundamental zone overlaps the entire Rodrigues space. For C_n ($n \neq 1$) the fundamental zone is bounded by two planes perpendicular to the n-fold axis, each at the distance $\tan(\pi/(2n))$ from $\mathbf{0}$.

Dihedral symmetries The fundamental zone for D_n is a prism with $2n$-sided polygons (at the distance $\tan(\pi/(2n))$ from $\mathbf{0}$) as prism bases, and $2n$ square prism faces at the distance 1. The bases are perpendicular to the n-fold axis and the faces are perpendicular to the two–fold axes (Fig. 1).

As an example, single orientations of trigonal Al_2O_3 are displayed in the fundamental zone of D_3 (Fig. 2a). The orientations were measured using OIM–system (Adams, Wright and Kunze 1993).

Tetrahedral symmetry The fundamental zone for group T is a regular octahedron with faces at the distance $\tan(\pi/6) = \sqrt{3}/3$ from $\mathbf{0}$ and perpendicular to the three–fold axes (Fig. 3a).

Octahedral symmetry The fundamental zone is a truncated cube with six octagonal faces at the distance $\tan(\pi/4) = \sqrt{2} - 1$ from the origin, and eight triangular faces at the distance $\tan(\pi/6) = \sqrt{3}/3$ (*cf* Frank 1988). The octagonal faces are perpendicular to the four–fold symmetry axes and triangular faces are perpendicular to the three–fold axes (Fig. 3b).

Icosahedral symmetry The fundamental zone is a regular dodecahedron with faces perpendicular to the five–fold symmetry axes at the distance $\tan(\pi/10)$ (Fig. 3c).

For completeness, let us determine the other zones symmetrically equivalent to the fundamental one. To find them and to have a better insight into the structure of the space transformations, consider the plane perpendicular to unit vector $\mathbf{l}$ intersecting the line determined by $\mathbf{l}$ at the point $\tan(\alpha/2)\,\mathbf{l}$. Rotation $\mathbf{c} = \tan(\omega/2)\mathbf{l}$ transforms such a plane onto another one, also perpendicular to the direction of $\mathbf{l}$ and intersecting this line at the point $\tan((\alpha+\omega)/2)\,\mathbf{l}$. Moreover, the distance (in the normal sense of Euclidean space) of a given point on the plane from the axis $\{\lambda\mathbf{l}; \lambda \in \mathsf{R}\}$ changes from its initial value, ρ_0, to

$$\rho = \rho_0 \mid \cos(\alpha/2)/\cos((\alpha+\omega)/2) \mid$$

after transformation, and the whole plane is rotated by the same (α–independent) angle $\omega/2$. (See Appendix C.)

The above statements allow solution to the problem of finding zones symmetrically

equivalent to the fundamental zone. For C_n it is trivial: the space is tessellated by n parallel planes at the distance $\mid \tan((1+2k)\pi/(2n)) \mid$, $(k = 0, ..., n-1)$ from $\mathbf{0}$. For D_n it is also simple; the schematic picture (Fig. 4) displays the zones for $n = 4$. For T and O the task requires some gymnastics of imagination but still it is easier to imagine the space partition than to describe it. The case of Y is complicated and one needs tedious analysis to get the full three dimensional picture. Fig. 5 shows some arbitrary chosen sections through the space for each of T, O and Y symmetries.

This tessellation is in fact the partition of the space into 'Voronoi polyhedra'. This is done by first choosing points corresponding to the symmetry operations, and then creating zones in such a way that all points of the zone have smaller angular distance to one of these distinguished points than to any other. The cell containing the identity is the fundamental zone. The same idea was realized by Yeates (1993) for Euler angles parameterization of rotations.

4.2 *MacKenzie cells*

Similarly to orientations, when analyzing misorientations of crystallites one must take into account that each one, say $\mathbf{r}$, is represented by symmetrically equivalent points $\{\mathbf{c}_\alpha \circ \mathbf{r} \circ \mathbf{c}_\beta,\ \mathbf{c}_\alpha \circ (-\mathbf{r}) \circ \mathbf{c}_\beta\}$, where $\mathbf{c}_\alpha$ and $\mathbf{c}_\beta$ denote crystal symmetries. However, a region can be selected to which all physically distinguishable misorientations, when operated upon by elements of the symmetry group, may be mapped only once (i.e., there are no other points in the cell symmetrically equivalent to it). In the Rodrigues parameterization it has a relatively simple shape. (Compare with that for cubic misorientations in Euler space described by Zhao and Adams 1988). In this work, such a domain is referred to as a MacKenzie cell (after Neumann 1991).

To find the boundaries of a MacKenzie cell for an arbitrary symmetry, it is necessary to first identify some properties of symmetry operations in Rodrigues space. Let $\mathbf{r}$ be a vector in Rodrigues space and let $\mathbf{c}_k$ $(k = 0, 1, ..., M-1)$ be rotations with the same M-fold rotation axis and rotation angle equal to $2k\pi/M$. The transformation $\mathbf{c}_n \circ \mathbf{r} \circ \mathbf{c}_m$ gives the new point $\mathbf{r}'$ symmetrically equivalent to $\mathbf{r}$. If $n = M - m$, i.e., if $\mathbf{c}_n = -\mathbf{c}_m$ then points $\mathbf{r}$ and $\mathbf{r}'$ lie in the same plane perpendicular to the rotation axis at the same distance from that axis. With the vertex on the axis they form an angle $2\pi m/M$ in the plane. (See Appendix D.) This statement, together with the equivalence of $\mathbf{r}$ to $-\mathbf{r}$, allow derivation of the MacKenzie cell for arbitrary symmetry.

For example, the MacKenzie cell for C_n is obtained by dividing the fundamental zone into two halves separated by a plane passing through the origin and perpendicular to the axis of symmetry. Points in these sections are related to each other by the inverse property (i.e., $\mathbf{r}$ is symmetrically equivalent to $-\mathbf{r}$). Each section is further reduced into n equivalent regions symmetrically distributed round the n-fold axis and rotated by $2\pi/n$ with respect to each other.

Using the guidelines discussed above, boundaries of the MacKenzie cells can be chosen for all symmetry groups. These are described briefly in the following paragraphs.

Cyclic symmetries For C_n ($n \neq 1$) the MacKenzie cell is part of the fundamental zone bounded by
1. the plane through **0** perpendicular to the n-fold axis,
2. two planes containing symmetry axis (i.e., both perpendicular to the planes bounding the fundamental zone) with dihedral angle equal to $2\pi/n$.

Dihedral symmetries The MacKenzie cell for D_n is part of the fundamental zone (prism) bounded by
1. the plane through **0** perpendicular to n-fold rotation axis (i.e., parallel to the prism bases),
2. two planes containing n-fold symmetry axis (i.e., both perpendicular to the bases) and each containing
– middle point of the prism face for n-even (Fig. 1a),
– side of the faces for n-odd (Fig. 1b),
with dihedral angle equal to π/n in both (even and odd) cases.

A set of misorientations corresponding to the sample of Al_2O_3 is displayed in Fig. 2b.

Tetrahedral symmetry The MacKenzie cell is 1/24 of fundamental zone with edges inside the zone being segments of two nearest (to each other) two–fold symmetry axes and one three–fold axis (Fig. 3a).

Octahedral symmetry The MacKenzie cell is 1/48 of fundamental zone with edges inside the zone being segments of one two–fold symmetry axis, one three–fold axis and one four–fold symmetry axis (see e.g., Neumann 1991).

Icosahedral symmetry The MacKenzie cell is 1/120 of fundamental zone with edges inside the zone being segments of one two–fold symmetry axis, one three–fold axis and one five–fold symmetry axis (Fig. 3c).

4.3 *Multiplicity*

Operations by symmetry elements will always map the misorientation inside the MacKenzie cell to a point outside of it except for those points which have a multiplicity greater than one, for which the misorientation may be mapped identically back to itself. Misorientations of high multiplicity necessarily lie upon the boundary of the MacKenzie cell. The Rodrigues space representation offers simple physical interpretation of these types of misorientations which, some claim, possess special properties (*cf* Field and Adams 1992).

General to all symmetries is the fact that the origin has the highest possible multiplicity $2N$, where N is the number of proper symmetry elements. (Equivalence of $\mathbf{r}$ and $-\mathbf{r}$ is included.) Moreover, points on the line determined by n-fold rotation axis are of multiplicity n. Thus, for example for cyclic symmetry C_n ($n \geq 2$), the n-fold axis posesses

multiplicity n, while the point at the origin has a multiplicity of $2n$. Moreover, other points on the plane through $\mathbf{0}$ perpendicular to symmetry axis have a multiplicity of one (when n is odd) or two (when n is even).

A description of multiplicity over the entire boundary of the MacKenzie cell for octahedral symmetry was recently given (Field 1995).

§5. Other applications

There are also other subjects where application of Rodrigues parameters seems to be advantageous compared with other parameterizations. First is in the analysis of the so-called rotation rate field. In this case, Rodrigues parameters make the calculations more simple. The other application lies in the relation of orientation distributions to pole figures. Straight projection lines offer obvious advantages over the curvilinear projection lines in the Euler parameterization. These are discussed in the following sections.

5.1 *Rotation rate field*

The rotation rate field or orientation flow has been used to model and investigate the evolution of crystallographic texture during plastic deformation of polycrystals (Bunge 1970). The rotation related to the small displacement $\mathbf{u}$ can be described by a vector of infinitesimal rotation

$$\mathbf{R} = \frac{1}{2}\mathrm{curl}(\mathbf{u}) \ .$$

The relations between infinitesimal increments of Euler angles and $\mathbf{R}$ in the considered context can be found in the paper by Bunge (1970). It is instructive to determine a similar relation for Rodrigues parameters.

Let the continuous rotation of a crystal due to plastic deformation after time $\mathrm{d}t$ be $\mathbf{R}\,\mathrm{d}t$ (i.e., $\mathbf{R}$ represents the vector of angular velocity). The corresponding rotation matrix δg is related to $\mathbf{R}\,\mathrm{d}t$ by

$$(\delta g)_{ij} = \delta_{ij} + \varepsilon_{ijk} R^k \mathrm{d}t \ . \tag{6}$$

On the other hand we can express $(\delta g)_{ij}$ using Rodrigues parameters $\delta\mathbf{r} = (\mathbf{r} + \mathrm{d}\mathbf{r}) \circ (-\mathbf{r})$, which are assumed to determine the same infinitesimal rotation. The appropriate components are given by Eq.(4). Because of Eq.(2) (and disregarding higher order terms) one has

$$(\delta g)_{ij} = \delta_{ij} - 2\varepsilon_{ijk}\frac{\delta_{kl} + \varepsilon_{klm} r^m}{1 + r^2}\mathrm{d}r^l \ .$$

Comparing this with Eq.(6) one gets

$$R^i = -2\frac{\delta_{ij} + \varepsilon_{ijk} r^k}{1 + r^2} v^j \ ,$$

where $v^i = \mathrm{d}r^i/\mathrm{d}t$ are components of the rotation rate $\mathbf{v}$ at the point $\mathbf{r}$. The inverse relation is

$$v^i = -\left(\delta_{ik} + r^i r^k + \varepsilon_{ijk} r^j\right) R^k/2 \ . \tag{7}$$

Thus having established $\mathbf{R}$ in the crystal coordinate system one can get the components of the rotation rate for each orientation (in the sample coordinate system). With established $\mathbf{R}$ the field $\mathbf{v}$ is right invariant and thus its magnitude is constant $\mid \mathbf{v} \mid = d_{ij} v^i v^j = R^i R^i/(4\pi^{2/3})$.

5.2 *Continuity equation*

The continuity equation is a formal way to say that with the continuous rotations of particular crystallites, the corresponding orientations flow continuously in orientation space. With $f = f(t, \mathbf{r})$ being a sufficiently smooth orientation distribution it has the form

$$\frac{\partial f}{\partial t} + \mathrm{div}(f\mathbf{v}) = 0$$

(Clément 1982 and Wierzbanowski and Clément 1985). The divergence operator can be calculated using Christoffel symbols (5)

$$\mathrm{div}(f\mathbf{v}) = (fv^i)_{,i} + \Gamma^i_{ij}(fv^j) = f_{,i}\, v^i + f\left(v^i{}_{,i} - 4v^i r^i/(1+r^2)\right) \ .$$

If $\mathbf{v}$ is given by Eq.(7) then the last term vanishes and $\mathrm{div}(f\mathbf{v}) = f_{,i}\, v^i$, i.e., in this case the continuity equation can be expressed as $\mathrm{d}f/\mathrm{d}t = 0$ (as it should be, because that field is invariant, i.e., in a sense constant on the space).

The field $\mathbf{v}$ might be useful in analyzing texture changes due to a given displacement $\mathbf{u}$ or rotation $\mathbf{R}$. For small Δt one has

$$f(\Delta t, \mathbf{r}) = f(0, \mathbf{r}) - \Delta t \frac{\partial f(0, \mathbf{r})}{\partial r^i} v^i \ .$$

This allows to predict the 'direction' of texture development or orientation flow due to given $\mathbf{R}$. In such a simple case the uniform texture is stable. This follows directly from the the invariance of the field. To change this, the field has to be orientation dependent.

5.3 *Pole figures and their projection lines*

The pole figure is a projection of the orientation distribution. The projection lines (integration paths) are those which correspond to rotations with established rotation axes, i.e., they coincide with geodesics and in the case of Rodrigues space they are straight lines.

They are of importance in the problem of reproducing orientation distributions from pole figures. In so called direct methods of reproduction the system of linear equations is built with values of the orientation distribution as unknowns and with each equation corresponding to one projection line (Pospiech 1980). The simplicity of the geometry of

projection lines in the case of Rodrigues space might be an advantage in building such procedures and analyzing ambiguity problems which arise there.

The integration path corresponding to point $\mathbf{y}$ on pole figure P_h consists of all orientations composed of:
— the rotation transforming unit vector $\mathbf{y}$ (in the sample coordinate frame) into the direction of the $\mathbf{e}_3$–axis,
— all rotations about $\mathbf{e}_3$, and finally
— the rotation transforming the $\mathbf{e}_3$–axis into pole $\mathbf{h}$ (in the crystal coordinate frame).
Rotations transforming unit vector $\mathbf{y}$ (with components given in the sample coordinate system) into $\mathbf{e}_3$ are of the form $\mathbf{r}_y = \lambda_y \mathbf{y} \times \mathbf{e}_3$, with $\lambda_y = 1/(1+\cos\alpha)$ and α being a polar angle of $\mathbf{y}$. Rotations with $\mathbf{e}_3$ as the rotation axis are $\mathbf{r}_\lambda = \lambda \mathbf{e}_3$. Rotations transforming direction $\mathbf{e}_3$ into unit vector $\mathbf{h}$ (with components given in the crystal coordinate system) are given by $\mathbf{r}_h = \lambda_h \mathbf{e}_3 \times \mathbf{h}$, with $\lambda_h = 1/(1+\cos\theta)$ and θ being the polar angle of $\mathbf{h}$. The line (parameterized by λ)

$$\underline{\mathbf{r}}(\lambda) = \mathbf{r}_h \circ \mathbf{r}_\lambda \circ \mathbf{r}_y$$

is the integration path, i.e., if (following Appendix B) the parameter λ is expressed by $\lambda = \tan(\omega/2)$ then the pole figure P_h^0 is related to the orientation distribution f through

$$P_h^0(\mathbf{y}) = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(\underline{\mathbf{r}}(\tan(\omega/2)))\mathrm{d}\omega = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{f(\underline{\mathbf{r}}(\lambda))}{1+\lambda^2}\mathrm{d}\lambda \ .$$

The pole figure P_h measured in the normal X–ray diffraction experiment, due to the Friedel's law, is the superposition of P_h^0 and P_{-h}^0, i.e., $P_h(\mathbf{y}) = (P_h^0(\mathbf{y}) + P_{-h}^0(\mathbf{y}))/2$. Moreover, if there are any crystal symmetries involved, the measured pole figure is an average of P_h for all symmetrically equivalent $\mathbf{h}$ directions.

While still posing a challenging problem, the geometry of projection lines is much simpler in Rodrigues space than for any other parameterization.

§6. Final remarks

Despite some general formulations contained in the paper, we want to emphasize practical applications of the Rodrigues parameterization, which can compete with Euler angles in the area of standardized orientation description. In conclusion, positive and negative attributes of these parameters will be stressed (from the viewpoint of crystallographic texture analysis, or more generally, analysis of orientations of symmetric objects).

As was already mentioned in the Introduction, simple relation of Rodrigues parameters to the rotation angle and axis allows simple interpretation of orientations as well as misorientations given by these parameters. On the same basis, one can also easily estimate the whole distribution of misorientation angle; its value at a given point ω is directly related to the total density of misorientations on a sphere of radius $\tan(\omega/2)$. Similarly, one can analyze distributions of the corresponding rotation axes; the value of

the distribution at $\mathbf{n}$ is related to the total distribution on a segment through $\mathbf{0}$, colinear to $\mathbf{n}$, and contained inside the fundamental zone.

The other important point is that, with the Rodrigues parameterization the asymmetric domains for orientations (fundamental zones) are not very complicated and, simultaneously, the domains for misorientations (MacKenzie cells) have much more simple shapes than for other parameters. Therefore, this parameterization seems to be the most reasonable choice for displaying misorientation data.

One should also mention the relatively simple procedure of transformation of orientations due to rotation. Using the rules given at the end of §4.1 it is easy to find how the orientation changes when a given rotation is applied. On the other hand, when starting and final orientations are given, one can easily trace the 'path' of direct rotation from one orientation to the other. Due to the principle of straight geodesic lines, it is a straight line segment through both points–orientations. (Symmetrically equivalent points have to be taken into account.) This principle is, in fact, the cause of most of the plausible features of the Rodrigues parameterization, from simple (planar) boundaries of asymmetric domains to straight projection lines in the pole figure projection.

It is worth noticing that the nature of the Rodrigues parameters is such that it allows 'index manipulation' in theoretical calculations. The analysis of the rotation rate field is a simple example. Analogous calculations based on, e.g., Euler angles are much more tedious.

As to drawbacks, the most serious negative attribute is that for cyclic symmetries the space is infinite. In this case, the parameterization (quaternions) can still be used in calculations. However, it seems to be advantageous to use other parameterizations for displaying the data graphically. Another drawback is that the Rodrigues parameterization is not 'isochoric' (*cf* Frank 1988). However, this is also feature of other used parameterizations. Moreover, the distortion is low for points close to the origin $\mathbf{0}$. E.g., in the case of cubic symmetry the value of the density coefficient changes inside the fundamental zone by a factor of less then 2.

Appendix A: Relation to rotation matrix

To derive the relation between components of a Rodrigues vector r^i and components of the orthogonal matrix g_{ij}, both representing the same rotation, the following procedure can be applied.

The relation for the product of permutation symbols is required in the derivation

$$\varepsilon_{ijk}\varepsilon_{lmn} = \det \begin{bmatrix} \delta_{il} & \delta_{im} & \delta_{in} \\ \delta_{jl} & \delta_{jm} & \delta_{jn} \\ \delta_{kl} & \delta_{km} & \delta_{kn} \end{bmatrix} \tag{8}$$

as well as $\varepsilon_{ijk}\varepsilon_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}$ which follows from the previous one. We will also need some other relations of a different nature: Let $\overline{g}$ be a rotation with the same axis

as g but half of the rotation angle. (Other overlined symbols correspond to $\overline{g}$, i.e., if ω is the rotation angle of g, then $\overline{\omega} = \omega/2$.) Obviously

$$\overline{g}_{ij}\overline{g}_{jk} = g_{ik} \tag{9}$$

and, moreover,

$$g_{ii} = 1 + 2\cos\omega = (1 + 2\cos\overline{\omega})^2 - 2(1 + 2\cos\overline{\omega}) = (\overline{g}_{ii})^2 - 2\overline{g}_{ii} \quad . \tag{10}$$

Analogous relations can be found for Rodrigues parameters. The first relates the parameters

$$r^i = n^i \tan(\omega/2) = n^i \frac{2\tan(\overline{\omega}/2)}{1 - \tan^2(\overline{\omega}/2)} = \frac{2\overline{r}^i}{1 - \overline{r}^2} \ , \tag{11}$$

whereas the second relates magnitudes of the vectors

$$1 + r^2 = 1 + \frac{4\overline{r}^2}{(1 - \overline{r}^2)^2} = \left(\frac{1 + \overline{r}^2}{1 - \overline{r}^2}\right)^2 \quad . \tag{12}$$

After this preparation one is ready to proceed with proper calculations.

It is easy to express the trace of g through r^i. Because $r^2 = \tan^2(\omega/2)$ and $g_{ii} = 1 + 2\cos\omega$, after eliminating ω one has

$$g_{ii} = (3 - r^2)/(1 + r^2) \ . \tag{13}$$

Hence, for $g_{ii} + 1 \neq 0$, the magnitude of $\mathbf{r}$ is given by

$$r^2 = (3 - g_{ii})/(1 + g_{ii}) \ . \tag{14}$$

To express r^i through g_{ij}, let us notice that $\mathbf{r}$ is colinear with $\mathbf{n}$ and thus remains unchanged under rotation g, i.e., $g_{ij}r^j = r^i$ or $(g_{ij} - \delta_{ij})r^j = 0$. This is a system of linear equations for r^j. Multiplying it by $(g_{ik} + \delta_{ik})$ one gets $(g_{kj} - g_{jk})r^j = 0$. The antisymmetric matrix can be expressed as $(g_{kj} - g_{jk}) = \varepsilon_{kjm}p^m$, where $p^m = \varepsilon_{mst}g_{st}$. Hence, $\varepsilon_{kjm}r^j p^m = 0$, i.e., vector $\mathbf{r}$ is colinear with $\mathbf{p}$ and thus, the solution of the system for orthogonal g is of the form $r^i = \alpha\varepsilon_{ijk}g_{jk}$. One can calculate α using Eq.(8) $r^2 = \alpha^2\varepsilon_{ijk}\varepsilon_{imn}g_{jk}g_{mn} = \alpha^2(3 - g_{ij}g_{ji})$. By a relation analogous to Eq.(10) and due to Eq.(13)

$$r^2 = \alpha^2\left(3 - (g_{ii})^2 + 2g_{ii}\right) = 16\alpha^2 r^2/(1 + r^2)^2 \ .$$

Thus $\alpha = \pm(1 + r^2)/4$. The sign '$-$' is chosen here to be in agreement with the convention used by Bunge (1982). Hence finally, after applying Eq.(14) one gets the expression

$$r^i = -\varepsilon_{ijk}g_{jk}/(1 + g_{ll}) \ . \tag{15}$$

which occurs when $g_{ll} \neq -1$. Otherwise, the direction of r^i is determined by $\pm\varepsilon_{ijk}g_{jk}$ and its magnitude is infinite.

Let us now express the symmetric part of the matrix g through $\mathbf{r}$. Later on the antisymmetric part, and finally g will be calculated. As to the symmetric part, first of all let us notice that

$$\overline{r}^i\overline{r}^l/\overline{\alpha}^2 = \varepsilon_{ijk}\varepsilon_{lmn}\overline{g}_{jk}\overline{g}_{mn} = (\delta_{il}(1-g_{mm}) + g_{il} + g_{li}),$$

where Eqs (8) and (9) and orthogonality relations ($\overline{g}_{in}\overline{g}_{ln} = \delta_{il} = \overline{g}_{mi}\overline{g}_{ml}$) were used. On the other hand, from Eqs (11) and (12) one gets

$$\overline{r}^i\overline{r}^l/\overline{\alpha}^2 = \frac{r^i r^l(1-\overline{r}^2)^2}{4\overline{\alpha}^2} = r^i r^l \frac{4(1-\overline{r}^2)^2}{(1+\overline{r}^2)^2} = \frac{4r^i r^l}{1+r^2} \quad .$$

and hence, the symmetric part of g is given by

$$\frac{g_{ij}+g_{ji}}{2} = \frac{1}{2}\delta_{ij}(g_{mm}-1) + \frac{2r^i r^j}{1+r^2} = \delta_{ij}\frac{1-r^2}{1+r^2} + \frac{2r^i r^j}{1+r^2} \ .$$

It is easier to find the antisymmetric part. Because $\varepsilon_{ijk}r^k = \alpha\varepsilon_{ijk}\varepsilon_{klm}g_{lm} = \alpha(g_{ij}-g_{ji})$ one has $(g_{ij}-g_{ji})/2 = -2\varepsilon_{ijk}r^k/(1+r^2)$. Summing symmetric and antisymmetric parts one gets

$$g_{ij} = \left((1-r^2)\delta_{ij} + 2r^i r^j - 2\varepsilon_{ijk}r^k\right)/(1+r^2) \ , \tag{16}$$

which is the sought expression for the matrix components.

Appendix B: Geodesic lines

Let us define $\xi := 1 + r^i r^i$. The equation of the geodesic line

$$\frac{\mathrm{d}^2 r^i}{\mathrm{d}\omega^2} + \Gamma^i_{jk}\frac{\mathrm{d}r^j}{\mathrm{d}\omega}\frac{\mathrm{d}r^k}{\mathrm{d}\omega} = 0 \ ,$$

after substituting Γ^i_{jk} (Eq.(5)), can be written in the form

$$\xi\frac{\mathrm{d}^2 r^i}{\mathrm{d}\omega^2} - \frac{\mathrm{d}r^i}{\mathrm{d}\omega}\frac{\mathrm{d}\xi}{\mathrm{d}\omega} = 0 \ .$$

Defining $s^i := \mathrm{d}r^i/\mathrm{d}\omega$ one gets $\xi\mathrm{d}s^i/\mathrm{d}\omega = s^i\mathrm{d}\xi/\mathrm{d}\omega$ or $\mathrm{d}(s^i/\xi)/\mathrm{d}\omega = 0$. The solution $s^i = a^i\xi$ means that

$$\frac{\mathrm{d}r^i}{\mathrm{d}\omega} = a^i\xi \quad , \tag{17}$$

where a^i are integration constants. Multiplying this equation consecutively by r^i and a^i one gets the system of two first order equations for ξ and $y := a^i r^i$

$$\frac{1}{2}\frac{\mathrm{d}\xi}{\mathrm{d}\omega} = y\xi \quad \text{and} \quad \frac{\mathrm{d}y}{\mathrm{d}\omega} = a^2\xi \ , \tag{18}$$

where $a^2 = a^i a^i$. Eliminating ξ from the right-hand sides one gets $a^2\mathrm{d}\xi/\mathrm{d}\omega = \mathrm{d}y^2/\mathrm{d}\omega$ and because $a^2\xi - y^2$ is non-negative

$$a^2\xi = y^2 + c^2 \ , \tag{19}$$

with c^2 being another integration constant. Substituting $a^2\xi$ in the second of Eqs (18) one obtains the equation $\mathrm{d}y/\mathrm{d}\omega = y^2 + c^2$ with the elementary solution $y = c\tan(c\omega + d)$. Thus from Eq.(19)

$$\xi = \left(\frac{c}{a}\right)^2 \left(1 + \tan^2(c\omega + d)\right) = \left(\frac{c}{a}\right)^2 \frac{1}{\cos^2(c\omega + d)} \ .$$

Finally from Eq.(17) one gets

$$r^i = a^i \left(\frac{c}{a}\right)^2 \int \frac{\mathrm{d}\omega}{\cos^2(c\omega + d)} = a^i \frac{c}{a^2} \tan(c\omega + d) + b^i \ .$$

Because of the nature of the equation of geodesic lines, the parameter ω can be replaced by any linear expression of it. This allows choice of suitable values for the constants c and d. Let $d = 0$. To have the same $\mathbf{r}$ corresponding to all $\omega + 2k\pi$ the quantity c must be a multiple of $1/2$; let $c = 1/2$. Substituting $a^i/(2a^2) \to a^i$ one finally obtains $r^i = a^i \tan(\omega/2) + b^i$.

Appendix C: Transformation of a plane perpendicular to the Rodrigues vector

Let $\mathbf{c} = \lambda\mathbf{l}$, where $\mathbf{l}$ is unit vector, $\lambda = \tan(\omega/2)$ and $\omega \in [0, \pi)$. The plane perpendicular to the Rodrigues vector $\mathbf{c}$ can be determined as

$$\mathbf{r}(\lambda_1, \lambda_2) = \lambda_0\mathbf{l} + \lambda_1\mathbf{k}_1 + \lambda_2\mathbf{k}_2 \ ,$$

where versors $\{\mathbf{l}, \mathbf{k}_1, \mathbf{k}_2\}$ are assumed to constitute a right-handed Carthesian coordinate frame and λ_s $(s = 1, 2)$ are extended from $-\infty$ to $+\infty$. Let the distance of the plane form $\mathbf{0}$ be determined by $\tan(\alpha/2)$ $(= \lambda_0)$. Using the composition relation one easily finds that for $\lambda\lambda_0 \neq 1$ $\mathbf{c} \circ \mathbf{r}(\lambda_1, \lambda_2)$ is given by

$$\mathbf{c} \circ \mathbf{r}(\lambda_1, \lambda_2) = \frac{1}{1 - \lambda\lambda_0} \left((\lambda + \lambda_0)\mathbf{l} + (\lambda_1 - \lambda_2\lambda)\mathbf{k}_1 + (\lambda_2 + \lambda_1\lambda)\mathbf{k}_2\right) \ .$$

Because the coefficients of $\mathbf{k}_s$ $(s = 1, 2)$ are linear functions of λ_s and the coefficient of $\mathbf{l}$ does not depend on λ_s, the image of the plane in transformation represented by $\mathbf{c}$ is another plane perpendicular to $\mathbf{l}$. Its distance from $\mathbf{0}$ is determined by the coefficient of the versor $\mathbf{l}$ and can be expressed in the form

$$\frac{\lambda + \lambda_0}{1 - \lambda\lambda_0} = \tan\left(\frac{\omega + \alpha}{2}\right) \ .$$

It is infinite when $\lambda\lambda_0 = 1$ with $\omega + \alpha$ equal π.

Let us consider also the distance of a given point of the plane from the line $\lambda\mathbf{l}$. Let the initial distance and the distance after transformation be ρ_0 and ρ, respectively. For specified λ_1, λ_2 there is $\rho_0 = \sqrt{\lambda_1^2 + \lambda_2^2}$. The sum of squares of coefficients of the vectors $\mathbf{k}_1$ and $\mathbf{k}_2$ in the expression for the distance after transformation is

$$\rho^2 = \frac{(\lambda_1^2 + \lambda_2^2)(1 + \lambda^2)}{(1 - \lambda\lambda_0)^2} = \rho_0^2 \frac{\cos^2(\alpha/2)}{\cos^2((\alpha + \omega)/2)} \ ,$$

when $\lambda\lambda_0 \neq 1$ and infinite in opposite (singular) case.

Calculating scalar and vector products of vectors $\lambda_1\mathbf{k}_1 + \lambda_2\mathbf{k}_2$ and $(\lambda_1 + \lambda_2\lambda)\mathbf{k}_1 + (\lambda_2 - \lambda_1\lambda)\mathbf{k}_2$ one easily finds the cosine and sine of the angle φ between them

$$\cos\varphi = 1/\sqrt{1+\lambda^2} = \cos(\omega/2) \ , \qquad \sin\varphi = \lambda/\sqrt{1+\lambda^2} = \sin(\omega/2) \ .$$

Hence the transformation causes the rotation of the whole plane by the same angle $\varphi = \omega/2$.

Appendix D: Transformation $\mathbf{c}_n \circ \mathbf{r} \circ \mathbf{c}_m$

Let $\mathbf{l}$ be a unit vector in Rodrigues space and let rotations $\mathbf{c}_k$ be defined by $\mathbf{c}_k = t_k\mathbf{l}$ where $t_k = \tan(k\pi/M)$. Thus, $\mathbf{c}_k$ are rotations with the same M-fold rotation axis $\mathbf{l}$. Let $\mathbf{r}$ be an arbitrary point in Rodrigues space. Application of the relation Eq.(3) reveals that the image $\mathbf{r}'$ of $\mathbf{r}$ in the transformation $\mathbf{c}_n \circ \mathbf{r} \circ \mathbf{c}_m$ is given by

$$\mathbf{r}' = \mathbf{c}_n \circ \mathbf{r} \circ \mathbf{c}_m = \frac{\mathbf{c}_n + \mathbf{c}_m + \mathbf{r} + \mathbf{c}_n \times \mathbf{r} - \mathbf{c}_m \times \mathbf{r} - (\mathbf{c}_m \cdot \mathbf{r})\mathbf{c}_n - (\mathbf{c}_n \cdot \mathbf{r})\mathbf{c}_m + (\mathbf{c}_n \cdot \mathbf{c}_m)\mathbf{r}}{1 - \mathbf{c}_n \cdot \mathbf{r} - \mathbf{c}_m \cdot \mathbf{r} - \mathbf{c}_n \cdot \mathbf{c}_m} \ . \tag{20}$$

Points $\mathbf{r}$ and $\mathbf{r}'$ are in the same plane perpendicular to $\mathbf{l}$ if $\mathbf{r}' \cdot \mathbf{l} = \mathbf{r} \cdot \mathbf{l}$. This condition leads to

$$\left(1 + (\mathbf{r} \cdot \mathbf{l})^2\right)(t_m + t_n) = 0 \ ,$$

which means that $t_n = -t_m$. Therefore point $\mathbf{r}$ and its image $\mathbf{r}'$, are in the same plane perpendicular to $\mathbf{l}$, if $\mathbf{c}_n = -\mathbf{c}_m$. Assuming that this condition is satisfied, relation (20) becomes

$$\mathbf{r}' = \frac{\mathbf{r} - 2\mathbf{c}_m \times \mathbf{r} + 2(\mathbf{c}_m \cdot \mathbf{r})\mathbf{c}_m - (\mathbf{c}_m \cdot \mathbf{c}_m)\mathbf{r}}{1 + \mathbf{c}_m \cdot \mathbf{c}_m} \ . \tag{21}$$

Now, let $\mathbf{h}$ be the projection of $\mathbf{r}$ onto the plane perpendicular to $\mathbf{l}$, with $\mathbf{h}'$ representing an analogous projection of $\mathbf{r}'$. They are given by $\mathbf{h} = \mathbf{r} - (\mathbf{r} \cdot \mathbf{l})\mathbf{l}$ and $\mathbf{h}' = \mathbf{r}' - (\mathbf{r}' \cdot \mathbf{l})\mathbf{l}$, respectively. With relations $\mathbf{r}' \cdot \mathbf{r}' = \mathbf{r} \cdot \mathbf{r}$ and $\mathbf{r}' \cdot \mathbf{l} = \mathbf{r} \cdot \mathbf{l}$, which follow directly from Eq.(21), there occurs

$$\mathbf{h}' \cdot \mathbf{h}' = \mathbf{h} \cdot \mathbf{h} \ ,$$

i.e., the distance of points $\mathbf{r}$ and $\mathbf{r}'$ from the rotation axis is the same. Moreover, the angle between the projections, say α, is now related to $\mathbf{h}$ and $\mathbf{h}'$ by

$$\cos\alpha = (\mathbf{h}' \cdot \mathbf{h})/(\mathbf{h} \cdot \mathbf{h}) \ .$$

This expression can be written in the form

$$\left((\mathbf{r} \cdot \mathbf{r}) - (\mathbf{r} \cdot \mathbf{l})^2\right)((1 + \mathbf{c}_m \cdot \mathbf{c}_m)\cos\alpha - (1 - \mathbf{c}_m \cdot \mathbf{c}_m)) = 2(\mathbf{c}_m \cdot \mathbf{r})^2 - 2(\mathbf{c}_m \cdot \mathbf{r})(\mathbf{c}_m \cdot \mathbf{l})(\mathbf{r} \cdot \mathbf{l}) \ .$$

The right side of the equation equals 0. Thus, for $\mathbf{r}$ not collinear with $\mathbf{l}$ (i.e., $(\mathbf{r}\cdot\mathbf{r}) - (\mathbf{r}\cdot\mathbf{l})^2 \neq 0$) the angle between the vectors $\mathbf{h}$ and $\mathbf{h}'$ is given by

$$\cos\alpha = \frac{1 - \mathbf{c}_m \cdot \mathbf{c}_m}{1 + \mathbf{c}_m \cdot \mathbf{c}_m} = \cos\left(\frac{2m\pi}{M}\right)$$

which means that α equals $2m\pi/M$ or $2(M-m)\pi/M$ whichever is smaller.

Therefore, by choosing m suitably one can divide Rodrigues space into symmetrically equivalent regions using planes containing the rotation axis, $\mathbf{l}$, and distributed radially with dihedral angles equal to $2\pi/M$. This statement (together with the equivalence between $\mathbf{r}$ and its inverse $-\mathbf{r}$) allows derivation of the MacKenzie cell for all considered symmetries.

References

Adams,B.L., Wright,S.I. and Kunze,K., 1993, *Metall. Trans. A*, **24**, 819.

Becker,R. and Panchanadeeswaran,S., 1989, *Textures and Microstructures*, **10**, 167.

Bunge,H.J., 1970, *Krist. Tech.*, **5**, 145.

Bunge,H.J., 1982, *Texture Analysis in Materials Science*, (London: Butterworths).

Clément,A., 1982, *Mat. Sci. Engng.*, **55**, 203.

Field,D.P. and Adams,B.L., 1992, *Met. Trans. A*, **23**, 2514.

Field,D.P., 1995, *Scripta Metall. Mater.*, **32**, 67.

Frank,F.C., 1988, *Metall. Trans. A*, **19**, 403.

Pospiech,J., 1980, *Kristall u. Technik*, **15**, 1481.

Morawiec,A. and Pospiech,J., 1989, *Textures and Microstructures*, **10**, 211.

Morawiec,A., 1995, to appear in *J. Appl. Cryst.* **28**.

Neumann,P., 1991, *Textures and Microstructures*, **14-18**, 53.

Randle,V., 1990, *Proc. R. Soc. Lond. A*, **431**, 61.

Randle,V., 1992, *Phil. Mag. Lett.*, **66**, 307.

Wierzbanowski,K. and Clément,A., 1985, *Phil. Mag.*, **51**, 145.

Zhao,J. and Adams,B.L., 1988, *Acta Cryst. A*, **44**, 326.

Yeates,T.O., 1993, *Acta Cryst. A*, **49**, 138.

Captions

1. The fundamental zones and MacKenzie cells for D_3 (a) and D_4 (b).

2. Orientations (a) and misorientations (b) present in a sample of trigonal Al_2O_3. The technique applied to obtain these measurements is described in the paper by Adams, Wright and Kunze 1993.

3. The fundamental zones and MacKenzie cells for tetrahedral (a), octahedral (b) and icosahedral (c) symmetries.

4. Schematic showing bounds of symmetrically equivalent zones for D_4. The sections (through $\mathbf{0}$) are perpendicular to four–fold axis (a) and two–fold axis (b).

5. Sections through $\mathbf{0}$ showing bounds of symmetrically equivalent zones for T (section perpendicular to two–fold axis), O (perpendicular to four–fold axis) and Y (perpendicular to five–fold axis).

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