Distributions of Misorientation Angles and Misorientation Axes for Crystallites with Different Symmetries

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Abstract

The misorientation angle is the simplest characteristic of the difference between orientations of two crystallites in a polycrystalline material. Another is the corresponding rotation axis. These quantities can also be determined when crystallites are of different types and possibly different symmetries, as in multiphase materials. With the assumption that crystallites are randomly oriented, distributions of misorientation angles and corresponding rotation axes are calculated. They depend on the symmetries of the crystallites and on the choice of bases of the crystal coordinate systems. All pairs of crystallographic point groups are considered. The approach can also be applied to non-crystallographic symmetries. The results can serve as reference functions for distributions corresponding to real materials. In the derivation, asymmetric domains of misorientation distributions are determined by choosing among equivalent rotations those with the smallest rotation angles. The property of Rodrigues parameterization of rotations is used, allowing the faces of the domains to be planar. Forms of the distributions follow from the shapes of these domains. The asymmetric domains are also applicable in the case of rotation functions, *i.e.* correlations of two mutually rotated Patterson functions.

1. Introduction

A simple way to define the terms orientation and misorientation of objects (crystallites) is by choosing a laboratory (sample) Cartesian coordinate system and attaching Cartesian coordinate systems to the objects. The orientation of an object can be defined as the rotation applied to the laboratory coordinate system that gives a coordinate system with axes in the same directions as the axes of the system of the object. Analogously, the misorientation of two objects is determined as the rotation applied to the coordinate system of the first object that leads to a system with axes

in the same directions as the axes of the system of the second object. Thus, formally, the orientation of an object can be treated as the misorientation between the laboratory coordinate system and the object. Therefore, results concerning misorientations are equally applicable to orientations although their meaning is special because one of the objects is the unique laboratory coordinate system.

A rotation can be determined by a rotation axis and a rotation angle. However, when the objects are symmetric, a number of rotations correspond to the misorientation and these, and generally any parameters, are not unique. To make the parameters unique, instead of the whole rotation space, one considers a certain part of it in which each physically distinct misorientation is represented only once. Many different names have been used for this region, *e.g.* asymmetric domain (or unit or region), symmetrically equivalent area, fundamental zone, MacKenzie cell. There, we use the first term as most suitable for the context of this paper. For some particular methods of determining the asymmetric domains, see Tollin, Main & Rossmann (1966), Pospiech (1972), Pospiech, Gnatek & Fichtner (1974), Rao, Jih & Hartsuck (1980), Bonnet (1980), Zhao & Adams (1988), Heinz & Neumann (1991) and Yeates (1993).

The simplest characteristic of misorientation is the smallest rotation angle of the equivalent rotations. It is called the misorientation angle. The first problem that we are concerned with is what the distribution of the misorientation angles is when the orientations of objects are random. Another problem is the distribution of misorientation axes (*i.e.* axes of rotations with the smallest rotation angles), again for randomly oriented objects. These distributions are influenced by symmetries of objects. To take into account all distinguishable configurations, it is sufficient to consider only proper symmetry operations. There is, however, a certain viewpoint from which improper rotations should also be included. This is considered in the last section of the paper, whereas, in the first four sections, all symmetry operations are assumed to be proper and all coordinate systems to be of the same kind (right-handed).

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The issues of misorientation-angle and misorientation-axis distributions have been addressed previously but only in the case of objects of one type (like crystallites in single-phase materials). MacKenzie & Thomson (1957) estimated the misorientation-angle distribution for octahedral symmetry numerically by the Monte Carlo method. MacKenzie (1958) and Handscomb (1958), using considerably different approaches, obtained an explicit formal expression for that distribution. The misorientation-angle distributions for cyclic and dihedral symmetries were reported by Grimmer (1979). The distribution of misorientation axes for octahedral symmetry was presented by MacKenzie (1964). Morawiec (1995, 1996) gave both types of distribution for all symmetries in three dimensions.* This paper is focused on the case for different symmetries of misoriented objects. It corresponds directly to two-phase polycrystalline materials with different crystallographic symmetries of phases. Distributions of misorientation angles and misorientation axes are tools in analysing intercrystalline misorientations and geometric features of grain boundaries (*cf.* Haessner & Sztwiertnia, 1988; Plutka & Hougardy, 1991; Gertsman, Tangri & Valiev, 1994). They have been used in investigations of orientation relationships between nuclei or growing grains and the matrix in the process of recrystallization and are equally important in studying the relationship between orientations of emerging grains and parent orientations in phase transformations. The model distributions are references for those that occur in real materials and are influenced by crystallographic textures and correlations between orientations of neighbouring grains. Because of new experimental techniques allowing measurements of large numbers of individual orientations (*cf.* Adams, Wright & Kunze, 1993), such statistical results are especially important.

Although we are interested in crystallites in multiphase polycrystalline materials, the results concern all symmetric objects in three dimensions. In particular, those related to asymmetric domains are fully applicable in the relatively close area of the rotation function defined as the correlation of two mutually rotated Patterson functions (Rossmann & Blow, 1962; Tollin & Rossmann, 1966). The function is used to search for structurally identical or similar molecular subunits within large molecules. Symmetries of the rotation functions are of the same kind as the symmetries of misorientation distributions.

It is relatively easy to determine the asymmetric domains when Rodrigues parameters of rotation are used. What matters here, however, is that in this parameterization it is straightforward to calculate the

misorientation-angle distributions and distributions of rotation axes based on shapes of appropriately chosen domains. The Rodrigues parameters $\{r^1, r^2, r^3\}$ of rotation (also called symmetric Euler parameters or Gibbs vector) are given by $r^i = \tan(\omega/2)k^i$, where ω ($0 \le \omega \le \pi$) is the rotation angle and k^i ($i = 1, 2, 3$) are Cartesian components of the unit vector $\mathbf{k}$ determining the rotation axis.* The three parameters will be briefly denoted by one vector symbol $\mathbf{r}$. All possible rotations fill infinite three-dimensional 'Rodrigues space' but every two antipodal points at infinity correspond to one rotation (by π). Vectors representing mutually inverse rotations differ by their sign. Composition of rotations $\mathbf{r}_1$ and $\mathbf{r}_2$ is given by $\mathbf{r}_2 \circ \mathbf{r}_1 = (\mathbf{r}_1 + \mathbf{r}_2 - \mathbf{r}_1 \times \mathbf{r}_2)/(1 - \mathbf{r}_1 \cdot \mathbf{r}_2)$. The Rodrigues parameterization has a special property making it suitable for the determination of asymmetric domains based on the misorientation angle. Let the angular distance between $\mathbf{r}_1$ and $\mathbf{r}_2$ be the smallest rotation angle of rotations leading from $\mathbf{r}_1$ to $\mathbf{r}_2$. In terms of Rodrigues vectors, it is given by $2\arctan[|\mathbf{r}_2 \circ (-\mathbf{r}_1)|]$. Let two different points be distinguished. Points at the same angular distance to each of them constitute two planes (in the Euclidean sense) in the Rodrigues space. For purposes of this paper, only planes equidistant to $\mathbf{0}$ and $\mathbf{r} = \tan(\omega/2)\mathbf{k}$ are needed; they are given by $\tan^{\pm 1}(\omega/4)\mathbf{k} + \mathbf{y}$, where $\mathbf{y}$ is an arbitrary vector perpendicular to $\mathbf{k}$ (*cf.* Frank, 1988; Morawiec, 1995).

Let two neighbouring crystallites have lattice symmetries described by point groups G_L and G_R. With Rodrigues vectors $\mathbf{s}_L$ and $\mathbf{s}_R$ corresponding to elements of G_L and G_R, points $\mathbf{r}_L$ and $\mathbf{r}_R$ representing orientations of the crystallites are equivalent to $\mathbf{s}_L \circ \mathbf{r}_L$ and $\mathbf{s}_R \circ \mathbf{r}_R$, respectively. The misorientation between the crystallites (the rotation leading from $\mathbf{r}_R$ to $\mathbf{r}_L$) is represented in the Rodrigues space by the point $\mathbf{r} = \mathbf{r}_L \circ (-\mathbf{r}_R)$. It is equivalent to $\mathbf{s}_L \circ \mathbf{r}_L \circ (-\mathbf{r}_R) \circ (-\mathbf{s}_R) = \mathbf{s}_L \circ \mathbf{r} \circ (-\mathbf{s}_R)$. This also means that points $\mathbf{r}$ and $\mathbf{s}_L \circ \mathbf{r} \circ \mathbf{s}_R$ are equivalent. Thus, the direct product (G_L, G_R) acts in the space of rotations and divides it into classes of equivalent points. The asymmetric domain constitutes a suitably chosen set of unique representatives of the classes.

For a one-phase material, both $\mathbf{s}_L$ and $\mathbf{s}_R$ are elements of the same symmetry group. The known results for $G_L = G_R$ (MacKenzie, 1958, 1964; Handscomb, 1958; Grimmer, 1979; Morawiec, 1995, 1996) constitute special cases of those considered in this paper with G_L and G_R allowed to be different. What matters, however, is that most of the distributions for $G_L \ne G_R$ can be reduced to those already published for $G_L = G_R$.

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* When writing the account on misorientation-angle distributions (Morawiec, 1995), the author was unaware of Grimmer's (1979) communication.

* The components of the unit vector indicating the rotation axis are the same in three orthonormal coordinate systems: initial, final and that in which the Rodrigues vector is determined and, thus, it is not necessary to specify the system when the rotation axes are considered.

The case of the one-phase material, *i.e.* with all crystallites of the same kind, has two special features. The first of them concerns their misorientation distribution. Because two misoriented objects are indistinguishable, their roles can be exchanged and, hence, values of the distribution at mutually inverse rotations (*i.e.* at opposite points r and $-r$ of the Rodrigues space) are the same. Therefore, these rotations are also considered to be equivalent and, thus, the asymmetric domain is half the size of that in the general case.* This additional 'symmetry', however, does not influence the distributions of misorientation angles and misorientation axes and, thus, it is immaterial for the main purpose of this paper. It is trivial to take it into account when the domain is sought.

As for the second feature, because the crystallites are indistinguishable, the crystal coordinate systems must be attached to each of them in the same way. Therefore, there exists a natural and unique choice for the reference alignment (or reference misorientation corresponding to **0**). On the other hand, when the crystallites are of different types, there are various possible settings of the crystal coordinate systems and the reference misorientation is not unique (*cf.* Fortes, 1984). For example, in the case of misorientations between h.c.p. and b.c.c. phases, bases of the crystal coordinate systems can be chosen in the standard way, *i.e.* (disregarding directions), for misorientation corresponding to **0**, the b.c.c. (001) plane is parallel to h.c.p. (0001). In some special cases, however, the other choices would be interesting, *e.g.* to have the b.c.c. (110) plane parallel to the h.c.p. (0001) plane as in the Burgers relation observed in b.c.c. to h.c.p. phase transformations in zirconium, titanium and their alloys (*cf.* Williams, Cahn & Barret, 1953).

The possibility of setting coordinate systems in various ways means that for objects with different symmetries the asymmetric domain is not 'fundamental'. Its shape and also the form of distributions of misorientation angle and misorientation axis depend on the choice of the reference misorientation. Therefore, although the method of determining the domains and the distributions is general, particular results presented below are valid only for the special setting of the crystal coordinate systems. It will be described as the standard choice of the systems. It is based on the table of stereograms of three-dimensional crystallographic point groups printed in *International Tables for X-ray Crystallography* (1952, pp. 26–27) with horizontal x axis and vertical y axis, both in the plane of the paper, and with the z axis perpendicular

to that plane. The first of the two settings for the monoclinic system is taken.

2. Pairs without non-trivial common symmetries

A symmetry element present in both G_L and G_R is considered to be a common symmetry element in specified coordinate systems if it has the same parameters when expressed explicitly in both coordinate systems. To give an example, let two crystals have symmetries described by the crystallographic point groups T and C_3. Each of these groups contains symmetry with a threefold rotation axis. If in the two crystal coordinate systems this axis is along the same line (*e.g.* the z axis), this symmetry element is considered to be common. But it is not a common element if the systems are chosen in the standard way with the threefold axis of C_3 along the z axis and the twofold rotation axes of T along the axes of the coordinate system.

If the pair (G_L, G_R) has *no* common symmetry elements other than the identity (**0**), each misorientation is represented in the Rodrigues space by $N = \#G_L \#G_R$ different symmetrically equivalent points, where $\#G$ denotes the order of the group G. Those equivalent to **0** are given by $s_L \circ \mathbf{0} \circ s_R = s_L \circ s_R$. They will be described as distinguished points. The space can be divided into regions with boundaries determined by points at the same angular distance from the two nearest distinguished points. Points inside such a region are closer to one $s_L \circ s_R$ than to any other. The method of obtaining these regions is the same as the tessellation into the so-called 'Voronoi polyhedra'. Similar ideas for Euler-angle parameterization in the context of rotation functions was presented by Yeates (1993). In the case of the Rodrigues parameters, regions' boundaries are planar, owing to the forementioned fact that points equidistant to two distinguished points lie on planes. The angular distance of a given point r from **0** is the same as the distance between $s_L \circ r \circ s_R$ and $s_L \circ s_R$. Thus, disregarding points at the boundaries, each region contains representatives of all classes of non-equivalent points and each class is represented only once in the region.* Therefore, each of the regions can serve as the asymmetric domain. It is most convenient to choose the one surrounding $\mathbf{0} \circ \mathbf{0} = \mathbf{0}$ because points of this region correspond to rotations with the smallest rotation angles. This asymmetric domain will be used to obtain the sought distributions.

In practice, to determine the domain, all distinguished points $s_L \circ s_R$ must be taken into considera-

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*Also the rotation function has that symmetry when it is an autocorrelation of the Patterson function (Moss, 1985).

*To take boundary points into account, additional rules would be necessary. But these points constitute a set of measure 0 and do not play any role in calculating the sought distributions.

tion. Excluding $\mathbf{0} \circ \mathbf{0}$, they are of the form $\mathbf{l}_i \tan(\omega_i/2)$, where $i = 1, 2, \ldots, (N-1)$, $\mathbf{l}_i$ are unit vectors and $0 < \omega_i \leq \pi$. The planes equidistant to the ith point and to $\mathbf{0}$ are given by $\left((\mathbf{l}_i; \tan^{\pm 1}(\omega_i/4)\right)$, where the symbol $(\mathbf{l}; d)$ denotes here (and later on) a plane given by all points $\mathbf{x}$ satisfying $\mathbf{l} \cdot \mathbf{x} = d \geq 0$, *i.e.* the plane perpendicular to the unit vector $\mathbf{l}$ at a distance d from $\mathbf{0}$, in the direction indicated by the vector. For $0 < \omega < \pi$, $\tan(\omega/4) < 1 < \tan^{-1}(\omega/4)$ and, moreover, $\tan^{\pm 1}(\pi/4) = 1$. Thus, the asymmetric domain composed of points located closer to $\mathbf{0}$ than to any other distinguished point is common of all half-spaces

determined by the conditions $\mathbf{l}_i \cdot \mathbf{x} \leq \tan(\omega_i/4)$ if $0 < \omega_i < \pi$ and by $\pm \mathbf{l}_i \cdot \mathbf{x} \leq 1$ if $\omega = \pi$.

2.1. *Misorientation-angle and misorientation-axis distributions*

Once the domain based on rotations with the smallest rotation angles is known, it is relatively easy to obtain the misorientation-angle distribution and the distribution of corresponding rotation axes for randomly oriented crystallites. The procedures allowing the calculation of these distributions from the shape of the
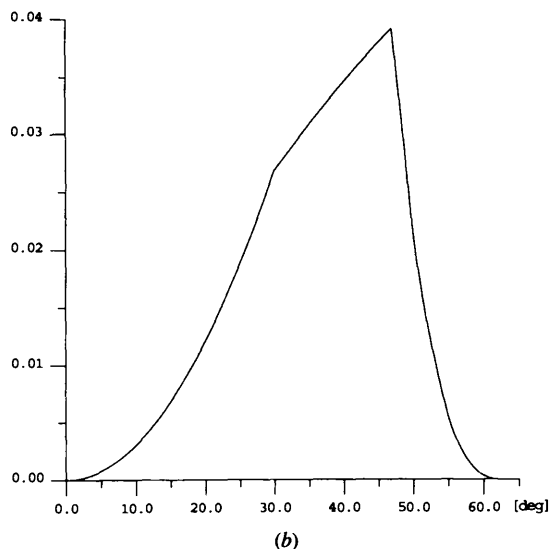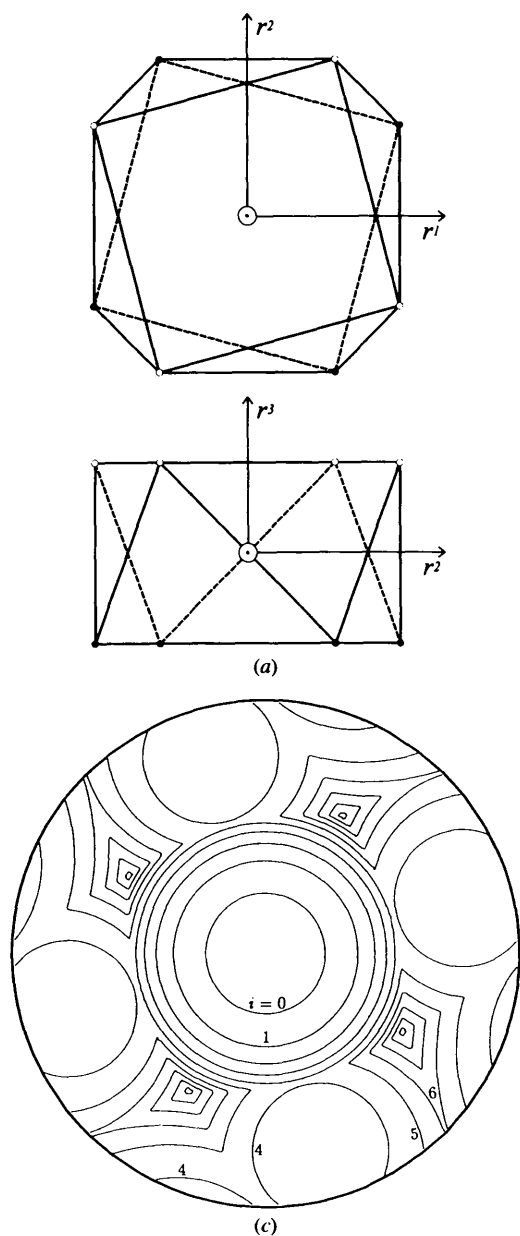

Fig. 1. Results for the pair (C_3, T) for reference alignment with the same line (z) as the threefold axis of C_3 and as twofold axis of T. (a) Projections of the asymmetric domain on the planes $r^3 = 0$ and $r^1 = 0$ of the Rodrigues space. Third coordinate, r^3, of vertices marked by o [●] is $\tan(\pi/12)$ $[-\tan(\pi/12)]$. Dashed lines correspond to 'invisible' edges. (b) Misorientation-angle distribution. (c) Stereographic projection of the upper hemisphere $(z \geq 0)$ of the distribution of misorientation axes q. The mirror image with respect to the vertical axis gives the projection of the lower hemisphere. The isolines are equidistant in the range of the distribution: isoline$(i) = \min(q) + (i + 0.5)[\max(q) - \min(q)]/10$, $i = 0, 1, \ldots, 9$, with $\min(q) = 2.1520 \times 10^{-2}$ and $\max(q) = 1.8040 \times 10^{-1}$. [Comparing this with extrema given by MacKenzie (1964) or Morawiec (1996), different normalizations of q must be taken into account.]

domain are described elsewhere (Morawiec, 1995, 1996). The first step is to find the density of random orientations in the Rodrigues space. It is equal to the invariant volume of the space $dV(\mathbf{r}) = \{r/[\pi(1 + r^2)]\}^2 \, dr \, d_2\mathbf{k}$, where $r = (\mathbf{r} \cdot \mathbf{r})^{1/2} = \tan(\omega/2)$, is the distance of the point $\mathbf{r}$ from $\mathbf{0}$ and $d_2\mathbf{k}$ denotes the infinitesimal element on the unit sphere. The value of the misorientation-angle distribution p at fixed ω is calculated by integrating the density over all rotation axes of misorientations contained inside the asymmetric domain. With the volume of the whole rotation space set to 1, the volume of the asymmetric domain equals $1/N$. If the normalization coefficient of N is taken into account, the general result can be formally expressed as

$$p(\omega) = [N/(2\pi^2)] \sin^2(\omega/2) \, \chi[\tan(\omega/2)],$$

where $\chi(r)$ is the solid angle based on the part of the sphere of radius r contained inside the asymmetric domain. When angles are given in degrees, p should be replaced by the distribution $\omega[\mathrm{deg}] \mapsto (\pi/180)p(\omega\pi/180)$.

The distribution q of rotation axes at $\mathbf{k}$ is equal to N times the integral of the density over angles of these rotations that are represented by Rodrigues vectors $\mathbf{r} = r\mathbf{k}$ and located inside the domain. It is given by

$$q(\mathbf{k}) = [N/(2\pi^2)]\left(\arctan[\lambda(\mathbf{k})] - \lambda(\mathbf{k})/\{1 + [\lambda(\mathbf{k})]^2\}\right),$$

where $\lambda(\mathbf{k})$ is the distance from point $\mathbf{0}$ to the boundary of the domain in the direction $\mathbf{k}$. If $(\mathbf{l}; d)$ is the bounding plane such that $\mathbf{k} \cdot \mathbf{l} > 0$, then $\lambda(\mathbf{k}) = d/(\mathbf{k} \cdot \mathbf{l})$. The distribution is normalized over all directions on the sphere.

The following general remark allows one to reduce significantly (roughly by half) the number of pairs (G_L, G_R) that should be analysed: the asymmetric domain of the pair (G_R, G_L) can be obtained by taking the inversion of the domain of (G_L, G_R) with respect to the origin of the coordinate system in the space of Rodrigues parameters. Based on the above expressions for the distributions p and q, it can easily be noticed that the misorientation-angle distributions of (G_L, G_R) and (G_R, G_L) are identical and the misorientation-axis distributions are related by $q_{(G_R, G_L)}(\mathbf{k}) = q_{(G_L, G_R)}(-\mathbf{k})$.

2.2. Example: (C_3, T)

Let us consider the pair (C_3, T) with crystal coordinate systems chosen in the standard way. There are no common symmetry elements other than the identity. Points $\{0, 0, \pm\tan(\pi/6)\}$ of the Rodrigues space represent symmetry operations of C_3 and are equivalent to $\mathbf{0}$. Because of them, the asymmetric domain is bounded by two planes $((0, 0, \pm 1); a)$, where $a = \tan(\pi/12) = 2 - 3^{1/2}$. Moreover, with the elements $\mathbf{s}_L = \{0, 0, -\tan(\pi/6)\}$ of C_3 and $\mathbf{s}_R = \{1, 1, 1\}$ of T, the distinguished point $\mathbf{s}_L \circ \mathbf{s}_R$ has coordinates $\{1, a, a\}$ and its distance from $\mathbf{0}$ is $b = (1 + 2a^2)^{1/2}$. Its presence leads to another bounding plane; it is given by

$((\alpha, \beta, \beta); c)$, where $\alpha = 1/b$, $\beta = a/b$ and $c = \tan[\arctan(b)/2] = \beta(1 + a)/(1 - a)$. In this way, a complete list of eight extra bounding planes is obtained. Their parameters are $((\alpha, \pm\beta, \pm\beta); c)$, $((\beta, \pm\alpha, \mp\beta); c)$, $((-\alpha, \pm\beta, \mp\beta); c)$ and $((-\beta, \pm\alpha, \pm\beta); c)$, where either upper or lower signs are valid. The shape of the domain is shown in Fig. 1(a).

2.2.1. *Misorientation-angle distribution.* The points of interest on the 'angle' axis are of the form $2\arctan(r_i)$ $(i = 1, \ldots, 5)$, where r_1 and r_2 are distances (from $\mathbf{0}$) of the faces of the domain, r_3 and r_4 are distances of the edges, and r_5 is the distance of all vertices. They are given by

$$r_1 = a, \quad r_2 = c, \quad r_3 = 3^{1/2}a, \quad r_4 = a^{1/2}, \quad r_5 = 5^{1/2}a.$$

Angles between normals to the three types of neighbouring plane are

$$\delta_1 = \arccos(\beta), \quad \delta_2 = \arccos[\beta(2\alpha - \beta)],$$
$$\delta_3 = \arccos(\alpha^2 - 2\beta^2).$$

Let α_i $(i = 1, 2)$ be r-dependent quantities defined by $\alpha_i = \alpha_i(r) = \arccos(r_i/r)$. With $r_0 = 0$, the function χ is given by

$$\chi(r) = \sum_{i=1}^{j} \chi_i(r) \quad \text{for} \quad r_{j-1} \le r < r_j \ (j = 1, \ldots, 5),$$

where

$$\chi_1(r) = 4\pi,$$
$$\chi_2(r) = -2S_1(\alpha_1),$$
$$\chi_3(r) = -8S_1(\alpha_2),$$
$$\chi_4(r) = 8S_2(\alpha_1, \alpha_2; \delta_1) + 4S_2(\alpha_2, \alpha_2; \delta_3),$$
$$\chi_5(r) = 4S_2(\alpha_2, \alpha_2; \delta_2).$$

$S_1(\rho)$ is the solid angle based on a spherical cap of angular radius ρ:

$$S_1(\rho) = 2\pi[1 - \cos(\rho)].$$

Moreover, $S_2(\rho_1, \rho_2; \xi)$ is the solid angle based on the common of two spherical caps of angular radii ρ_1 and ρ_2 and angular distance ξ between their centres. It can be expressed as

$$S_2(\rho_1, \rho_2; \xi) = 2[\pi - C(\rho_1, \rho_2; \xi) - \cos(\rho_1)C(\rho_1, \xi; \rho_2) - \cos(\rho_2)C(\rho_2, \xi; \rho_1)],$$

where $C(\rho_1, \rho_2; \xi) = \arccos\{[\cos(\xi) - \cos(\rho_1)\cos(\rho_2)]/ [\sin(\rho_1)\sin(\rho_2)]\}$ [see Handscomb (1958) or Morawiec (1995)]. The distribution $(\pi/180)p(\omega\pi/180)$, *i.e.* with argument given in degrees, is displayed in Fig. 1(b). The corresponding maximum misorientation angle is 61.8561°. The mean misorientation angle and the standard deviation are 36.4058 and 10.5826°, respectively.

2.2.2. *Distribution of rotation axes.* Let (k^1, k^2, k^3) be components of a unit vector $\mathbf{k}$ determining a rotation

axis. To obtain the distribution q of rotation axes corresponding to the smallest rotation angle, it is sufficient to know the function λ. It is given by

$$\lambda(\mathbf{k}) = \min\{r_1/|k^3|, r_2/d_2\},$$

where

$$d_2 = \max\{\alpha k^1 \pm \beta k^2 \pm \beta k^3, \beta k^1 \pm \alpha k^2 \mp \beta k^3,$$
$$- \alpha k^1 \pm \beta k^2 \mp \beta k^3, -\beta k^1 \pm \alpha k^2 \pm \beta k^3\}.$$

In each of the four arguments of max, either upper or lower signs are valid. The stereographic projection of q is given in Fig. 1(c).

3. Pairs with common symmetries

It is easy to notice that the approach applied to pairs without common symmetry elements must be modified when such elements are present. It follows directly from the fact that some of the products $\mathbf{s}_L \circ \mathbf{s}_R$ are no longer different. There are distinguished points overlapping each other and for them the planes of equidistant points cannot be constructed. From another viewpoint, for a given common symmetry operation $\mathbf{s}$, the conjugate points $\mathbf{r}$ and $\mathbf{s} \circ \mathbf{r} \circ (-\mathbf{s})$ have equal rotation angles. Thus, it is impossible to built asymmetric domains of points with smallest rotation angles because different but equivalent points with the same angle exist, and additional surfaces to separate such points are necessary.

However, in order to calculate the misorientation-angle and the misorientation-axis distributions, it is sufficient to consider the Voronoi tessellation of the Rodrigues space based on different distinguished points. The cell surrounding $\mathbf{0}$ will be called the 'large cell'. It contains misorientations with the smallest rotation angles but there are still equivalent points (with equal angles) inside it. The sought distributions can be obtained based solely on the shape of the large cell. A small additional effort allows determination of asymmetric domains. The following subsection contains some details concerning equivalences within the large cell and clarifies a way of determining locations of the additional surfaces cutting off the asymmetric domain from the cell.

3.1. Auxiliary construction

In order to investigate the role of the common symmetry elements, let us concentrate on the case when rotations with the same rotation axis determined by the unit vector $\mathbf{l}$ are applied on both sides of $\mathbf{r}$ but the axis is m-fold on the right side and n-fold on the left side. To have a nontrivial common symmetry element, the numbers m and n are assumed to have a nontrivial ($\neq 1$) common divisor. Thus, points symmetrically equivalent to $\mathbf{r}$ are of the form $\mathbf{r}' = \mathbf{s}_L \circ \mathbf{r} \circ \mathbf{s}_R$, where

$\mathbf{s}_R = \tan(i_m\pi/m)\mathbf{l}$ and $\mathbf{s}_L = \tan(i_n\pi/n)\mathbf{l}$, with $i_m = 0, \ldots, m-1$ and $i_n = 0, \ldots, n-1$. Let a plane perpendicular to $\mathbf{l}$ in the Rodrigues space be determined by all $\mathbf{r}$ satisfying $\mathbf{r} \cdot \mathbf{l} = \tan(\omega/2) = $ constant. A short calculation shows that $\mathbf{r}' \cdot \mathbf{l} = \tan(\omega/2 + i_m\pi/m + i_n\pi/n)$. This means that the plane perpendicular to $\mathbf{l}$ and located at a distance $\tan(\omega/2)$ from $\mathbf{0}$ is transformed onto a plane perpendicular to $\mathbf{l}$ and at a distance $|\tan(\omega/2 + (i_m/m + i_n/n)\pi)|$. Owing to the periodicity of tan, the number of overlapping planes (i.e. the number of planes with the same value of $\mathbf{r}' \cdot \mathbf{l}$) is equal to the number of different pairs (i_m, i_n) satisfying $(i_m/m + i_n/n)\pi = k\pi$ (with $k = 0, 1$). This number, in turn, is equal to the largest common divisor of m and n, denoted here by $E(m, n)$. The total number of pairs (i_m, i_n) is mn. Thus, the number of different images of the initial plane is $F(m, n) = mn/E(m, n)$.

From a slightly different point of view, there are $F(m, n)$ different distinguished points $\tan[k\pi/F(m, n)]\mathbf{l}$, $k = 0, \ldots, F(m, n) - 1$, equivalent to $\mathbf{0}$. The two points nearest to $\mathbf{0}$ are $\pm\tan[\pi/F(m, n)]\mathbf{l}$. They give rise to the two surfaces $(\pm\mathbf{l}; \tan\{\pi/[2F(m, n)]\})$ bounding the zone of points close to $\mathbf{0}$. But there are still $E(m, n)$ equivalent points inside that zone.

To eliminate them, equivalences within the transformed plane must be considered. The image, $\mathbf{r}'$, is in the same plane as the initial point, $\mathbf{r}$, when $\mathbf{r}' \cdot \mathbf{l} = \mathbf{r} \cdot \mathbf{l}$. Let α be the angle between projections $\mathbf{h} = \mathbf{r} - \tan(\omega/2)\mathbf{l}$ and $\mathbf{h}' = \mathbf{r}' - \tan(\omega/2)\mathbf{l}$ of the vectors $\mathbf{r}$ and $\mathbf{r}'$ on the considered plane. For $\mathbf{r}'$ satisfying $\mathbf{r}' \cdot \mathbf{l} = \mathbf{r} \cdot \mathbf{l}$, there occurs $\mathbf{r}' \cdot \mathbf{r}' = \mathbf{r} \cdot \mathbf{r}$ and, thus, $\mathbf{h}' \cdot \mathbf{h}' = \mathbf{h} \cdot \mathbf{h}$. Hence, for $\mathbf{r}$ not collinear with the rotation axis, one has $\cos(\alpha) = (\mathbf{h}' \cdot \mathbf{h})/(\mathbf{h} \cdot \mathbf{h}) = \cos(2i_m\pi/m)$, where i_m ($0 \le i_m < m$) satisfies $i_mn + i_nm = kmn$ for $i_n = 0, \ldots, n-1$ and $k = 0, 1$. This means that $\alpha = 2\pi j/E(m, n)$, $j = 0, \ldots, E(m, n)$. Thus, all $E(m, n)$ equivalent points on the considered plane are at the same distance from the axis $\mathbf{l}$; they are distributed symmetrically around that axis and, therefore, the plane can be divided radially into $E(m, n)$ equivalent regions with angles between dividing half-lines equal to $2\pi/E(m, n)$.

In summary, when symmetries with the same rotation axis (of foldness m and n) occur, the task of finding the asymmetric domain can be simplified by the following rules: There are two bounding planes perpendicular to the axis at a distance $\tan\{\pi/[2F(m, n)]\}$ from $\mathbf{0}$. Moreover, the region between these planes can be radially divided into $E(m, n)$ identical and equivalent parts, of which one can be selected as the domain.

The latter division is caused by the presence of the common $E(m, n)$-fold rotation axis. It can be performed by introducing $E(m, n)$ symmetrically distributed half-planes having the rotation axis as their common edge, with the dihedral angle between closest pairs equal to $2\pi/E(m, n)$. Positions of the dividing half-planes in the Rodrigues space are not unique but, on the other hand,

when there is more than one axis corresponding to common symmetry operations, the half-planes must be properly arranged. It is *not* sufficient to establish proper dihedral angles and to satisfy the condition that the half-planes have the axes as their edges; the asymmetric domain must be built of such points **r** that application of all angle-preserving symmetry operations of the type s ∘ **r** ∘ (−s) to the points of the domain gives the large cell. All common symmetry operations constitute a group. It is a subgroup of both G_L and G_R. Thus, the subgroup determines the positions of the half-planes. If it is known, one can easily deduce which points of the large cell are equivalent and, hence, where the half-planes should be located.

3.2. Notation

The following notation allows us to make the description of the domains more concise. Let us assume that (G_L', G_R') is a pair without common symmetry elements. The expression

$$(G_L, G_R) \to (G_L', G_R')/G_C$$

will be used when the asymmetric domain of (G_L', G_R') constitutes the large cell for (G_L, G_R) and a group G_C determines equivalences [due to (G_L, G_R)] between points of the large cell. In this section, where only proper rotations are considered, G_C is simply the group of common elements of G_L and G_R. In this case, the relation between the volumes of the domains of (G_L, G_R) and (G_L', G_R') can be expressed by $\#G_R\#G_L = \#G_C\#G_R'\#G_L'$.

For simplicity, if one of G_R' and G_L' is the trivial symmetry group C_1, instead of (C_1, G) or (G, C_1), only the symbol G will be used; if G_C is trivial C_1, its symbol and the slash ('/') will be omitted.

At this point, the crucial fact is that once the asymmetric domain of (G_L', G_R') is known, it is straightforward to deduce from this notation the form of the domain of the pair (G_L, G_R). Moreover, the misorientation-angle distribution and the distribution of the corresponding axes for (G_L, G_R) are the same as for (G_L', G_R'). The latter statement follows from the fact that the geometric figure of the large cell has (at least) the point symmetry of the common subgroup. Transformation of the outer planes bounding the asymmetric domain (*i.e.* these that are not through **0**) by elements of the subgroup gives the planes bounding the large cell. But these outer planes of the domain constitute the only factor influencing the sought misorientation-angle and misorientation-axis distributions. Therefore, to obtain the distributions, the large cell can be used. In order to have proper normalization of the distributions, the normalizing factor must correspond to the volume of the large cell. Thus, N is equal to $\#G_L'\#G_R'$ or

$$N = \#G_L\#G_R/\#G_C.$$

This guarantees that the formulae for p and q for the case without common symmetry elements also are correct when such elements are present.

3.3. Special case: subgroups

When one of the groups, say G_L, is a crystallographic subgroup of the other one (G_R), the coordinate system can be arranged in such a way that all elements of the subgroup are common symmetry operations. The large cell of (G_L, G_R) is nothing but the asymmetric domain of the group $G_R \sim (C_1, G_R)$ alone. Thus, there occurs $(G_L, G_R) \to G_R/G_L$. The misorientation-angle distribution and the distribution of rotation axes of the system are the same as those for the higher symmetry G_R. In particular, if $G_R = G = G_L$, then $(G, G) \to G/G$. (The additional equivalence between **r** and −**r** is not taken into account.)

In order to give an example for the case with one group being subgroup of the other, let us consider the pair (C_3, T) once more. This time, the threefold axes of both symmetries are assumed to have the same direction in the state of reference alignment (non-standard arrangement). Therefore, there are three half-planes in the Rodrigues space with a threefold axis as their common edge and dihedral angles of $2\pi/3$ and, thus, the appropriate domain for (C_3, T) is one third of that for tetrahedral symmetry, *i.e.* of the regular octahedron with faces at a distance $3^{1/2}/3$ from its centre. Hence, the corresponding misorientation-angle distribution and distribution of rotation axes are the same as for tetrahedral symmetry alone. The appropriate formulae and graphs for this symmetry can be found elsewhere (Morawiec, 1995, 1996). Because the domain and the distributions are different to those obtained in §2.2, this example is simultaneously a visualization of the previously given statement that the shape of the asymmetric domain, and also misorientation-angle and misorientation-axis distributions, depends on the choice of the crystal coordinate systems.

4. Solutions for proper crystallographic symmetries

To solve the problem for proper crystallographic symmetries, all possible pairs of 11 crystallographic groups consisting of proper symmetry operations must be considered. Most of these pairs satisfy subgroup-group relationship, *i.e.* one group is a crystallographic subgroup of the other. [See *e.g.* the subgroup diagram for crystallographic groups in *International Tables for X-ray Crystallography* (1952), pp. 36–37.] Although it is tempting to take advantage of this fact, it would be necessary to choose the crystal coordinate system in such way that the subgroup-group relation is geometrically satisfied as in the above (second) example for (C_3, T) and, thus, awkward crystal coordinate systems would have to be accepted in some cases. Therefore,

Table 1. *Asymmetric domains of the pairs (G_L, G_R) with groups G_L and G_R containing proper symmetry operations*

The first column and first row contain groups G_L and G_R, respectively. Entries of the table correspond to the right side of the arrow $\rightarrow$. The large cell of (G_L, G_R) is the same as the asymmetric domain of the pair (group) given on the left side of the slash. The group on the other side of the slash determines the symmetry of sets of equivalent points within the large cell. The entries on the diagonal, *i.e.* for $G_R = G = G_L$, are given by G/G, *e.g.* $(O, O) \rightarrow O/O$.

	O	T	D_6	D_4	D_3	C_6	D_2	C_4	C_3
C_2	O/C_2	T/C_2	D_6/C_2	D_4/C_2	D_6	C_6/C_2	D_2/C_2	C_4/C_2	C_6
C_3	(C_3, O)	(C_3, T)	D_6/C_3	D_{12}	D_3/C_3	C_6/C_3	D_6	C_{12}	
C_4	O/C_4	O/C_2	D_{12}/C_2	D_4/C_4	D_{12}	C_{12}/C_2	D_4/C_2		
D_2	O/D_2	T/D_2	D_6/D_2	D_4/D_2	D_6/D_1	D_6/C_2			
C_6	$(C_3, O)/C_2$	$(C_3, T)/C_2$	D_6/C_6	D_{12}/C_2	D_6/C_3				
D_3	$(C_3, O)/D_1$	$(C_3, T)/D_1$	D_6/D_3	D_{12}/D_1					
D_4	O/D_4	O/D_2	D_{12}/D_2						
D_6	$(C_3, O)/D_2$	$(C_3, T)/D_2$							
T	O/T								

further on, the standard choice of the systems will be assumed: for cyclic and dihedral symmetries, the principal axis is along the z axis and the twofold axis of the latter is along the x axis; for T and O, two- and fourfold axes, respectively, are along the axes of the coordinate system.

The form of the asymmetric domain for combinations involving only cyclic symmetries follows directly from the 'auxiliary construction'. The region between the forementioned planes $((0, 0, \pm 1); \tan\{\pi/[2F(m, n)]\})$ represents the large cell of (C_m, C_n). On the other hand, it is also the asymmetric domain of $C_{F(m,n)}$. The common subgroup is $C_{E(m,n)}$. With the introduced notation, these statements can be expressed by

$$(C_m, C_n) \rightarrow C_{F(m,n)}/C_{E(m,n)}.$$

Also, the pair (C_m, D_n) can easily be solved. Its large cell has the form of a prism with bases on planes $((0, 0, \pm 1); \tan\{\pi/[2F(m, n)]\})$ and faces determined by planes $(\pm(\sin(i_m/m + i_n/n)\pi, \cos(i_m/m + i_n/n)\pi, 0); 1)$. The prism is the same as that constituting the asymmetric domain of $D_{F(m,n)}$. The group of common symmetry operations is $C_{E(m,n)}$. The half-planes cutting the domain of $D_{F(m,n)}$ have their edges on the principal axis. In the symbolic notation, the result has the form

$$(C_m, D_n) \rightarrow D_{F(m,n)}/C_{E(m,n)}.$$

The domain for the pair (D_m, D_n) can be obtained by using the solution for (C_m, D_n) and by noticing that the only difference is due to an additional common twofold rotation axis along the x axis. This leads to another bounding plane (more precisely, to two half-planes); it is perpendicular to the z axis, this time. Formally, the result can be expressed as

$$(D_m, D_n) \rightarrow D_{F(m,n)}/D_{E(m,n)},$$

where D_1 represents the symmetry with a twofold axis along the x axis.

For each of the already considered pairs, the distinguished points are the same as those of a single group. Among the remaining non-trivial pairs (*i.e.*

those not satisfying the subgroup–group relationship in the standard arrangement), the same can be applied to (C_4, T) and (D_4, T). For both pairs, the large cell is the same as the domain of the octahedral group; there occurs

$$(C_4, T) \rightarrow O/C_2 \quad \text{and} \quad (D_4, T) \rightarrow O/D_2.$$

The important point is that, in all above cases and those satisfying the subgroup–group relationship, the sought misorientation-angle and misorientation-axis distributions are determined by the corresponding group (G) on the left side of the slash (*i.e.* C_n, D_n, T and O) regardless what is on the right side. This means that they can be obtained directly from the results for $(G, G) \rightarrow G/G$.[*] Detailed accounts of these distributions have already been given (MacKenzie, 1958, 1964; Handscomb, 1958; Grimmer, 1979; Morawiec, 1995, 1996), and this means that the problem has already been solved for a large number of possible cases with different G_R and G_L as well.

In order to obtain results for the remaining pairs, let us notice that in the standard arrangement the products (C_6, T), (D_3, T) and (D_6, T) differ from (C_3, T) by symmetry elements that are common symmetry elements for these pairs. Simple analysis shows that

$$(C_6, T) \rightarrow (C_3, T)/C_2, \quad (D_3, T) \rightarrow (C_3, T)/D_1,$$
$$(D_6, T) \rightarrow (C_3, T)/D_2$$

and, thus, solutions for these systems follow from the first example for (C_3, T). Finally, for the last four non-trivial pairs, there occurs

$$(C_6, O) \rightarrow (C_3, O)/C_2, \quad (D_3, O) \rightarrow (C_3, O)/D_1,$$
$$(D_6, O) \rightarrow (C_3, O)/D_2.$$

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[*] For example, the distributions for (D_4, T) are the same as those for (O, O).

Therefore, to complete the task for all pairs of crystallographic groups with proper rotations, it remains to consider (C_3, O). This case is discussed in §4.1. All results are summarized in Table 1.

4.1. The pair (C_3, O)

The system (C_3, O) is related to (D_6, O), which is the most interesting combination from the practical viewpoint owing to the application to metals with 'cubic' and 'hexagonal' phases. It would be called 'hexagonal-cubic' in papers by Bonnet (1980) and Heinz & Neumann (1991). Worth noticing is the fact that, in the assumed configuration, different from the already

considered cases, vertices of the asymmetric domain of (C_3, O) are at different distances from $\mathbf{0}$. Therefore, to calculate the misorientation-angle distribution, an additional formula for the solid angle based on a common one of three spherical caps is necessary.

It is straightforward to find the first six planes bounding the asymmetric domain. Because of the threefold (of C_3) and fourfold (of O) rotation axes along the z axis, there exist bounding planes $((0, 0, \pm 1);$ $\tan[\pi/24])$. Moreover, fourfold rotation axes (of O) along x and y axes lead to $((\pm 1, 0, 0); \tan[\pi/8])$ and $((0, \pm 1, 0); \tan[\pi/8])$, respectively. But there are still symmetrically equivalent points in the described region. To eliminate them, eight additional planes are required.
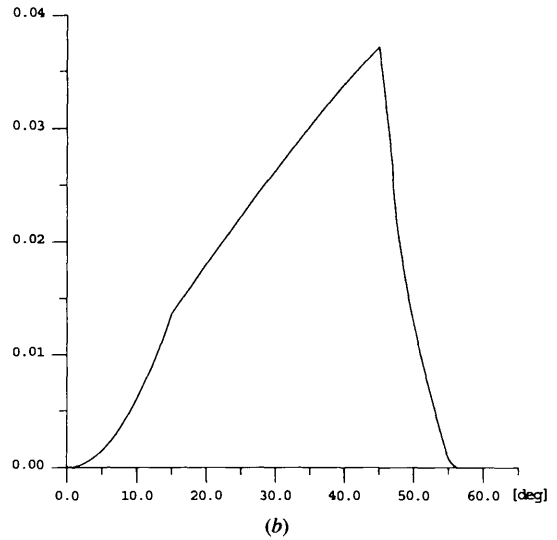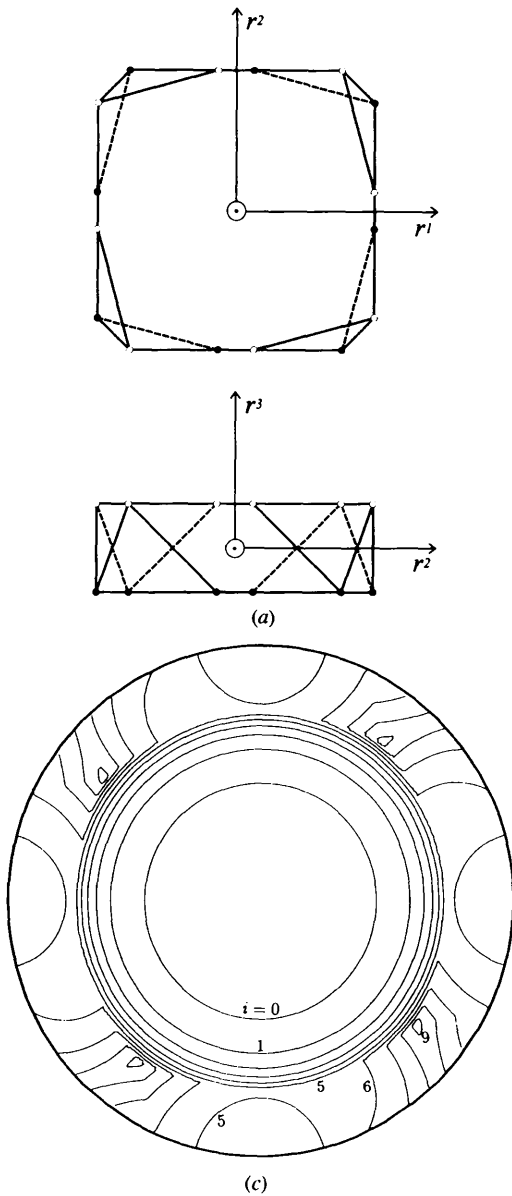

Fig. 2. Results for the pair (C_3, O). (a) Projections of the asymmetric domain. The third coordinate of vertices marked by o [•] is $\tan(\pi/24)$ $[-\tan(\pi/24)]$. (b) Misorientation-angle distribution. (c) Distribution of axes corresponding to the smallest rotation angle. The isolines are as in Fig. 1(c) with $\min(q) = 5.4355 \times 10^{-3}$ and $\max(q) = 2.7906 \times 10^{-1}$.

These are the same planes as those given in the first example for (C_3, T): $((\alpha, \pm\beta, \pm\beta); c)$, $((\beta, \pm\alpha, \mp\beta); c)$, $((-\alpha, \pm\beta, \mp\beta); c)$, $((-\beta, \pm\alpha, \pm\beta); c)$. (Either upper or lower signs are valid.) The symbols a, b, c, α and β denote the same quantities as in the case of (C_3, T). The asymmetric domain is displayed in Fig. 2(a). See also Heinz & Neumann (1991) for a stereopair of the domain of the 'cubic–hexagonal' system (O, D_6).

4.1.1. *Misorientation-angle distribution.* The essential points on the 'angle' axis are $2\arctan(r_i)$ $(i = 1, \ldots, 7)$, where r_1, r_2 and r_3 are distances (from $\mathbf{0}$) of the faces of the domain, r_4 and r_6 are distances of its edges, and r_5 and r_7 are distances of vertices. They are given by

$$r_1 = \tan(\pi/24), \quad r_2 = \tan(\pi/8), \quad r_3 = c,$$
$$r_4 = (r_1^2 + r_2^2)^{1/2}, \quad r_5 = (r_1^2 + r_2^2 + r_1^2 r_2^2)^{1/2}, \quad r_6 = a^{1/2},$$
$$r_7 = (a + r_1^2 + ar_1^2)^{1/2}.$$

Angles between normals to the four types of neighbouring planes are δ_1, δ_2 [the same as for (C_3, T)], $\delta_3 = \arccos(\alpha)$ and $\delta_4 = \pi/2$. As before, α_i $(i = 1, 2, 3)$ depend on r and are given by $\alpha_i = \arccos(r_i/r)$. With $r_0 = 0$, the formula for χ takes the form

$$\chi(r) = \sum_{i=1}^{j} \chi_i(r) \quad \text{for} \quad r_{j-1} \le r < r_j \ (j = 1, \ldots, 7),$$

where

$$\chi_1(r) = 4\pi,$$
$$\chi_2(r) = -2S_1(\alpha_1),$$
$$\chi_3(r) = -4S_1(\alpha_2),$$
$$\chi_4(r) = -8S_1(\alpha_3),$$
$$\chi_5(r) = 8S_2(\alpha_1, \alpha_2; \delta_4) + 8S_2(\alpha_2, \alpha_3; \delta_3)$$
$$\quad + 8S_2(\alpha_1, \alpha_3; \delta_1),$$
$$\chi_6(r) = -8S_3(\alpha_1, \alpha_2, \alpha_3; \delta_3, \delta_1, \delta_4),$$
$$\chi_7(r) = 4S_2(\alpha_3, \alpha_3; \delta_2).$$

Here, $S_3(\rho_1, \rho_2, \rho_3; \xi_1, \xi_2, \xi_3)$ is the solid angle based on the common of three spherical caps with angular radii ρ_i $(i = 1, 2, 3)$; the symbol ξ_k $(k = 1, 2, 3)$ denotes the angular distance between the centres of the caps with radii ρ_i and ρ_j, where $i \ne j \ne k \ne i$. (For example, ξ_1 is the angular distance between the centres of caps with radii ρ_2 and ρ_3.) The function can be expressed as

$$S_3(\rho_1, \rho_2, \rho_3; \xi_1, \xi_2, \xi_3)$$
$$= -\pi + [S_2(\rho_1, \rho_2; \xi_3) + S_2(\rho_2, \rho_3; \xi_1)$$
$$\quad + S_2(\rho_3, \rho_1; \xi_2)]/2 + \cos(\rho_1)C(\xi_2, \xi_3; \xi_1)$$
$$\quad + \cos(\rho_2)C(\xi_3, \xi_1; \xi_2) + \cos(\rho_3)C(\xi_1, \xi_2; \xi_3).$$

The outline of the derivation of this formula is given in Appendix *A*. The graph of the distribution $(\pi/180)p(\omega\pi/180)$ is shown in Fig. 2(b). The maximum misorientation angle, the mean misorientation angle

and the standard deviation are 56.6003, 33.2220 and 11.0604°, respectively.

4.1.2. *Distribution of rotation axes.* The appropriate function λ has the form

$$\lambda(\mathbf{k}) = \min\{r_1/|k^3|, r_2/\max\{|k^1|, |k^2|\}, r_3/d_2\},$$

where d_2 was given in the first example for (C_3, T). See Fig. 2(c) for the stereographic projection of the distribution q.

5. Solutions for groups with improper symmetry operations

The complete rotation space is composed of two separate components of proper and improper rotations. The relation (improper rotation) = (proper rotation) $\circ$ (a fixed improper rotation) provides a one-to-one correspondence between the components. Using it, a Rodrigues vector can be ascribed to an improper rotation. Thus, in the general description involving improper rotations, a misorientation is determined by a Rodrigues vector and a flag indicating to which of two 'spaces' it belongs. Additional rules would be necessary to write down the composition relation for vectors that may correspond to improper rotations.

Before going further, let us mention that, despite its importance, there is some confusion concerning the role of the improper symmetry operations in texture analysis, particularly their influence on the shape of the asymmetric region. A correct and complete treatment of the subject is not to be found in the literature. Although the problem is not very complicated, there are some subtle elements involved.

When improper symmetries are taken into account (*i.e.* the groups G_R and G_L are allowed to contain improper symmetry operations), objects without such symmetries occur in two distinguishable enantiomorphous forms and there are two possible approaches for studying (mis)orientation distributions:

1. ignore improper symmetries and consider the distinguishable forms as separate phases with their own characteristics, *e.g.* textures;

2. extend the domain of distributions on both right- and left-handed forms, *i.e.* on both components of the complete rotation space. (The presence of improper symmetries means that there are mutually equivalent regions in separated components.)

The first approach seems to be favoured by the texture community (*cf.* Bunge, 1982, pp. 100 ff.). When this approach is applied, there are four* 'misorientation spaces' to be considered. In the case of the second approach, there are only two such spaces, *i.e.* two components of rotation manifold; compared with the first approach, the handedness of misoriented objects is

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* Two types of chirality of the first object times two chiralities for the second object.

missing. This is not incorrect because misorientation, as it is defined, is not supposed to carry information about the original features of objects but only about their relative features. Knowing the misorientation, it is impossible to guess the orientation of an object and, analogously, it is impossible to guess its handedness unless orientation and handedness of the other object are known.

In the special case, when the first object is the laboratory coordinate system, the difference disappears because the handedness of this system is *a priori* known. Thus, in the first approach, only two spaces remain and, in the second, (mis)orientation automatically carries the information on the handedness of the second object.

The previous sections, where only proper rotations were considered, provide the full solution of the problem (of misorientation-angle and misorientation-axis distributions) in the sense of the first approach. With the second approach, the issue is more complex. The composition of two symmetries on both sides of a proper rotation is a proper rotation if both symmetries are proper or if they are improper. Besides the case when both symmetry groups contain inversion, *these two configurations are distinguishable* and, as such, can be treated separately from the viewpoint of texture analysis (see Fig. 3). From another viewpoint (of
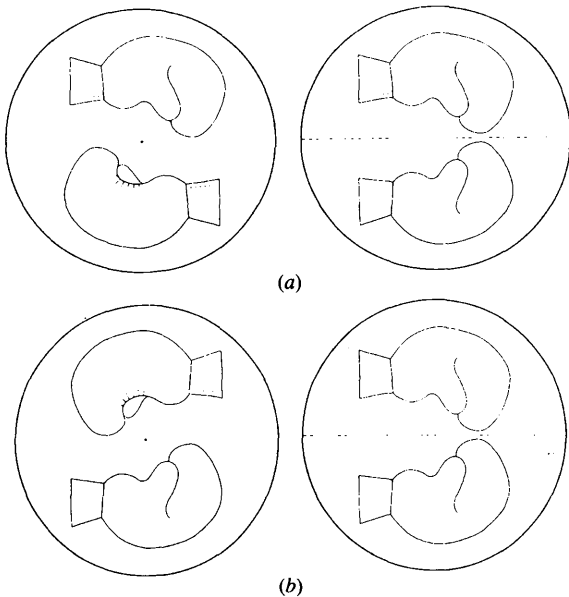

(a)

(b)

Fig. 3. The symmetries of the first object and the second one are C_i (inversion) and C_s (mirror plane), respectively. When both symmetry operations are applied, the initial configuration (a) is changed to the final one (b). The same result can be obtained by applying proper operation of rotation by π about an axis perpendicular to the mirror plane, which is equal to (inversion) $\circ$ (mirror plane). Although these two configurations are equivalent, one can be distinguished from the other: in (a) left gloves of both objects are related by simple translation, whereas in (b) this occurs for right gloves.

Table 2. *Groups P(G) and Q(G) corresponding to the crystallographic groups (G) containing improper symmetry operations*

For a group G without improper symmetry operations, there occurs $P(G) = Q(G) = G$. The relation $P(D_{3h}) = D_3^{(y)}$, where $D_3^{(y)}$ denotes D_3 with principal axis along z and twofold axis along y, appears in the first table because in *International Tables for X-ray Crystallography* (1952) the twofold axis of D_{3h} is fixed as vertical (y) whereas it is horizontal (x) for D_3.

G	C_s	S_4	C_{2v}	C_{3h}	C_{3v}	C_{4v}	D_{2d}	C_{6v}	D_{3h}	T_d
P(G)	C_1	C_2	C_2	C_3	C_3	C_4	D_2	C_6	$D_3^{(y)}$	T
Q(G)	C_2	C_4	D_2	C_6	D_3	D_4	D_4	D_6	D_6	O

G	C_i	C_{2h}	C_{3i}	C_{4h}	C_{6h}	D_{2h}	D_{3d}	D_{4h}	D_{6h}	T_h	O_h
P(G) = Q(G)	C_1	C_2	C_3	C_4	C_6	D_2	D_3	D_4	D_6	T	O

boundary properties, for example), however, these configurations are the same and this means that additional equivalences between rotations must be taken into account. This leads to new Voronoi tessellations and new asymmetric domains. Following the conventional approach, it is appropriate to consider the rotation angle only for proper rotations. Thus, in order to calculate the distributions of misorientation angles and distributions of corresponding rotation axes, only parts of the asymmetric domains contained inside the first component of the rotation manifold are needed. What considerably simplifies the task is that they can be described in a way similar to that used in the previous sections, *i.e.* by specifying $(G'_L, G'_R)/G_C$ with groups G'_L, G'_R and G_C containing only proper symmetry operations. This automatically gives the sought distributions and the forms of the domains can be deduced. The group on the right side of the slash (G_C) still determines equivalences between points with the same rotation angles but it does not represent the group of common symmetry operations any more.

Appropriate expressions will be listed below for the following separately considered cases:

(A) Both groups G_R and G_L contain only proper symmetry operations. There are no equivalences between points in different components of the rotation manifold and, thus, the asymmetric domain must consist of two parts; one part in each of the components. With the correspondence between proper and improper rotations established by the relation (improper rotation) = (proper rotation) $\circ$ (inversion), both components can be tessellated in the same way. The asymmetric domain can be obtained by choosing (as its part in each of the components) the same region as the domain for (G_L, G_R) in the previous section.

In all remaining cases, there are equivalences between points in different components and the asymmetric domain can be confined to the component of the identity.

Table 3. *Asymmetric domains of the pairs (G_L, G_R) for groups G_L and G_R containing improper symmetry operations but without inversion*

The diagonal entries of the table for $G_R = G = G_L$ would be given by $P(G)/Q(G)$, e.g., for (T_d, T_d), one would have $P(T_d)/Q(T_d) = T/O$. The symbol $C_2^{(\cdot)}$ denotes C_2 with rotation axis along $(\cdot)$ and $D_n^{(\cdot)}$ denotes D_n with principal axis along z and twofold axis along $(\cdot)$. The axis w is the bisector of the angle between x and y.

	T_d	D_{3h}	C_{6v}	D_{2d}	C_{4v}	C_{3v}	C_{3h}	C_{2v}	S_4
C_s	O	$D_3^{(y)}/C_2$	D_6	D_4	D_4	$D_3^{(y)}$	C_3/C_2	D_2	C_4
S_4	T/C_4	D_{12}	$D_6^{(w)}/C_2$	D_2/C_4	D_4/C_2	$D_6^{(w)}$	C_{12}	$D_2^{(w)}/C_2$	
C_{2v}	O/C_2	$D_6/C_2^{(x)}$	C_6/D_2	D_4/C_2	C_4/D_2	$C_6/C_2^{(x)}$	D_6		
C_{3h}	(C_3, O)	$D_3^{(y)}/C_6$	D_6/C_3	D_{12}	D_{12}	$D_3^{(y)}/C_3$			
C_{3v}	(C_3, O)	$D_3^{(y)}/D_3$	C_6/D_3	D_{12}	$C_{12}/C_2^{(x)}$				
C_{4v}	$O/D_2^{(w)}$	$D_{12}/C_2^{(x)}$	C_{12}/D_2	$D_4/D_2^{(w)}$					
D_{2d}	T/D_4	$D_{12}/C_2^{(y)}$	D_{12}/C_2						
C_{6v}	$(C_3, O)/C_2$	D_6/D_3							
D_{3h}	$(C_3, O)/C_2^{(y)}$								

(*B*) Only one of the groups contains improper symmetry operations. Let it be G_L. The distinguished points of the first component are obtained by composing proper symmetry operations of G_L with all elements of G_R. Therefore, the tessellation of the first component and, thus, the appropriate asymmetric domain are the same as the tessellation and the domain for $(P(G_L), G_R)$, where $P(G)$ is the subgroup of G consisting of proper rotations (Table 2).

(*C*) Both groups G_R and G_L contain inversion. Inversion commutes with all rotations and, thus, the configuration of objects obtained by applying improper symmetry operations on both sides of their misorientation can be obtained by applying some proper operations of the symmetry groups. The asymmetric domain is the same as that for $(P(G_L), P(G_R))$ from the previous section.

(*D*) Both groups G_R and G_L contain improper symmetry operations but only one of them, say G_L, contains inversion. The two resulting configurations of objects (first obtained by applying proper symmetry operations to both sides, second, by applying improper operations) are distinguishable (Fig. 3) but corresponding rotations are considered to be equivalent. To simplify the description of the asymmetric domain, let $I(G)$ denote a group generated from generators of G and inversion. Moreover, let $Q(G) = P(I(G))$ (Table 2). The asymmetric domain in the space of proper rotations is the same as the domain of $(P(G_L), Q(G_R))$ from the previous section.

With the sought distributions in mind, the contents of points (*A*)–(*D*) can be collected in a brief statement: if one of the groups (say G_R) contains only proper symmetry operations *or* one of them (G_L) contains inversion then the distributions of misorientation angles and corresponding axes for the pair (G_L, G_R) are the same as for $(P(G_L), Q(G_R))$.

(*E*) Both groups G_R and G_L contain improper symmetry operations but none of them contains inversion. Analogously to point (*D*), the application of proper symmetry operations to both sides of the proper rotation leads to a different configuration from the application of improper operations. As for the asymmetric domains, they must be determined separately for particular pairs because there is no simple relation to the results of the previous sections. As before, the subgroup diagram can be used to reduce the number of cases that should be considered. If the group G_L is a crystallographic subgroup of G_R, then there exists a setting in which all elements of G_L are common symmetry operations. In such a case, all distinguished points in the first component correspond to elements of $P(G_R)$, i.e. the asymmetric domain of the pair is part of the domain of $P(G_R)$. More precisely, it is given by $P(G_R)/Q(G_L)$. This approach has the disadvantage of forcing one to accept awkward settings for crystal coordinate systems. The results corresponding to the standard settings of the coordinate systems (*International Tables for X-ray Crystallography*, 1952) are given in Table 3.

As in the previous section, the sought distributions of misorientation angle and misorientation axis are fully determined by the pair or group given on the left side of the slash. The distributions for most of them are already known. The only complication appears when that group happens to be $D_n^{(\cdot)}$; in order to obtain the misorientation axis distribution q from that for D_n, the latter must be rotated around the z axis by the angle between $(\cdot)$ and the x axis. The misorientation-angle distribution in that case is the same as for D_n.

To close this article, it is worth mentioning that the case of indistinguishable objects has a third feature: the misorientation-angle and misorientation-axis distributions are determined by their proper symmetry operations regardless of the other elements of the complete symmetry group, i.e. it does not matter whether the group contains inversion or other improper rotations or it does not. It follows directly from the applicable points (*A*), (*C*) and (*E*).

APPENDIX A

Solid angle based on the common of three spherical caps

The solid angle S_3 based on the common of three spherical caps can be expressed as

$$S_3 = Q + \sum_{i=1}^{3} R_i - (T_i - T_i^0),$$

where T_i is the solid angle based on the ith cap, i.e. $T_i = S_1(\rho_i)$, Q is the solid angle corresponding to the hexagon $(O_1 P_3 O_2 P_1 O_3 P_2)$ with vertices at the centres of the caps and the outer cross points of the caps' edges (see Fig. 4), T_i^0 is the solid angle based on the part of the ith cap that is outside the hexagon; if ψ_i is the internal vertex angle of the hexagon at the centre of the ith cap, then $T_i^0 = [1 - \psi_i/(2\pi)]T_i$, R_i is the common one of caps with radii ρ_j and ρ_k, where $i \neq j \neq k \neq i$ $(i, j, k = 1, 2, 3)$ and, thus, $R_i = S_2(\rho_j, \rho_k; \xi_i)$.

Q is equal to the sum of solid angles based on the four spherical triangles $(O_1 P_3 O_2)$, $(O_2 P_1 O_3)$, $(O_3 P_2 O_1)$ and $(O_1 O_2 O_3)$, of which the hexagon is composed. For each spherical triangle, the solid angle is equal to the sum of its internal vertex angles minus π. The vertex angles, in turn, can be expressed through the side angles ρ_i and ξ_i
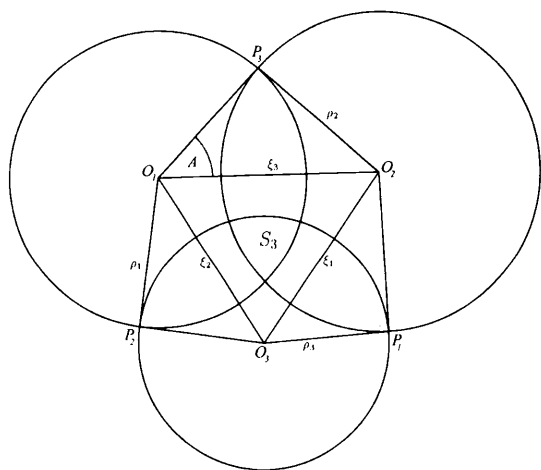

Fig. 4. Schematic diagram for the derivative of S_3.

using the cosine theorem of spherical geometry [e.g. $A = C(\rho_1, \xi_3; \rho_2)$]. Also, ψ_i is the sum of three such angles with a vertex at the centre of the ith cap. The final result reduces to the formula for $S_3(\rho_1, \rho_2, \rho_3; \xi_1, \xi_2, \xi_3)$ given in the main body of the paper.

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