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# A Unique Description of the Relative Orientation of Neighbouring Grains

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## Abstract

If $N$ denotes the number of symmetry rotations of a crystal lattice, the number, $n$, of different rotations connecting two orientations of this lattice is a multiple of $N$ and a factor of $2N^2$. Among these $n$ equivalent rotations those with minimum angle are considered. Usually one, but in exceptional cases two or three, of these has its axis in the standard stereographic triangle and is called a disorientation. How equivalent disorientations are connected by symmetry rotations and how the number, $n$, of equivalent rotations can be found for any disorientation are shown. Additional conditions for selecting a unique reduced rotation among the disorientations are proposed.

## Introduction

The relative orientations of neighbouring grains in a one-phase polycrystalline substance can be described by different rotations due to the point group of the grain. In determining experimentally (*e.g.* Chaudhari & Matthews, 1971) or theoretically (*e.g.* Warrington, 1974) the frequency with which relative orientations of neighbouring grains occur, it is necessary to choose a unique one among the several equivalent descriptions of the relative orientation, which we shall call the reduced rotation. A reduced rotation, therefore, represents a class of equivalent rotations. The number, $n$, of equivalent rotations is not the same for each class. We show how $n$ can be determined. This number is needed for investigations of special relative orientations of neighbouring grains of the type initiated by Warrington (1974, 1975; Warrington & Boon, 1975).

The reduced rotations and the numbers of equivalent rotations have been determined for the cubic holohedry by Grimmer (1974). The present paper extends these results to all seven holohedries. It needs further extensions in two directions: the determination of 'standard' distributions and the extension from holohedral to arbitrary point groups.

The simplest assumption about the distribution of the relative orientations of neighbouring grains is that they are completely accidental, which gives rise to 'standard' probability distributions to which measured frequency distributions can be compared. The standard probability distribution of the disorientation angle has been determined for the cubic holohedry by Handscomb (1958) and by Mackenzie (1958) and for the remaining holohedries by Grimmer (1979). The standard probability distribution of the rotation axis has been determined by Mackenzie (1964) for the cubic holohedry.

The extension of the results in the present paper and in Grimmer (1979) from the holohedral to arbitrary point groups is in progress.

The connection between our work and the well-known texture analysis of Bunge (1969) is as follows: Bunge investigates the orientation of the grains with respect to the piece of material in which they are contained. He, therefore, combines the point group of the grain with the symmetry of the piece. We are interested in the relative orientation of neighbouring grains and combine the point groups of the two neighbours.

The notions of 'reduced rotation' and of 'disorientation' are closely connected. Every reduced rotation is a disorientation, *i.e.* a minimum angle rotation about an axis in a standard stereographic triangle. However, there are some disorientations that are not reduced rotations. Representing rotations by angles less than $\pi$ in the usual way by points in the interior of a sphere with radius $\pi$, the disorientations form a closed connected subset $\mathscr{D}$ of the sphere. The set of reduced rotations, called an 'asymmetric unit', contains all the interior points of $\mathscr{D}$ but not all the points on its surface. The number, $n$, of equivalent rotations is the same for each class represented by a point in the interior, but is often lower for classes represented by a surface point.

## 1. Equivalent rotations and disorientations

The relative orientation of two congruent crystal lattices, 1 and 2, can be described by different rotations. If **R** is a rotation that maps lattice 1 onto lattice 2, we can carry out a symmetry rotation of lattice 1 before and a symmetry rotation of lattice 2 afterwards, and we can exchange the roles of lattices 1

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and 2. **R** and **R′** are therefore called *hexagonally* (or *tetragonally*, ...) *equivalent* if the hexagonal (or tetragonal, ...) holohedry contains two rotations **S** and **T** such that

$$\mathbf{R}' = \mathbf{SRT} \quad \text{or} \quad \mathbf{R}' = \mathbf{SR}^{-1}\mathbf{T}. \tag{1}$$

This definition thus generalizes the cubic equivalence introduced by Grimmer (1974). Let $N$ be the number of symmetry rotations of the lattice. We show in the Appendix that the number, $n$, of different equivalent rotations is always a multiple of $N$ and a factor of $2N^2$. Therefore, we can write $n$ as

$$n = 2N^2/M, \tag{2}$$

where $M$ is a factor of $2N$. Table 1 lists the possible values of $M$.

We shall see later that there exist equivalence classes with $n = 2N^2/M$ different rotations for all the values of $M$ in Table 1 except those between brackets; for example, there are hexagonal equivalence classes with 288, 144, 72, 36, 24, and 12 different rotations. $M = 1$, *i.e.* $n = 2N^2$ for most equivalence classes whereas, for the class consisting of the symmetry rotations, $M$ has the maximum value, *i.e.* $M = 2N$ and $n = N$.

For each holohedry we shall define a '*standard stereographic triangle*' (SST), which comprises $1/2N$ of the full solid angle. For each rotation angle that occurs in an equivalence class, this class contains at least one rotation with this angle that acts in the positive sense around an axis in (the interior or on the boundary of) the SST. The minimum-angle rotations in the positive sense around an axis in the SST are called *disorientations*.

To picture the sets of disorientations for the different holohedries (Figs. 2, 5, 7), we shall use the following representation of the set of rotations: with each rotation we associate a point, the radius vector of which corresponds in direction to axis and sense and in length to the angle $\theta$ of the rotation. In this way we obtain a one-to-one correspondence between rotations with angles less than 180° and points in the interior of a full solid sphere, and between rotations with angle 180°

Table 1. *The number, $N$, of rotations in the holohedry, the maximum number, $2N^2$, of equivalent rotations and the factors, $M$, of $2N$*

Except for the values of $M$ within brackets there exist equivalence classes with n = $2N^2/M$ different rotations

| Crystal system | $N$ | $2N^2$ | $M$ |
|---|---|---|---|
| Triclinic | 1 | 2 | 1 2 |
| Monoclinic | 2 | 8 | 1 2 4 |
| Orthorhombic | 4 | 32 | 1 2 4 8 |
| Rhombohedral | 6 | 72 | 1 2 (3) 4 6 12 |
| Tetragonal | 8 | 128 | 1 2 4 8 16 |
| Hexagonal | 12 | 288 | 1 2 (3) 4 (6) 8 12 24 |
| Cubic | 24 | 1152 | 1 2 (3) 4 6 8 12 16 (24) 48 |

and pairs of diametrically opposed points on the surface of the sphere. Let $\mathscr{D}$ be the closed subset of the solid sphere that corresponds to the disorientations.

Consider the point $P$ representing a disorientation the angle $\theta$ of which is not maximal, $\theta < \theta_m$, *i.e.* there exist (inequivalent!) disorientations with the same axis but larger angle. The number of rotations in the corresponding equivalence class is proportional to the solid angle under which $\mathscr{D}$ appears from $P$. (In the case of several equivalent disorientations, we have to take the sum of the corresponding solid angles.) For example, each equivalence class represented by an interior point of $\mathscr{D}$ contains the maximum number of $2N^2$ equivalent rotations; the equivalence class represented by the origin contains $1/2N$ times the maximum number, namely the $N$ symmetry rotations.*

Our representation of the set of rotations not being conformal, the connection between solid angle and number of equivalent rotations breaks down for $\theta = \theta_m$. In Figs. 3, 5 and 7, which show schematically the maximum angle surface of the set of disorientations, we shall therefore indicate also the number $M$ ($M$ times the number of different inequivalent rotations equals $2N^2$).

To determine the rotations that are equivalent, we shall represent rotations by pairs of quaternions. They are defined with respect to an orthogonal coordinate system: if $\xi$, $\eta$ and $\zeta$ denote the angles between the rotation axis and the $x$, $y$, and $z$ axes of our orthogonal coordinate system, the pair of quaternions that corresponds to a rotation with angle $\theta$ is

$$\pm[\cos\tfrac{1}{2}\theta, \cos\xi\sin\tfrac{1}{2}\theta, \cos\eta\sin\tfrac{1}{2}\theta, \cos\zeta\sin\tfrac{1}{2}\theta]. \tag{3}$$

This representation has the following advantages.

(*a*) *Continuity.* Neighbouring rotations are always described by neighbouring quaternion pairs and *vice versa*.

(*b*) *Ease of interpretation.* Axis and angle of the rotation can immediately be read off the quaternion: $[a,b,c,d]$ denotes a rotation, the angle of which is given by the first component

$$\theta = 2\arccos|a|,$$

and the axis by the three remaining components

$$(b^2+c^2+d^2)^{-1/2}(b,c,d)\ [=(1-a^2)^{-1/2}(b,c,d)].$$

The rotation is right-handed if $a \geq 0$, left-handed if $a \leq 0$.

(*c*) *Convenience of notation and of multiplying rotations.* Compared with the usual matrix representation of rotations, quaternions are somewhat simpler

* The number of rotations with $\Sigma = 11$ given in Table 1 of Warrington (1974) and in Table 2 of Warrington & Boon (1975) should be 288 instead of 300. (Notice that $\Sigma = 13$, 17, 19, 21 and 25 correspond to two equivalence classes each.) In each of the cases 17*b*, 19*b*, and 23*c* of Table II in Warrington (1975), the number of equivalent rotations is 144.

to write and to multiply: matrix multiplication gets replaced by quaternion multiplication.

$$[a,b,c,d][a',b',c',d'] = [aa' - bb' - cc' - dd',\; ab' + ba' + cd' - dc',\; ac' - bd' + ca' + db',\; ad' + bc' - cb' + da'].$$

(*d*) *Ease of recognizing equivalent rotations.* We shall see that, looking at two quaternion pairs, it is easy to decide whether or not they correspond to equivalent rotations.

## 2. Hexagonal lattice

### 2.1. *Hexagonally equivalent quaternions*

We choose the $z$ axis of the orthogonal coordinate system parallel to the sixfold symmetry axis and the $x$ axis parallel to a twofold symmetry axis of the lattice. The group of hexagonal symmetry rotations is generated by the 60° rotation about the $z$ axis ($\pm[\frac{1}{2}\sqrt{3}, 0, 0, \frac{1}{2}]$) and the 180° rotation about the $x$ axis ($\pm[0,1,0,0]$). Computing all the quaternions that are hexagonally equivalent to $\pm[a,b,c,d]$, we find that they are obtained as follows. Let pair 1 be one of the six pairs of numbers in Fig. 1 and pair 2 one of the three pairs connected by a line to pair 1. As the first component of the quaternion, let us choose either the inner or the outer number of pair 1. The second component is then respectively the inner or the outer number of pair 2, the third component the other number of pair 2, and the fourth component the other number of pair 1, *e.g.* $[\frac{1}{2}(d+\sqrt{3}a), c, b, \frac{1}{2}(a-\sqrt{3}d)]$. We obtain in this way $6\times 3\times 2$ quaternions that are all different if all the 12 numbers in Fig. 1 are different. All the quaternions that are *hexagonally equivalent* to $[a,b,c,d]$ are obtained by arbitrary sign changes of the components in these 36 quaternions. If the absolute values of all the 12 numbers in Fig. 1 are different, then none of them will be 0 and we obtain $36\times 16 = 576$ different quaternions, which are all hexagonally equivalent, and correspond to 288 hexagonally equivalent rotations.

### 2.2. *Disorientations*

As a representative of the equivalence class, let us choose a quaternion all the components of which are non-negative and with first component equal to the largest among the absolute values of the 12 numbers in Fig. 1. Let us call one of these quaternions

$$[\alpha, \beta, \gamma, \delta]. \tag{4}$$

Two other such quaternions are

$$[\alpha, \tfrac{1}{2}(\beta+\sqrt{3}\gamma), \tfrac{1}{2}|\gamma-\sqrt{3}\beta|, \delta] \tag{5}$$

and

$$[\alpha, \tfrac{1}{2}|\beta-\sqrt{3}\gamma|, \tfrac{1}{2}(\gamma+\sqrt{3}\beta), \delta]. \tag{6}$$

$b \geq \sqrt{3}c$ is satisfied by (4) if $\beta \geq \sqrt{3}\gamma$, by (5) if $\beta \leq \sqrt{3}\gamma$, but never by (6). We may therefore require our representative to satisfy

$$a \geq \begin{cases} b \geq \sqrt{3}c \geq 0 & \\ d \geq 0 & \\ \frac{1}{2}(a+\sqrt{3}d) & \textit{i.e. } a \geq \sqrt{3}d \\ \frac{1}{2}|a-\sqrt{3}d| & [\leq \frac{1}{2}(a+\sqrt{3}d)] \\ \frac{1}{2}(d+\sqrt{3}a) & \textit{i.e. } a \geq (2+\sqrt{3})d \\ \frac{1}{2}|d-\sqrt{3}a| & [\leq \frac{1}{2}(d+\sqrt{3}a)] \\ \frac{1}{2}(b+\sqrt{3}c) & (\leq b) \\ \frac{1}{2}|b-\sqrt{3}c| & [\leq \frac{1}{2}(b+\sqrt{3}c)] \\ \frac{1}{2}(c+\sqrt{3}b) & \\ \frac{1}{2}|c-\sqrt{3}b| & [\leq \frac{1}{2}(c+\sqrt{3}b)] \end{cases}, \tag{7}$$

*i.e.*

$$a \geq \begin{cases} b \geq \sqrt{3}c \geq 0 \\ \frac{1}{2}(\sqrt{3}b+c) \\ (2+\sqrt{3})d \geq 0. \end{cases} \tag{8}$$

Our choice in (8) of a quaternion with first component as large as possible and with the other three components satisfying certain restrictions corresponds to choosing a rotation with minimum rotation angle and rotation axis in a certain stereographic triangle, which we shall call the *standard stereographic triangle* (SST). Such rotations will be called *disorientations*.

Although (8) does depend on our choice of an orthogonal coordinate system, Fig. 2 no longer depends

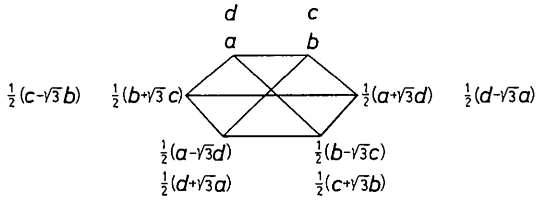


Fig. 1. The components of hexagonally equivalent quaternions.

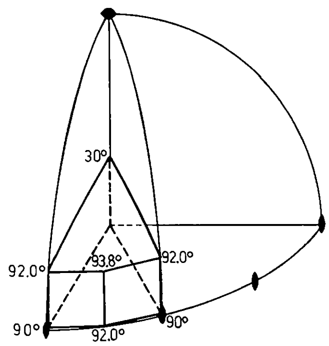


Fig. 2. The set of disorientations, *i.e.* of rotations defined by (8). Each rotation is hexagonally equivalent to a rotation in this set.

Table 2. *Connection between equivalent disorientations*

Disorientations with $\theta = \theta_m$ are equivalent if they lie symmetrically with respect to one of the planes determined by the pairs of directions given in column 1; column 2 shows how the equivalent disorientations are connected by symmetry rotations.

| Pair of directions | Connection between equivalent disorientations |
|---|---|
| $[2+\sqrt{3}, 1, 1]$ and $[1,0,0]$ | $\pm[0,0,0,1]\,[a,a,c,d]\,[0,0,1,0] = \pm[a,a,d,c]$ |
| $[2+\sqrt{3}, 1, 1]$ and $[\sqrt{3}, 1, 0]$ | $\pm[0,\frac{1}{2},-\frac{1}{2}\sqrt{3},0]\,[a, b, 2a-\sqrt{3}b, d]\,[0,0,0,1]$ $= \pm[a, \frac{1}{2}(\sqrt{3}a+d), \frac{1}{2}(a-\sqrt{3}d), 2b-\sqrt{3}a]$ |
| $[2+\sqrt{3}, 1, 1]$ and $[0,0,1]$ | $\pm[0,\frac{1}{2}\sqrt{3},\frac{1}{2},0]\,[a, b, c, (2-\sqrt{3})a]\,[0,1,0,0]$ $= \pm[a, \frac{1}{2}(\sqrt{3}b+c), \frac{1}{2}(b-\sqrt{3}c), (2-\sqrt{3})a]$ |

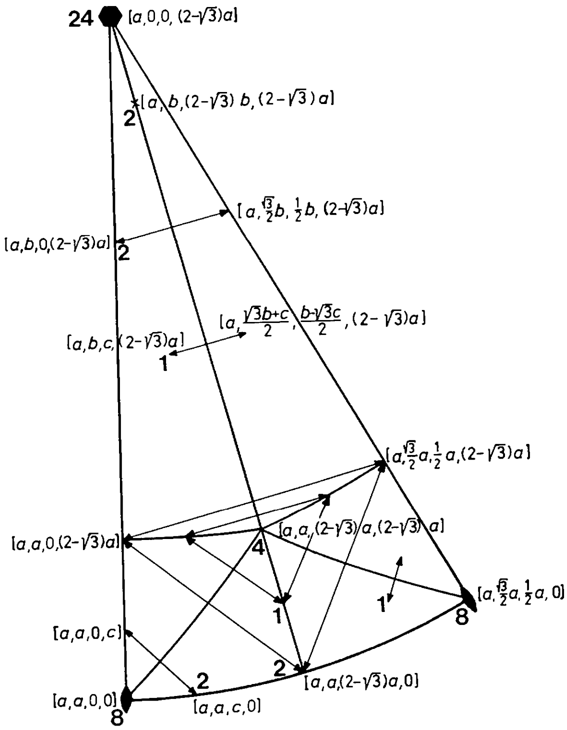


Fig. 3. The maximum angle surface of the set of disorientations. Equivalent disorientations are connected by arrows. A number $M$ indicates that there are $288/M$ rotations ($576/M$ quaternions) in the equivalence class.

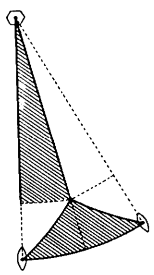

Fig. 4. The hatched areas indicate the reduced rotations in the maximum angle surface of the set of disorientations.

on it because we did not indicate the position of the $x$, $y$, and $z$ axes in this figure. [Without changing our choice of an orthogonal coordinate system we could have chosen, instead of (8), other restrictions corresponding to a set congruent to the one shown in Fig. 2 but lying in another of the 24 stereographic triangles into which the sphere is divided by the mirror planes of the hexagonal holohedry.]

### 2.3. *Reduced rotations*

Consider a disorientation with $\theta < \theta_m$. The corresponding quaternion with positive first component satisfies (8) with $a >$ instead of $a \geq$. It follows that this disorientation is the only one in its equivalence class. However, if $\theta = \theta_m$ there may be several equivalent disorientations. The situation is illustrated in Fig. 3, which shows schematically the maximum angle surface of the set of disorientations.

Table 2 shows how equivalent disorientations are connected by symmetry rotations.

We conclude from Fig. 3 that we arrive at a unique representative of each equivalence class, if we supplement (8) as follows:

$$\begin{aligned} &\text{if} \quad a = b, && \text{then} \quad c \geq d; \\ &\text{if} \quad a = \tfrac{1}{2}(\sqrt{3}b + c), && \text{then} \quad \tfrac{1}{2}(b - \sqrt{3}c) \geq d; \\ &\text{if} \quad a = (2+\sqrt{3})d, && \text{then} \quad b \geq (2+\sqrt{3})c. \end{aligned} \tag{9}$$

The rotations that correspond to quaternions satisfying (8), (9) will be called *reduced rotations*. Each disorientation with $\theta < \theta_m$ is a reduced rotation, the disorientations with $\theta = \theta_m$ that are reduced rotations are shown in Fig. 4.

## 3. Non-hexagonal lattices

With a method analogous to that used for the hexagonal lattice, results were derived also for the lattices of other symmetry. The tetragonal and orthorhombic cases turned out to be most similar to the

Table 3. *Choice of an orthogonal coordinate system, equivalent quaternions and definition of the disorientations for orthogonal, tetragonal and cubic holohedry*

| Holohedry | Orthorhombic | Tetragonal | Cubic |
|---|---|---|---|
| Choice of<br>$z$ axis parallel to<br>$x$ axis parallel to | <br>twofold axis<br>twofold axis | <br>fourfold axis<br>twofold axis | <br>fourfold axis<br>fourfold axis |
| Equivalent quaternions are obtained by arbitrary sign changes of the four components in the quaternions obtained from | $[a,b,c,d]$<br>by the permutations<br>(1)<br>(12) (34)<br>(13) (24)<br>(14) (23)<br>(*i.e.*<br>$[a,b,c,d]$<br>$[b,a,d,c]$<br>$[c,d,a,b]$<br>$[d,c,b,a]$) | $[a,b,c,d]$<br>$2^{-1/2}[a+d, b+c, b-c, a-d]$<br>by the permutations<br>(1)<br>(12) (34)<br>(13) (24)<br>(14) (23)<br>(14)<br>(23)<br>(1342)<br>(1243) | $[a,b,c,d]$<br>$2^{-1/2}[a+b, a-b, c+d, c-d]$<br>$2^{-1/2}[a+c, a-c, b+d, b-d]$<br>$2^{-1/2}[a+d, a-d, b+c, b-c]$<br>$\frac{1}{2}[a+b+c+d, a+b-c-d,$<br>$a-b+c-d, a-b-c+d]$<br>$\frac{1}{2}[a+b+c-d, a+b-c+d,$<br>$a-b+c+d, a-b-c-d]$<br><br>by all 24 permutations |
| Conditions for disorientation | $a \geq \begin{cases} b \geq 0 \\ c \geq 0 \\ d \geq 0 \end{cases}$ | $a \geq \begin{cases} b \geq c \geq 0 \\ 2^{-1/2}(b+c) \\ (\sqrt{2}+1)d \geq 0 \end{cases}$ | $a \geq \begin{cases} (\sqrt{2}+1)b \\ b+c+d \end{cases}$<br>$b \geq c \geq d \geq 0$ |

Table 4. *Connection between equivalent disorientations*

Disorientations with $\theta = \theta_m$ are equivalent if they lie symmetrically with respect to one of the planes determined by the pairs of directions given in column 2; column 3 shows how the equivalent disorientations are connected by symmetry rotations.

| Holohedry | Pair of directions | Connection between equivalent disorientations |
|---|---|---|
| Orthorhombic | [1,1,1] and [1,0,0] | $\pm[0,0,0,1]\,[a,a,c,d]\,[0,0,1,0] = \pm[a,a,d,c]$ |
| | [1,1,1] and [0,1,0] | $\pm[0,1,0,0]\,[a,b,a,d]\,[0,0,0,1] = \pm[a,d,a,b]$ |
| | [1,1,1] and [0,0,1] | $\pm[0,0,1,0]\,[a,b,c,a]\,[0,1,0,0] = \pm[a,c,b,a]$ |
| Tetragonal | $[\sqrt{2}+1, 1, 1]$ and [1,0,0] | $\pm[0,0,0,1]\,[a,a,c,d]\,[0,0,1,0] = \pm[a,a,d,c]$ |
| | $[\sqrt{2}+1, 1, 1]$ and [1,1,0] | $\pm 2^{-1/2}[0,1,-1,0]\,[a, b, \sqrt{2}a-b, d]\,[0,0,0,1]$<br>$= \pm[a, 2^{-1/2}(a+d), 2^{-1/2}(a-d), \sqrt{2}b-a]$ |
| | $[\sqrt{2}+1, 1, 1]$ and [0,0,1] | $\pm 2^{-1/2}[0,1,1,0]\,[a, b, c, (\sqrt{2}-1)a]\,[0,1,0,0]$<br>$= \pm[a, 2^{-1/2}(b+c), 2^{-1/2}(b-c), (\sqrt{2}-1)a]$ |
| Cubic | $[1, 1, \sqrt{2}-1]$ and [1,0,0] | $\pm 2^{-1/2}[0,0,1,1]\,[a, (\sqrt{2}-1)a, c, d]\,[0,0,1,0]$<br>$= \pm[a, (\sqrt{2}-1)a, 2^{-1/2}(c+d), 2^{-1/2}(c-d)]$ |

hexagonal one. The cubic case, which has been described by Grimmer (1974), is included here for comparison.

### 3.1. *Orthorhombic, tetragonal and cubic lattices*

The results for orthogonal, tetragonal and cubic holohedry are shown in Table 3.

Fig. 5 tells us that, as in the hexagonal case, disorientations can also in the orthorhombic, tetragonal and cubic cases be equivalent only if $\theta = \theta_m$, *i.e.* if they lie in the maximum angle surface. Table 4 shows how the equivalent disorientations are connected by symmetry rotations.

We obtain a unique reduced rotation if we supplement the conditions for disorientations (Table 3) by the conditions given in Fig. 6.

### 3.2. *Triclinic, monoclinic and rhombohedral lattices*

The results for triclinic, monoclinic and rhombohedral holohedry are shown in Table 5.

Fig. 7 shows that in contrast to the previous cases there are now equivalent disorientations that do not lie in the maximum angle surface. In the triclinic system they lie in the plane separating the rotations that are disorientations from those that are not, for which we chose the plane $z=0$. The rotations in this plane consist of pairs of equivalent disorientations lying symmetrically with respect to the origin. The two rotations of each pair are connected by $\mathbf{R}_2 = \mathbf{R}_1^{-1}$.

In the monoclinic and rhombohedral systems equivalent disorientations in the maximum angle surface are connected by 90° rotations about the twofold axis. This connection can be expressed with symmetry rotations as $\mathbf{R}_2 = \mathbf{R}_1^{-1}\mathbf{S}_x$. Finally, consider the plane normal to the threefold axis in the rhombohedral case, a plane containing the twofold axis in the monoclinic case, for which we chose the plane $z = 0$. Equivalent disorientations in these planes lie symmetrically with respect to the twofold axis and are connected by symmetry rotations as follows:

$$\mathbf{R}_2 = \mathbf{S}_x\mathbf{R}_1\mathbf{S}_x,$$

*i.e.* $\pm[0, 1, 0, 0][a, b, c, 0][0, 1, 0, 0] = \pm[a, b, -c, 0]$.

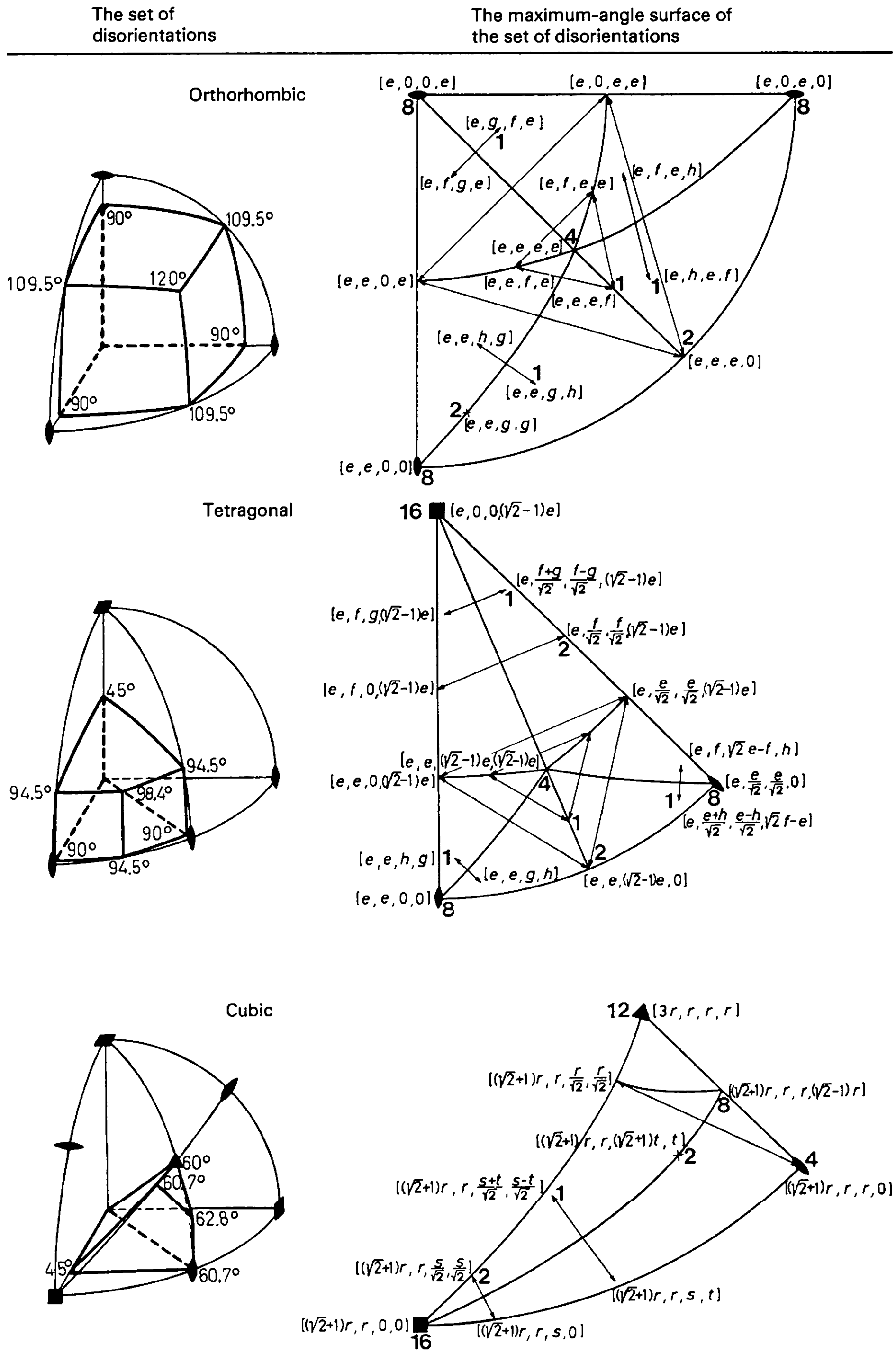


Fig. 5. Disorientations for orthorhombic, tetragonal and cubic holohedry.

We obtain a unique reduced rotation if we supplement the conditions for disorientations (Table 5) by the conditions given in Fig. 8.

| Holohedry | Orthorhombic | Tetragonal | Cubic |
|---|---|---|---|
| Supplementary conditions | If $a = b$, then $c \geq d$<br>If $a = c$, then $b \geq d$<br>If $a = d$, then $b \geq c$ | If $a = b$, then $c \geq d$<br>If $\sqrt{2}a = b + c$, then $b - c \geq \sqrt{2}d$<br>If $a = (\sqrt{2} + 1)d$, then $b \geq (\sqrt{2} + 1)c$ | If $a = (\sqrt{2} + 1)b$, then $c \leq (\sqrt{2} + 1)d$ |
| Reduced rotations in the maximum angle surface | | | |

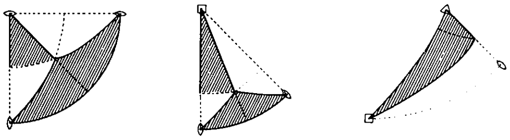

Fig. 6. Reduced rotations for orthorhombic, tetragonal and cubic holohedry. The hatched areas indicate the reduced rotations in the maximum angle surface of the set of disorientations.

| Holohedry | Triclinic | Monoclinic | Rhombohedral |
|---|---|---|---|
| Supplementary conditions | If $d = 0$, then $c > 0$, or ($c = 0$ and $b \geq 0$). | If $a = b$ and $d > 0$, then $c > 0$. If $d = 0$, then $c \geq 0$. | If $a = b$ and $d > 0$, then $c > 0$. If $d = 0$, then $c \geq 0$. |
| Reduced rotations in the maximum angle surface | | | |
| Reduced rotations in the surface '$z = 0$' | | | |

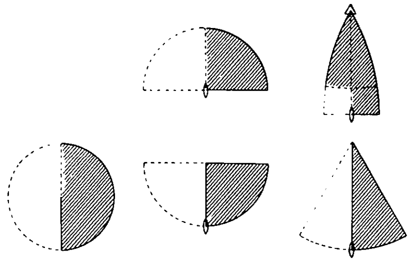

Fig. 8. Reduced rotations for triclinic, monoclinic, and rhombohedral holohedry. The hatched areas indicate the reduced rotations in the maximum angle and the '$z = 0$' surfaces of the set of disorientations.

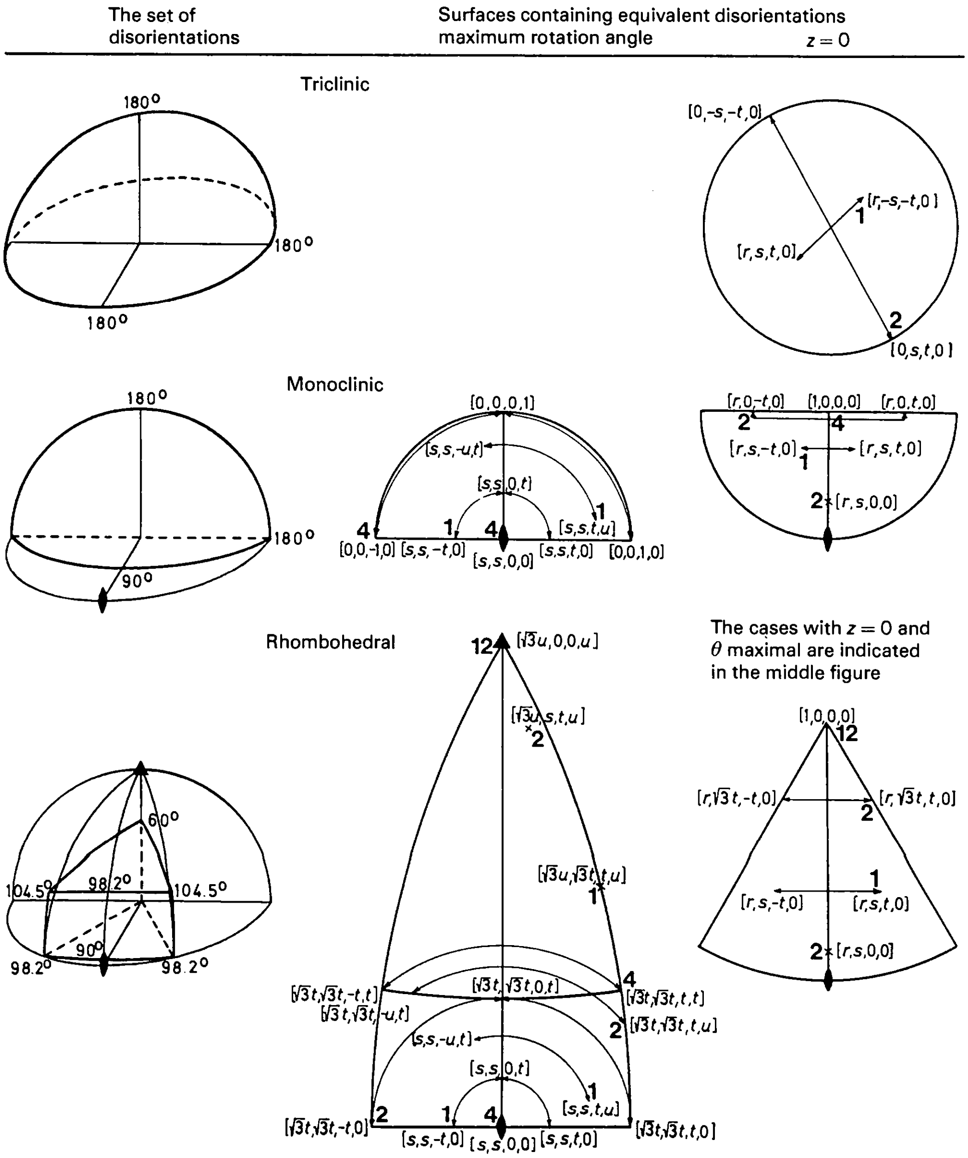


Fig. 7. Disorientations for triclinic, monoclinic and rhombohedral holohedry.

Table 5. *Choice of an orthogonal coordinate system, equivalent quaternions and definition of the disorientations for triclinic, monoclinic and rhombohedral holohedry*

| Holohedry | Triclinic | Monoclinic | Rhombohedral |
|---|---|---|---|
| Choice of | | | |
| $z$ axis parallel to | | | threefold axis |
| $x$ axis parallel to | | twofold axis | twofold axis |
| Equivalent quaternions are obtained by arbitrarily combining the following transformations | | | |
| Arbitrary sign changes in components | 1 | 1, 2 | 1, 2 |
| Simultaneous sign changes in components | 2, 3 and 4 | 3 and 4 | 3 and 4 |
| The following permutation combined with a sign change | | $\begin{pmatrix} a & b & c & d \\ b & a & d & -c \end{pmatrix}$ | $\begin{pmatrix} a & b & c & d \\ b & a & d & -c \end{pmatrix}$ |
| applied to | $[a,b,c,d]$ | $[a,b,c,d]$ | $[a,b,c,d]$<br>$[a, \frac{1}{2}(b + \sqrt{3}c), \frac{1}{2}(-c + \sqrt{3}b), d]$<br>$[a, \frac{1}{2}(b - \sqrt{3}c), \frac{1}{2}(-c - \sqrt{3}b), d]$<br>$[b, \frac{1}{2}(a + \sqrt{3}d), \frac{1}{2}(d - \sqrt{3}a), c]$<br>$[b, \frac{1}{2}(a - \sqrt{3}d), \frac{1}{2}(d + \sqrt{3}a), c]$<br>$\frac{1}{2}[a + \sqrt{3}d, b - \sqrt{3}c, c + \sqrt{3}b, d - \sqrt{3}a]$<br>$\frac{1}{2}[a - \sqrt{3}d, b + \sqrt{3}c, c - \sqrt{3}b, d + \sqrt{3}a]$<br>$\frac{1}{2}[a + \sqrt{3}d, b + \sqrt{3}c, c - \sqrt{3}b, d - \sqrt{3}a]$<br>$\frac{1}{2}[a - \sqrt{3}d, b - \sqrt{3}c, c + \sqrt{3}b, d + \sqrt{3}a]$ |
| Conditions for disorientation | $a \geq 0$<br>$d \geq 0$ | $a \geq b \geq 0$<br>$d \geq 0$ | $a \geq \begin{cases} b \geq \sqrt{3}\lvert c \rvert \\ \sqrt{3}d \geq 0 \end{cases}$ |

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## APPENDIX

The aim of this Appendix is to prove that the number of different equivalent rotations is a multiple of the number, $N$, of symmetry rotations of the lattice and a factor of $2N^2$.

We saw that if $\mathbf{R}$ is a rotation that maps a lattice 1 onto a congruent lattice 2, the relative orientation of these two lattices can be described also by the rotation that we obtain by preceding $\mathbf{R}$ with a symmetry rotation of lattice 1 and following it with a symmetry rotation of lattice 2, and by exchanging the roles of lattices 1 and 2. Mathematically speaking, we associate with each crystal system a group $\mathscr{G}$ of automorphisms of the three-dimensional rotation group $SO_3$. The automorphism $\{\mathbf{S}, \mathbf{U}, \mathbf{T}\} \in \mathscr{G}$ acts as follows on $SO_3$:

$$\{\mathbf{S}, \mathbf{U}, \mathbf{T}\}\mathbf{R} = \mathbf{S}\ \mathbf{U}(\mathbf{R})\ \mathbf{T},$$

where $\mathbf{S}$ and $\mathbf{T}$ are elements of the group $\mathscr{H}$ of symmetry rotations of the lattice and $\mathbf{U}$ is either $\mathbf{U}_+$ or $\mathbf{U}_-$ defined by $\mathbf{U}_+(\mathbf{R}) = \mathbf{R}$ and $\mathbf{U}_-(\mathbf{R}) = \mathbf{R}^{-1}$. Two rotations, $\mathbf{R}$ and $\mathbf{R}'$, have been called equivalent if there exists an element $g \in \mathscr{G}$ such that $\mathbf{R}' = g(\mathbf{R})$. $\mathscr{G}$ has $2N^2$ elements, where $N$ denotes the number of elements in $\mathscr{H}$. The elements of $\mathscr{G}$ that leave a chosen rotation $\mathbf{R}$ invariant form a subgroup $\mathscr{G}'$ of $\mathscr{G}$. Let $M$ be the number of elements in $\mathscr{G}'$. The number of rotations equivalent to $\mathbf{R}$ is thus

$$n = 2N^2/M.$$

From the fact that for each choice of $\mathbf{U}$, $\mathbf{T}$ and $\mathbf{R}$ the $N$ rotations $\{\mathbf{S}, \mathbf{U}, \mathbf{T}\}\mathbf{R}$ with $\mathbf{S} \in \mathscr{H}$ are different, it follows that $2N^2/M$ is a multiple of $N$, which completes the proof.

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