

supported by the oscillation picture showing 500 and 500 in Fig. 13.

No attempt will be made in this paper to give a full theoretical interpretation of the various diffraction phenomena. Obviously this is impossible as long as the correct diffraction condition has not been realized, which can only be done either by changing the wavelength of the monochromatic radiation (valid in the cases of multiple diffraction $\bar{1}\bar{1}, 0, 2$, 703, 804, 304), or by varying the lattice constants (to be done for 500, 802). Consequently, completely new equipment is needed. On the other hand, it will be advisable to use strictly monochromatized and polarized radiation in order to simplify the influence of polarization, which has not been discussed here since it is unnecessary in those cases where the reflections involved belong to the same zone and all waves have the same plane of incidence.

Unfortunately, the indices of some of the planes relevant to secondary reflections are most probably incorrect in the previous short communication (Jagodzinski, 1978), since their intensities could not be checked on account of the data available. This difficulty arises from the inaccuracy of the diffraction condition for reflections on other but the zero layer line, because of the large horizontal and vertical angles of aperture. This problem has to be solved with the aid of more precise diffraction geometry.

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Disorientation Between Any Two Lattices

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Abstract

The concept of disorientation, previously used for studying the statistical distribution of the relative orientation of identical cubic crystals, is defined in this work for any two lattices. Using the proposed definition, an algorithm is presented, allowing all the known relative orientations between the two lattices to be conveniently classed. As an example, a unified classification of the numerous mutual orientations of the Al and CuAl₂ crystals is suggested. The unit quaternion method used by Grimmer [*Acta Cryst.* (1974), **A30**, 685–688] for identical cubic lattices is here proved efficient for discussing the pair axis/angle disorientations in more complicated cases: cubic

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1/cubic 2; tetragonal 1/tetragonal 2; hexagonal 1/hexagonal 2; cubic/tetragonal; cubic/orthorhombic and cubic/hexagonal. The general expressions of equivalent quaternions are given for any point group of lattice 1 or lattice 2.

1. Introduction

In a preceding paper, Bonnet & Cousineau (1977) presented results concerning a numerical method used to find the relative orientations of two equal or different lattices 1 and 2, such that two small multiple cells *M*₁ and *M*₂ are coincident or near-coincident to within a small deformation. Their results were classified in

increasing order of the volumes of cells $M1$ and $M2$. The relative orientations given were those found by the numerical method.

In this work a unique and convenient description of these relative orientations is suggested so as to compare rapidly results of different origins. Handscomb (1958), Mackensie (1958) and later Grimmer (1974) treated this problem for the special case of cubic lattices with the aid of the disorientation concept. In particular, they found by different ways that a rotation $\leq 62.80^\circ$ is sufficient to superimpose two cubic lattices. Next, Warrington (1975) determined the standard stereographic triangle for the two identical hexagonal lattices having point group 622.

In this paper, the definition of the disorientation of a lattice 2 with respect to a fixed lattice 1 is extended to any system lattice 1/lattice 2. In accordance with this definition a computer program is proposed allowing the treatment of numerous data, for example the system Al/CuAl₂. Moreover, the method proposed by Grimmer (1974) to treat the cubic cases is systematically used in the computer program to derive the possible quaternions related to any two lattices. This method allows an upper limit for the rotation angles representing all the relative orientations between any two lattices to be determined. Results are presented for six different associations of cubic, tetragonal, hexagonal and orthorhombic lattices which are often encountered in practice.

2. The definition of disorientation

An orthonormal reference frame $F_i (i = 1, 2)$ is attached to each lattice 1 and 2. Hereafter, lattice 1 is fixed in space. By convention its Bravais cell is more symmetric than that of lattice 2 when the two lattices are of different species. Initially $F2$ is superposed on $F1$ (axes (Ox_1, Oy_1, Oz_1)), so that the two Bravais cells (vectors a_i, b_i, c_i) are such that

$$\begin{aligned} Ox_1 // a_i \\ Oz_1 // a_i \times b_i, \quad i = 1, 2. \end{aligned} \quad (1)$$

Lattice 2 is first rotated by an angle θ around an axis whose direction cosines in $F1$ are denoted α, β, γ . The corresponding rotation matrix in $F1$ is $[R]_{F1}$. This rotation describes, for instance, an experimental relative orientation of two crystal lattices. If the crystals are of different species this relative orientation is most often presented by the parallelism of lattice planes or lattice rows.

Let us now suppose that the frames $F1$ and $F2$ are rotated by all lattice symmetry rotations of lattices 1 and 2. These symmetry rotations are denoted by the matrices $[A_i]_{F1}$ ($i = 1, \dots, m$) and $[B_j]_{F2}$ ($j = 1, \dots, n$), respectively. The product mn represents the number of possible descriptions of the same situation provided

that the two lattices are differentiated. An elementary matrix calculation leads to the equivalent relative orientations of the new frame $F2$ with respect to the new frame $F1$. They are obtained here by the matrices R_{ij} such that

$$R_{ij} = [A_i]_{F1}^{-1} [R]_{F1} [B_j]_{F2}, \quad (2)$$

where $i = 1, \dots, m, j = 1, \dots, n$.

Since these rotations are global invariant operators, their real eigenvalues may be referred to a fixed orthonormal frame, here chosen to be $F1$ for simplicity. In $F1$, the rotation angles are denoted θ_{ij} and the direction cosines of the rotation axis $\alpha_{ij}, \beta_{ij}, \gamma_{ij}$. For all rotations R_{ij} the following relations are adopted by convention:

$$\left. \begin{aligned} -\pi < \theta_{ij} \leq \pi \\ \gamma_{ij} > 0 \end{aligned} \right\} \quad (3a)$$

$$\left. \begin{aligned} \text{or, if } \gamma_{ij} = 0, \quad \alpha_{ij} > 0 \\ \text{or, if } \gamma_{ij} = 0 \quad \text{and} \quad \alpha_{ij} = 0, \quad \beta_{ij} = 1 \end{aligned} \right\} \quad (3b)$$

Taking (3a) and (3b) into account, the disorientation is uniquely defined by the rotation R_{ij} (direction cosines

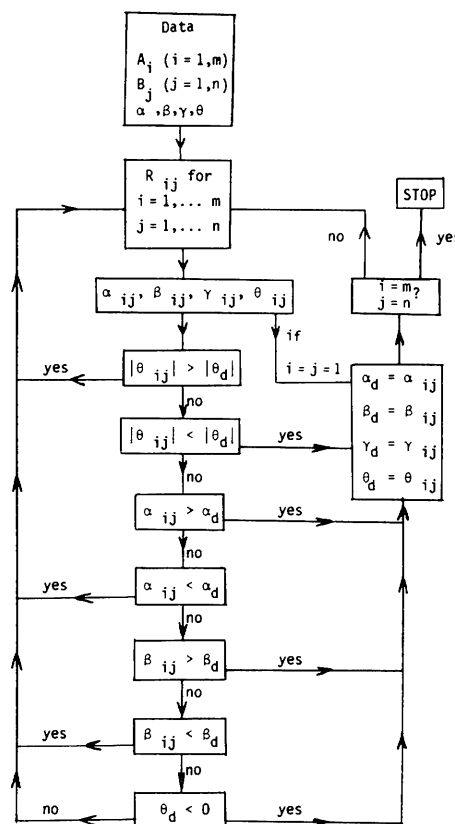


Fig. 1. Algorithm defining disorientation. Simplified flow chart of the computer program.

$\alpha_d = \alpha_{ij}$, $\beta_d = \beta_{ij}$, $\gamma_d = \gamma_{ij}$, rotation angle $\theta_d = \theta_{ij}$) having the following properties:

- (i) $|\theta_d|$ has the smallest possible value.
- (ii) Condition (i) being fulfilled, α_d has the greatest possible value.
- (iii) Condition (ii) being fulfilled, β_d has the greatest possible value.
- (iv) If conditions (i), (ii), (iii) are fulfilled for two rotations, the disorientation is that for which $\theta_d > 0$.
- (v) If the lattices are identical, lattices 1 and 2 can be interchanged. As a result θ_d is taken as $|\theta_d|$.

By using the above definition, a small computer program has been written in Fortran IV, the flow chart of which is presented in Fig. 1. The data can be introduced either by orientation relationships between lattice planes and lattice rows, or by rotation matrices $[R]_{F1}$, or by components $\alpha\theta$, $\beta\theta$, $\gamma\theta$ of the rotation vector.

3. A unified classification of the Al/CuAl₂ mutual orientations

The above computer program has been applied to the system Al/CuAl₂ for which mutual orientations are numerous. Since the review of Bonnet & Durand

(1972), several new mutual orientations have been observed (Bonnet, 1974; Kang & Laird, 1975). The latter concern mutual orientations of CuAl₂ precipitates growing on the surface of a solid solution of copper in Al.

Table 1 shows that all the disorientation angles are between -52.7 and 58.0° , the directions of the axes all being contained in the triangle $[100]$, $[110]$, $[001]$ of the frame $F1$ (Fig. 2). This property is demonstrated in the

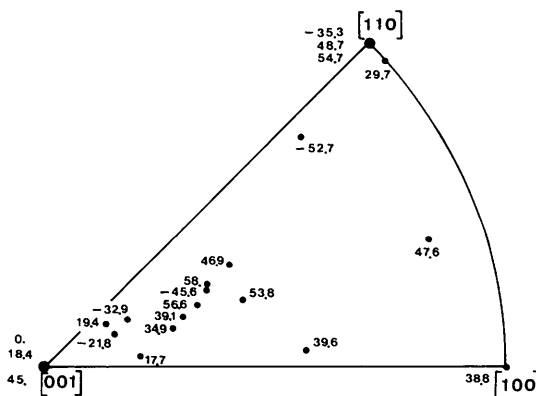


Fig. 2. The mutual orientations between Al and CuAl₂ reported as disorientations. The maximum disorientation angle is 58° .

Table 1. *The classification of the mutual orientations of Al and CuAl₂ in terms of disorientations*

Equivalent orientation relationships to those reported in the literature.							
Disorientation angle	Axis	Plane 1/Plane 2 row 1/row 2	References	Disorientation angle	Axis	Plane 1/Plane 2 row 1/row 2	References
-52.7	0.712	(111)//(211)	Vaughan & Silcock (1967)	38.8	1.	(001)//(011)	Heimendahl & Wassermann (1962)
	0.643	[011]//[120]	Davies & Hellowell (1970)		0.	[100]//[100]	Vaughan & Silcock (1967)
	0.280				0.		
-45.6	0.615	(021)//(211)	Vaughan & Silcock (1967)	0.546	(111)//(211)	Davies & Hellowell (1970)	
	0.297	[112]//[111]		0.200	[101]//[111]	Bonnet (1974)	
	0.731			0.814			
-35.3	0.714	(111)//(110)	Vaughan & Silcock (1967)	0.857	(131)//(011)	Vaughan & Silcock (1967)	
	0.700	[211]//[111]		0.049	[101]//[111]		
	0.003			0.513			
-32.9	0.342	(001)//(115)	Kang & Laird (1975)	0.	(001)//(001)	Guinier (1942)	
	0.196	[110]//[411]		0.	[010]//[110]	Takahashi (1960)	
	0.919			1.			
-21.8	0.296	(111)//(211)	Bonnet & Durand (1972)	0.664	(112)//(001)	Kang & Laird (1975)	
	0.138	[011]//[135]		0.372	[131]//[110]		
	0.945			0.649			
0	/	(001)//(001)	Ellwood & Bagley (1949)	0.939	(011)//(010)	Bonnet (1974)	
17.7	0.398	(111)//(121)	Davies & Hellowell (1970)	0.317	[111]//[101]	Kang & Laird (1975)	
	0.046	[011]//[135]	Bonnet & Durand (1972)	0.707	(001)//(111)		
	0.916			0.	[110]//[110]		
18.4	0.	(001)//(001)	Mehl, Barrett & Rhines (1932)	0.695	(001)//(011)	Vaughan & Silcock (1967)	
	0.	[310]//[100]	Guinier (1942)	0.239	[010]//[111]		
	1.			0.678			
19.4	0.259	(111)//(121)	Kraft & Albright (1962)	0.707	(112)//(110)	Kang & Laird (1975)	
	0.187	[110]//[210]	Davies & Hellowell (1970)	0.707	[111]//[001]		
	0.948			0.			
29.7	0.736	(111)//(121)	Lawson, Kerr & Lewis (1972)	0.590	(112)//(001)	Kang & Laird (1975)	
	0.677	[110]//[111]		0.244	[110]//[100]		
	0.011			0.769			
34.9	0.518	(111)//(211)	Bonnet & Durand (1972)	0.612	(111)//(211)	Davies & Hellowell (1970)	
	0.154	[011]//[113]		0.314	[110]//[011]	Proulx (1973)	
	0.842			0.726			

example of § 4.4. The new orientation relationships in column 3 of Table 1 are equivalent to those reported in the literature but are classified according to the disorientation definition.

4. Discussion on disorientation for any lattice 1/lattice 2. Examples

In order to discuss the disorientations between two identical cubic lattices, Grimmer (1974) used an elegant method requiring the properties of unit quaternions related to lattice rotations, in particular the multiplication law of unit quaternions (Du Val, 1964). This method has proved to be efficient in discussing the disorientation angle limits even in the more complicated cases treated here. In the following paragraph, a small number of typical expressions are derived for the unit quaternions representing all the equivalent rotations described above by (2).

4.1. Typical expressions of unit quaternions

Let us consider any two lattices, each having an initial orientation described by (1). Here, no rhombo-

hedral Bravais cells are used in order to write simply the quaternions related to symmetry rotations $[A_i]_{F1}$ and $[B_j]_{F2}$. Then, let us rotate lattice 2 by $[R]_{F1}$, the corresponding unit quaternion of which is denoted (a_0, a_1, a_2, a_3) , with

$$\begin{aligned} a_0 &= \cos \theta/2, & a_1 &= \alpha \sin \theta/2, \\ a_2 &= \beta \sin \theta/2, & a_3 &= \alpha \sin \theta/2. \end{aligned}$$

Combining two by two the symmetry elements of the two lattices by using the multiplication law of unit quaternions leads to the expressions for $m \times n$ equivalent quaternions. Their elements, linear functions of a_0, a_1, a_2, a_3 , are obtained by a small computer program. A careful observation of the listing provides all the typical expressions representing the $m \times n$ quaternions. Table 2 groups 24 typical expressions derived for the cases : cubic 1 (432)/cubic 2 (432) – expressions (5.1) to (5.6); hexagonal 1 (622)/hexagonal 2 (622) – expressions (5.1) and (5.7) to (5.14); and cubic (432)/hexagonal (622) – all expressions except (5.8) and (5.10) to (5.14). They are also available for any other combination of lattice 1/lattice 2 as shown in Table 3 because they also represent all the other com-

Table 2. Typical expressions of unit quaternions for any lattice 1/lattice 2

(a_0, a_1, a_2, a_3)	(5.1)
$2^{-1/2}(a_0 + a_1, a_1 - a_0, a_2 + a_3, a_3 - a_2)$	(5.2)
$2^{-1/2}(a_0 + a_2, a_1 - a_3, a_2 - a_0, a_1 + a_3)$	(5.3)
$2^{-1/2}(a_0 + a_3, a_1 + a_2, a_2 - a_1, a_3 - a_0)$	(5.4)
$2^{-1}(a_0 + a_1 + a_2 + a_3, a_1 + a_2 - a_0 - a_3, a_2 + a_3 - a_0 - a_1, a_1 + a_3 - a_0 - a_2)$	(5.5)
$2^{-1}(a_0 - a_1 - a_2 - a_3, a_2 - a_0 - a_1 - a_3, a_3 - a_0 - a_1 - a_2, a_0 + a_2 + a_3 - a_1)$	(5.6)
$2^{-1}(a_0 + a_3\sqrt{3}, a_2\sqrt{3} - a_1, -a_1\sqrt{3} - a_2, a_3 - a_0\sqrt{3})$	(5.7)
$2^{-1}(a_0 - a_3\sqrt{3}, a_2\sqrt{3} - a_1, -a_1\sqrt{3} - a_2, a_3 + a_0\sqrt{3})$	(5.8)
$2^{-1}(a_3 + a_0\sqrt{3}, a_2 - a_1\sqrt{3}, -a_1 - a_2\sqrt{3}, a_3\sqrt{3} - a_0)$	(5.9)
$2^{-1}(a_3 - a_0\sqrt{3}, a_2 - a_1\sqrt{3}, -a_1 - a_2\sqrt{3}, -a_3\sqrt{3} - a_0)$	(5.10)
$2^{-1}(2a_0, a_1 + a_2\sqrt{3}, a_2 - a_1\sqrt{3}, 2a_3)$	(5.11)
$2^{-1}(a_0 + a_3\sqrt{3}, -2a_1, -2a_2, a_3 - a_0\sqrt{3})$	(5.12)
$2^{-1}(a_0\sqrt{3} + a_3, 2a_2, -2a_1, -2a_0 + a_3\sqrt{3})$	(5.13)
$2^{-1}(2a_0, a_2\sqrt{3} - a_1, -a_1\sqrt{3} - a_2, 2a_3)$	(5.14)
$8^{-1/2}(a_0\sqrt{3} + a_1\sqrt{3} + a_2 - a_3, -a_0\sqrt{3} + a_1\sqrt{3} + a_2 + a_3, a_0 - a_1 + a_2\sqrt{3} + a_3\sqrt{3}, a_0 + a_1 - a_2\sqrt{3} + a_3\sqrt{3})$	(5.15)
$8^{-1/2}(a_0\sqrt{3} + a_1 + a_2\sqrt{3} + a_3, -a_0 - a_1\sqrt{3} + a_2 + a_3\sqrt{3}, -a_0\sqrt{3} + a_1 + a_2\sqrt{3} - a_3, a_0 - a_1\sqrt{3} + a_2 - a_3\sqrt{3})$	(5.16)
$8^{-1/2}(a_0\sqrt{3} + a_1\sqrt{3} - a_2 + a_3, -a_0\sqrt{3} + a_1\sqrt{3} - a_2 - a_3, a_0 - a_1 - a_2\sqrt{3} - a_3\sqrt{3}, a_0 + a_1 + a_2\sqrt{3} - a_3\sqrt{3})$	(5.17)
$8^{-1/2}(a_0 + a_1\sqrt{3} + a_2 + a_3\sqrt{3}, a_0\sqrt{3} + a_1 - a_2\sqrt{3} - a_3, -a_0 + a_1\sqrt{3} + a_2 - a_3\sqrt{3}, -a_0\sqrt{3} + a_1 - a_2\sqrt{3} + a_3)$	(5.18)
$2^{1/2}(pa_0 + qa_3, qa_1 + pa_2, -pa_1 + qa_2, -qa_0 + pa_3)$	(5.19)
$2^{1/2}(pa_1 + qa_2, -qa_0 - pa_3, pa_0 - qa_3, -qa_1 + pa_2)$	(5.20)
$p(a_0 + a_2) + q(a_1 + a_3), p(a_2 - a_0) + q(a_1 - a_3), p(a_3 - a_1) + q(a_2 - a_0), p(a_1 + a_3) + q(-a_0 - a_2)$	(5.21)
$p(a_1 + a_3) + q(a_0 + a_2), p(a_3 - a_1) + q(a_0 - a_2), p(a_2 - a_0) + q(a_3 - a_1), p(a_0 + a_2) + q(-a_1 - a_3)$	(5.22)
$p(a_0 + a_1) + q(a_2 - a_3), p(a_2 + a_3) + q(a_0 - a_1), p(a_1 - a_0) + q(a_2 + a_3), p(a_2 - a_3) + q(-a_0 - a_1)$	(5.23)
$p(a_2 - a_3) + q(a_0 + a_1), p(a_0 - a_1) + q(a_2 + a_3), p(a_2 + a_3) + q(a_1 - a_0), p(-a_0 - a_1) + q(a_2 - a_3)$	(5.24)

binations of point groups $[A_i]$, $[B_j]$. For the last six expressions, the values p and q are $(\sqrt{3} + 1)/4$ and $(\sqrt{3} - 1)/4$, respectively.

The problem is now to describe, from these typical expressions, all the set of $m \times n$ equivalent quaternions. Let us denote more generally (a_0, a_1, a_2, a_3) one of the 24 typical expressions of Table 2. Arbitrary permutations and sign changes of the four elements define a set of unit quaternions for which the general expression is*

$$(\varepsilon_i a_i, \varepsilon_j a_j, \varepsilon_k a_k, \varepsilon_l a_l), \quad (4)$$

where $\varepsilon_i, \varepsilon_j, \varepsilon_k, \varepsilon_l = \pm 1$, the subscripts i, j, k, l being any number among 0, 1, 2, 3. Depending on the combination of the point groups $[A_i]$, $[B_j]$, the number of permutations and sign changes representing the equivalent rotations R_{ij} are determined by two rules. These rules are presented in Table 4 for the above six examples with the aid of parameters defined below.

* In this expression, there is no summation over terms of the form $\varepsilon_i a_i$.

Table 3. Lattice 1/lattice 2 combinations related to quaternions of Table 2

lattice 2 \ lattice 1	cubic	tetragonal	orthorhombic	hexagonal	monoclinic	triclinic
cubic	X	X	X	X	X	X
tetragonal		X	X	X	X	X
orthorhombic			X	X	X	X
hexagonal				X	X	X
monoclinic					X	X
triclinic						X

Table 4. Expressions of the permutation and sign rules applying to the typical expressions listed in Table 2

The point groups of the lattices are in brackets in the first column.

lattice 1/lattice 2	typical expressions	permutation rule	sign rule
cubic 1/cubic 2 (432)/(432)	5.1 to 5.6	—	
tetrag. 1/tetrag. 2 (422)/(422)	5.1 and 5.4	$i + l = 3$	$\varepsilon_i \varepsilon_j \varepsilon_k \varepsilon_l = (-1)^i \varepsilon_{jkl}$
hexag 1/hexag 2 (622)/(622)	5.1 5.7 to 5.14	$\varepsilon_{ijkl} = (-1)^{i+1}$	$\varepsilon_i \varepsilon_j \varepsilon_k \varepsilon_l = 1$
cubic/tetrag (432)/(422)	5.1 to 5.6	$i + l = 3$	$\varepsilon_i \varepsilon_j \varepsilon_k \varepsilon_l = (-1)^{l+1} \varepsilon_{jkl}$
cubic/ortho (432)/(222)	5.1 to 5.6		
cubic/hexag (432)/(622)	5.1 to 5.7, 5.9, 5.15 to 5.24	$\varepsilon_{ijkl} = (-1)^i$	$\varepsilon_i \varepsilon_j \varepsilon_k \varepsilon_l = 1$

4.2. Permutation rule

The permutation rule is sometimes simple. For instance, if

$$i + l = 3, \quad (5)$$

the allowed permutations are

$$(a_0, a_1, a_2, a_3), (a_3, a_1, a_2, a_0), (a_1, a_0, a_3, a_2), (a_2, a_0, a_3, a_1), \\ (a_0, a_2, a_1, a_3), (a_3, a_2, a_1, a_0), (a_1, a_3, a_0, a_2), (a_2, a_3, a_0, a_1).$$

In some cases, the permutation rule is expressed by using a parameter ε_{ijkl} for which the whole set of possible subscripts (i, j, k, l) is defined by circular permutations from $(0, 1, 2, 3)$ or $(0, 3, 2, 1)$. In the former case $\varepsilon_{ijkl} = +1$, in the latter case $\varepsilon_{ijkl} = -1$ (see Fig. 3). For instance, the permutation rule

$$\varepsilon_{ijkl} = (-1)^{l+1} \quad (6)$$

allows four permutations:

$$(a_0, a_1, a_2, a_3); (a_2, a_3, a_0, a_1); \\ (a_1, a_0, a_3, a_2); (a_3, a_2, a_1, a_0).$$

4.3. Sign rule

For each permutation of (a_0, a_1, a_2, a_3) , the final subscripts i, j, k, l in (4) are known. The allowed values for $\varepsilon_i, \varepsilon_j, \varepsilon_k, \varepsilon_l$ are now determined either by (Table 4)

$$\varepsilon_i \varepsilon_j \varepsilon_k \varepsilon_l = 1 \quad (7)$$

or by an expression depending on a parameter ε_{ijk} . This parameter is equal to ± 1 according to a positive or negative reading sequence of the subscripts ijk around the circle in Fig. 3, with i, j, k equal to 0, 1, 2 or 3. Observation of the sign rules in Table 4 indicates that three out of four values of ε are independent.

Choosing $\varepsilon_i a_i \geq 0$, the sign of the rotation angle θ is determined from (3) and (4) by

$$\text{sign}(\varepsilon_i a_i) \quad \text{if} \quad a_i a_i \neq 0, \\ \text{sign}(\varepsilon_j a_j) \quad \text{if} \quad a_i = 0, \quad a_i \neq 0, \quad a_j \neq 0, \quad (8) \\ \text{sign}(\varepsilon_k a_k) \quad \text{if} \quad a_i = 0, \quad a_j = 0, \quad a_i \neq 0,$$

also

$$\theta = \pi \quad \text{if} \quad a_i = 0.$$

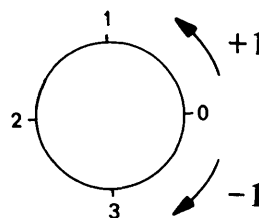


Fig. 3. The variables ε_{jkl} and ε_{ijkl} are equal to ± 1 according to the reading sequence of the indices jkl or $ijkl$ around the circle.

4.4. Stereographic standard triangle (SST) and disorientation. Example

Combining the general definition of disorientation given in § 2 and the results of Table 4 allows, for each of the six examples treated, the determination of:

(i) the area of the stereographic projection inside which the disorientation axis $[\alpha, \beta, \gamma]$ is defined. This area defines in turn a stereographic standard triangle referred to the frame $F1$ (Fig. 4*a, b, c, d*);

(ii) some inequalities, denoted 'disorientation inequalities' in Table 5, subdivided into two sets. These two sets are differentiated by the presence of a sign + or - before a_1, a_2, a_3 . Here, a_0 is taken to be positive. The interest of these inequalities is that if a quaternion (a_0, a_1, a_2, a_3) completely verifies one of these two sets, it is the disorientation quaternion;

(iii) the upper limits of $|\theta_d|$ corresponding to a rotation axis lying in the SST. These limits, determined by each disorientation inequality, apply in definite domains of the SST, denoted I, II, III, IV, V in Table 5. Fig. 4(*a, b, c, d*) shows the boundaries of each domain. The poles A, B, C, D, E, F, G , related to cubic/hexagonal lattices, correspond to the irrational directions: $A[u, 0, v]$; $B[u, v(1 + \sqrt{2}), v]$; $C[v(\sqrt{2} - 1), u, v]$; $D[0, u, v]$; $E[u, v\sqrt{2}, 0]$; $F[1/\sqrt{2}, 1/\sqrt{2}, 0]$; $G[v\sqrt{2}, u, 0]$; where $u = (\sqrt{2} - 1)(\sqrt{3} - 1)$ and $v = 2\sqrt{2} - \sqrt{3} - 1$.

As an example, the case cubic (432)/tetragonal (422) is now briefly presented. Let us now write the quaternions equivalent to the quaternion (a_0, a_1, a_2, a_3) , each having $a_0 \geq 0$ as first term. From the permutation and sign rules, they are: (a_0, a_1, a_2, a_3) ; $(a_0, -a_1, -a_2, a_3)$;

Table 5. Inequalities related to disorientation: limits of the disorientation angle versus the direction cosines $[\alpha, \beta, \gamma]$ of the disorientation axis

lattice-1/lattice 2	disorientation inequalities	upper limit of $ \text{tg}(\theta_d/2) $	maxi. disor.
cubic 1/cubic 2 (432)/(432)	I $a_0 \geq 2^{-1/2} (a_0 \pm a_1)$	$(\sqrt{2} - 1)/\alpha$	$(1, 1, \sqrt{2} - 1)$
	II $a_0 \geq 2^{-1} (a_0 \pm a_1 \pm a_2 \pm a_3)$	$1/(\alpha + \beta + \gamma)$	$ \theta_d = 62.80^\circ$
tetra.1/tetra.2 (422)/(422)	I $a_0 \geq \pm a_1$	$1/\alpha$	$(1, \sqrt{2}-1, \sqrt{2}-1)$
	II $a_0 \geq 2^{-1/2} (a_0 \pm a_3)$	$2/(\alpha + \beta)$	
	III $a_0 \geq 2^{-1/2} (\pm a_1 \pm a_2)$	$(\sqrt{2} - 1)/\gamma$	$ \theta_d = 98.42^\circ$
hexa.1/hexa. 2 (622)/(622)	I $a_0 \geq \pm a_1$	$1/\alpha$	$(1, 2-\sqrt{3}, 2-\sqrt{3})$
	II $a_0 \geq 2^{-1} (a_0 \sqrt{3} \pm a_3)$	$(2 - \sqrt{3})/\gamma$	
	III $a_0 \geq 2^{-1} (\pm a_1 \sqrt{3} \pm a_2)$	$2/(\alpha\sqrt{3} + \beta)$	$ \theta_d = 93.84^\circ$
cubic /tetra (432)/(422)	I $a_0 \geq 2^{-1/2} (a_0 \pm a_1)$	$(\sqrt{2} - 1)/\alpha$	$(1, 1, \sqrt{2} - 1)$ or
	II $a_0 \geq 2^{-1} (a_0 \pm a_1 \pm a_2 \pm a_3)$	$1/(\alpha + \beta + \gamma)$	$(1, \sqrt{2} - 1, 1)$
	III $a_0 \geq 2^{-1/2} (a_0 \pm a_3)$	$(\sqrt{2} - 1)/\gamma$	$ \theta_d = 62.80^\circ$
cubic/ortho. (432)/(222)	I $a_0 \geq 2^{-1/2} (a_0 \pm a_1)$	$(\sqrt{2} - 1)/\alpha$	$(1, 1, \sqrt{2} - 1)$ or
	II $a_0 \geq 2^{-1} (a_0 \pm a_1 \pm a_2 \pm a_3)$	$1/(\alpha + \beta + \gamma)$	$(1, \sqrt{2} - 1, 1)$ or
	III $a_0 \geq 2^{-1/2} (a_0 \pm a_3)$	$(\sqrt{2} - 1)/\gamma$	$(\sqrt{2} - 1, 1, 1)$
	IV $a_0 \geq 2^{-1/2} (a_0 \pm a_2)$	$(\sqrt{2} - 1)/\beta$	$ \theta_d = 62.80^\circ$
cubic/hexag. (432)/(622)	I $a_0 \geq 2^{-1/2} (a_0 \pm a_1)$	$(\sqrt{2} - 1)/\alpha$	$(1 + \sqrt{6} - \sqrt{2} - \sqrt{3},$
	II $a_0 \geq 2^{-1/2} (a_0 \pm a_2)$	$(\sqrt{2} - 1)/\beta$	$3 - \sqrt{6} + \sqrt{2} - \sqrt{3},$
	III $a_0 \geq 2^{1/2} (p a_0 \pm q a_3)$	$(2\sqrt{2} - \sqrt{3} - 1)/(\sqrt{3} - 1)\gamma$	$-1 - \sqrt{3} + 2\sqrt{2})$
	IV $a_0 \geq p(a_0 \pm a_2) \pm q(a_1 + a_3)$	$(3 - \sqrt{3})/[(\sqrt{3} - 1)(\alpha + \gamma) + \beta(\sqrt{3} + 1)]$	$ \theta_d = 56.60^\circ$
	V $a_0 \geq p(a_0 \pm a_1) \pm q(a_2 - a_3)$	$(3 + \sqrt{3})/[(\sqrt{3} - 1)(\beta - \gamma) + \alpha(\sqrt{3} + 1)]$	

$(a_0, a_1, -a_2, -a_3)$; $(a_0, -a_1, a_2, -a_3)$; (a_0, a_2, a_1, a_3) ; $(a_0, -a_2, -a_1, a_3)$; $(a_0, a_2, -a_1, -a_3)$; $(a_0, -a_2, a_1, -a_3)$. By using a stereographic projection it can be easily shown that one and only one of the eight above quaternions has a related rotation axis $[\alpha, \beta, \gamma]$ such that $\gamma \geq 0$ and $\alpha \geq \beta \geq 0$, the rotation angle θ being positive or negative. If the term a_0 of this latter quaternion hereafter supposed to be (a_0, a_1, a_2, a_3) is greater than all the terms of typical expressions (5.1) to (5.6), Table 2, it is deduced that this quaternion describes disorientation according to the definition of § 2. These latter conditions are expressed by the disorientation inequalities,

Table 5. The sign + or - in these inequalities depends only on the sign of θ_d , positive or negative. When one inequality becomes strictly an equality, it defines the limits of $|\theta_d|$. $|\theta_d|$ maximal is found on the limits of domains I, II, III.

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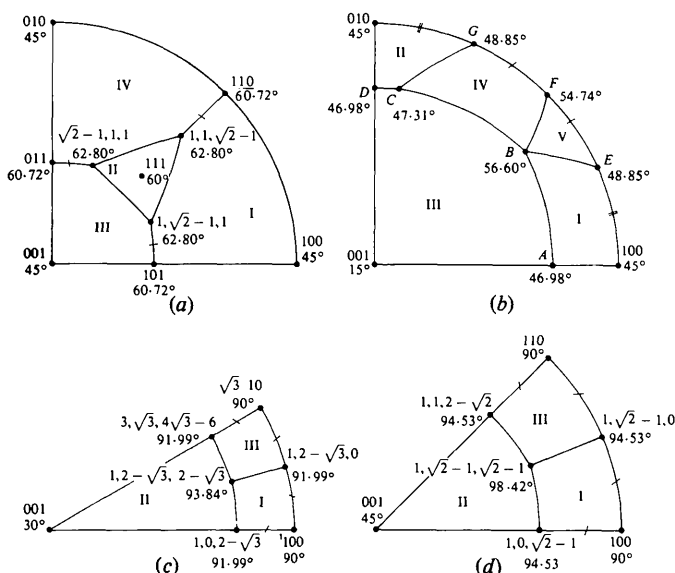


Fig. 4. Standard stereographic triangles with domains of maximum disorientation angles $|\theta_d|$. (a) cubic 1/cubic 2 [100, 110, 111], cubic/tetragonal: [100, 110, 001], cubic/orthorhombic [100, 010, 001], (b) cubic/hexagonal, (c) hexagonal 1/hexagonal 2, (d) tetragonal 1/tetragonal 2. Equal angular spacings are slashed / or //.

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On the Space Group of Spinel, $MgAl_2O_4$

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Abstract

The controversial space-group problem of spinel, $MgAl_2O_4$, whether it is $Fd\bar{3}m$ or $F43m$, was studied by electron diffraction. It was confirmed that the ap-

pearance of 'forbidden reflections' such as $\{200\}$ was caused by the double reflection process of reflections with high indices on the non-zero-order Laue zone. Consequently, the space group of spinel is $Fd\bar{3}m$, and the assignment of the space group to $F43m$ is ruled out.