5. Concluding remarks

Ambiguity in some of the structure-factor values can, in its turn, lead to ambiguous values of the function of electron-density distribution calculated as the sum (1). In this case the most representative (*i.e.* giving the least r.m.s. error) is the 'mean' synthesis (2) which is the general form of the best synthesis of Blow & Crick (1959). However, the possible deviation from the mean may vary for different points in the unit cell and is characterized by r.m.s. error σ_r.

Formulas (8)-(10) estimate the individual values σ_r for the case when the errors in the structure factors are regarded as independent and their spread is known. [This spread is characterized by A_s and B_s in (3)]. The values σ_r are closely related to Harker peaks at weighted Patterson syntheses. The derived formulas may be used by various approaches where knowledge of individual values ρ_r is required.

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Coincidence Orientations of Grains in Rhombohedral Materials

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Abstract

In experimental investigations and computer simulations of the structure and properties of grain boundaries, the results are usually discussed with reference to the special case of coincidence boundaries, where the two neighbouring grains have a three-dimensional lattice of symmetry translations in common. For historical reasons this lattice is called the coincidence site lattice or CSL. A systematic determination of CSL's for the case of grains with a lattice of rhombohedral Bravais type is presented. It is shown that a number of investigations of the structure of grain boundaries in alumina (α-Al_2O_3) have to be reinterpreted in the light of the present results. A central result is the Σ-rhomb theorem, which expresses the ratio Σ of unit-cell volumes of the CSL and the rhombohedral crystal lattice in terms of four integral parameters that describe the axis and angle of the rotation connecting the rhombohedral lattices of the two neighbouring grains and in terms of their axial ratio c/a. Two types of coincidence rotations, *i.e.* of rotations generating CSL's, may be distinguished, *viz* common rotations, which generate CSL's with the same Σ for every value of c/a, and specific rotations, which generate CSL's with a low value of Σ only for a few values of the axial ratio. The Σ-rhomb theorem makes it possible to determine systematically not only all common rotations with Σ up to a given maximum value Σ_c but also all specific rotations with $\Sigma \le \Sigma_c$ and with c/a in any given interval about the experimental value of c/a for the material in question. It is shown that the multiplicities of the CSL's generated by a given rotation in a hexagonal and in a rhombohedral lattice with the same value of c/a differ by at most a factor 3.

1. Introduction

Metals and ceramics are used in polycrystalline form for most of their applications. The boundaries between the crystallites often control mechanical and corrosion properties of the materials to a large extent. For this reason, great efforts are taken in the production and heat treatment of modern engineering materials to optimize the size of the grains and the impurity content of the boundaries between them as well as the distribution of additional phases. Significant improvements have been obtained in this way, *e.g.* in the toughness and strength of steels or in the tensile strength of ceramics.

Boundaries between regions with the same crystal structure will be considered in the present work. They will be called *grain boundaries* and include the special case of twin boundaries.

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A polycrystal has a higher energy than a single crystal with the same mass. The additional energy per unit area of a grain boundary depends on the relative orientation of the two neighbouring grains and on the orientation of the boundary. Brandon, Ralph, Ranganathan & Wald (1964) observed preferred orientations in cubic metals and interpreted them with the so-called coincidence-site-lattice model. The original formulation of this model is obtained by imagining the two neighbouring lattices continued across the interface. The points that are then common to both lattices form the *coincidence site lattice* (CSL). If a large fraction of the points of one of the two lattices consists of coincidence sites and if the interface coincides with a densely occupied net plane of the CSL, then the model predicts a minimum of the interfacial energy per unit area.

Consider two crystal lattices that have a CSL in common. After a translation of one of the lattices there will be either no points left in coincidence or the points in coincidence will form a lattice which differs from the old CSL at most by a translation. The translations that do not destroy the coincidence sites form another lattice, called the *displacement shift complete* or DSC lattice, introduced by Bollmann (1970, 1982). This lattice is of an importance similar to that of the CSL for the discussion of grain boundaries, as will be shown below.

Computer simulations of grain boundaries have shown that certain translations that destroy the coincidence sites will reduce the interfacial energy in many cases (Vitek, Sutton, Smith & Pond, 1980). This has been confirmed experimentally, *e.g.* by high-resolution electron microscopy (Ichinose & Ishida, 1985). Therefore one no longer defines the coincidence site lattice, despite its name, as a point lattice but as a lattice of translations. It consists of the symmetry translations that are common to the lattices of the two neighbouring grains. *The term 'lattice' will be used in the following in the sense of 'translation lattice'. The CSL may be defined as the finest lattice contained in both crystal lattices*; *the DSC lattice as the coarsest lattice that contains both crystal lattices.* The CSL determined by the two crystal lattices is reciprocal to the DSC lattice determined by the reciprocal crystal lattices (Grimmer, 1974). This is true for two arbitrary crystal lattices that have a one-, two- or three-dimensional CSL in common. If the two lattices are congruent, then one lattice can be transformed into the other by means of a rotation. This rotation will be called a *coincidence rotation* if the two lattices have a three-dimensional CSL in common. In the following, attention will be restricted to congruent lattices and three-dimensional CSL's. The volume ratio of primitive cells for the CSL and the crystal lattice is then always a positive integer Σ, called the *multiplicity* of the CSL, Whereas the cell volume of the CSL is Σ times larger than the cell volume V of the crystal lattice, the cell volume of the DSC lattice is Σ times smaller than V (Bonnet & Durand, 1975). The vectors of the DSC lattice are the geometrically possible Burgers vectors of dislocations in the grain boundary (Hirth & Balluffi, 1973). These Burgers vectors are DSC vectors of small length as a result of energy considerations.

If the crystal lattice can be characterized by an axial ratio c/a, *i.e.* if the lattice belongs to one of the Bravais classes *tP*, *tI*, *hP* or *hR*, one can distinguish between common and specific coincidence rotations according to whether the rotation generates a CSL for all or only for discrete values of c/a. Periodic nets of dislocations have often been observed experimentally in the boundary plane if the rotation which maps the (translation) lattice of one crystal onto the other is close to a coincidence rotation with a small value of Σ, either of the common type or of the specific type with c/a close to the experimental value. It is energetically favourable in these cases to maintain the atomic arrangement of an ideal coincidence boundary locally and to compensate the required shift of atoms with a periodic array of grain boundary dislocations. A review of early observations of such arrays in cubic crystals has been given by Balluffi, Komem & Schober (1972). More recently, periodic arrays of grain boundary dislocations have been observed also in hexagonal (Hagège, Nouet & Delavignette, 1980) and rhombohedral (Lartigue & Priester, 1984) materials.

Computer simulations of minimum-energy boundaries showed that the atoms at grain boundaries sit at the corners of simple polyhedra, called 'structural units' (Vitek *et al.*, 1980). The representation of the boundary structure often becomes particularly simple for coincidence boundaries with low values of Σ (Sutton & Vitek, 1983). It can be shown that the description of the boundary by structural units is equivalent to the description by grain boundary dislocations (Bishop & Chalmers, 1968; Brokman & Balluffi, 1981).

The determination of all possible coincidence orientations with low values of Σ is therefore an important basis for the investigation of grain boundaries. Systematic methods to find these orientations have been developed for cubic lattices (Acton & Bevis, 1971; Pumphrey & Bowkett, 1971; Fortes, 1972; Grimmer, Bollmann & Warrington, 1974; Mykura, 1980). Analogous results have been obtained also for tetragonal (Erochine & Nouet, 1983) and hexagonal lattices for fixed values of c/a (Warrington, 1975; Bonnet, Cousineau & Warrington, 1981; Bleris, Nouet, Hagège & Delavignette, 1982; Grimmer & Warrington, 1985).

In the case of lattices that can be characterized by c/a, one is interested in the common coincidence rotations as well as the specific rotations in an approximately 2% wide interval centred around the experimental value of c/a. The present work gives a systematic method for determining all coincidence rotations of rhombohedral lattices with c/a in a given interval and with multiplicity Σ up to a given maximum value Σ_c. Similar results have been obtained also for hexagonal lattices (Grimmer, 1989).

The present work starts by giving the form of the rotation matrix in rhombohedral lattice coordinates for an arbitrary rotation. These coordinates are suitable for the derivation of the conditions which the rotation must satisfy in order to generate a CSL of given multiplicity. The coincidence rotations may be characterized by a quadruple consisting of four integers without common divisor, of which three are proportional to the direction cosines of the rotation axis and the fourth is needed in addition to determine the rotation angle. A central result is the Σ-rhomb theorem, which gives Σ in terms of the quadruple and the axial ratio of the lattice.

It is convenient for the investigations that follow to characterize planes by their Miller–Bravais indices and directions by their Weber indices. The Σ-rhomb theorem is reformulated in terms of these indices and it is shown how the well known results on the multiplicity of coincidence rotations for the primitive, body-centred and face-centred cubic lattices follow from it as special cases.

The rotations that describe the relative orientation of two rhombohedral crystal lattices can be grouped into equivalence classes due to the trigonal symmetry of these lattices. Such a class can contain up to 72 different rotations. Computer programs have been developed which determine the classes of common rotations with multiplicity Σ less or equal to a given value Σ_c as well as the classes of specific rotations with $\Sigma \le \Sigma_c$ and c/a in a given interval.

Subsequently it is shown how the previous lack of a method to determine these classes systematically has influenced recent work on the interpretation of TEM images of grain boundaries in α-alumina.

The final section contains a proof that the multiplicity of the CSL's generated by the same rotation in a hexagonal and in a rhombohedral lattice with the same value of c/a differ by at most a factor of 3.

2. Rotations in rhombohedral coordinates, rhombohedrally equivalent rotations

2.1. *The rotation matrix in rhombohedral lattice coordinates*

Consider a basis defined by three vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ of equal length L with equal angles α between them and which span a primitive cell of the rhombohedral lattice. Define τ by

$$\tau = (\cos\alpha)/(1+2\cos\alpha) \tag{1}$$

i.e.

$$\cos\alpha = \tau/(1-2\tau). \tag{2}$$

Table 1. *Parameter values for the special cases of cubic lattices and for the limiting cases of linearly dependent vectors* $\mathbf{e}_1$, $\mathbf{e}_2$ *and* $\mathbf{e}_3$

	τ	c/a	$\cos\alpha$	α(°)
$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ parallel	1/3	∞	1	0
Face-centred cubic (f.c.c.)	1/4	$\sqrt{6}$	1/2	60
Primitive cubic (p.c.)	0	$\sqrt{3/2}$	0	90
Body-centred cubic (b.c.c.)	−1	$\sqrt{3/8}$	−1/3	109·47
$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ coplanar	$-\infty$	0	−1/2	120

A rotation with angle $\Theta = 2\theta$ and axis $\mathbf{n} = [n_1, n_2, n_3]$ normed to length $L/(1-2\tau)^{1/2}$ is given by the matrix

$$R = \begin{pmatrix} C^2+(1-2\tau)(X^2-Y^2-Z^2)+2\tau(CY-CZ-YZ) & 2[\tau X(Z+X-C)-(1-\tau)CZ+(1-2\tau)XY] & 2[\tau X(X+Y+C)+(1-\tau)CY+(1-2\tau)ZX] \\ 2[\tau Y(Y+Z+C)+(1-\tau)CZ+(1-2\tau)XY] & C^2+(1-2\tau)(Y^2-Z^2-X^2)+2\tau(CZ-CX-ZX) & 2[\tau Y(X+Y-C)-(1-\tau)CX+(1-2\tau)YZ] \\ 2[\tau Z(Y+Z-C)-(1-\tau)CY+(1-2\tau)ZX] & 2[\tau Z(Z+X+C)+(1-\tau)CX+(1-2\tau)YZ] & C^2+(1-2\tau)(Z^2-X^2-Y^2)+2\tau(CX-CY-XY) \end{pmatrix}, \tag{3}$$

where

$$(C, X, Y, Z) = \pm(\cos\theta, n_1\sin\theta, n_2\sin\theta, n_3\sin\theta). \tag{4}$$

The parameters $\pm(C, X, Y, Z)$, which (together with τ) determine R, will be called a (rhombohedral) quadruple. They satisfy the normalization condition

$$C^2+(1-2\tau)(X^2+Y^2+Z^2) + 2\tau(YZ+ZX+XY) = 1. \tag{5}$$

The non-primitive hexagonal cell has a basis

$$\mathbf{f}_1 = \mathbf{e}_1 - \mathbf{e}_2$$
$$\mathbf{f}_2 = \mathbf{e}_2 - \mathbf{e}_3 \tag{6}$$
$$\mathbf{f}_3 = \mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3$$

and axes $a = |\mathbf{f}_1|$, $c = |\mathbf{f}_3|$. The axial ratio c/a satisfies

$$c/a = [3/(2-6\tau)]^{1/2}. \tag{7}$$

Table 1 gives as examples parameter values for the special cases of the three cubic lattices and for the two limiting cases of linearly dependent vectors $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$.

2.2. *The Miller–Bravais–Weber notation*

In dealing with rhombohedral and hexagonal crystals it is convenient for many purposes to express the orientation of crystal planes by means of four-term Miller–Bravais indices instead of three-term Miller indices. Orthogonality between planes and directions is then expressed most simply if four-term indices are used also for crystal directions, as proposed by Weber (1922). Advantages of this combination have been pointed out by Frank (1965). The combination is nowadays often referred to as Miller–Bravais indices. We prefer to speak of Miller–Bravais–Weber indices.

They are based on a coordinate system defined by the four vectors

$$\begin{aligned} \mathbf{g}_1 &= \mathbf{f}_1/3 &&= (\mathbf{e}_1-\mathbf{e}_2)/3 \\ \mathbf{g}_2 &= \mathbf{f}_2/3 &&= (\mathbf{e}_2-\mathbf{e}_3)/3 \\ \mathbf{g}_3 &= -(\mathbf{f}_1+\mathbf{f}_2)/3 &&= (\mathbf{e}_3-\mathbf{e}_1)/3 \\ \mathbf{g}_4 &= \mathbf{f}_3/3 &&= (\mathbf{e}_1+\mathbf{e}_2+\mathbf{e}_3)/3. \end{aligned} \tag{8}$$

The vector $\mathbf{g}_4$ is parallel to the threefold axis of the rhombohedral lattice. The vectors $\mathbf{g}_1$, $\mathbf{g}_2$, $\mathbf{g}_3$ are parallel to twofold axes; they have equal length, and the angle between any two of them is 120°; $\mathbf{g}_1+\mathbf{g}_2+\mathbf{g}_3=0$.

The *Weber indices* $[x\,y\,z\,s]$ of the rotation axis $[X\,Y\,Z]$ are defined by the equation

$$\mathbf{e}_1X+\mathbf{e}_2Y+\mathbf{e}_3Z=\mathbf{g}_1x+\mathbf{g}_2y+\mathbf{g}_3z+\mathbf{g}_4s \tag{9}$$

with

$$x+y+z=0. \tag{10}$$

It follows that

$$\begin{aligned} x &= X-Y \\ y &= Y-Z \\ z &= Z-X \\ s &= X+Y+Z. \end{aligned} \tag{11}$$

The third Weber index z is often replaced by a point for brevity because it is determined by the remaining components, $z=-x-y$. Instead of the rhombohedral quadruple $(C\,X\,Y\,Z)$, also the five-term symbol

$$(C\,x\,y\,z\,s)=(C\;\;X-Y\;\;Y-Z\;\;Z-X\;\;X+Y+Z) \tag{12}$$

or the four-term symbol

$$(C\,x\,y\,.\,s)=(C\;\;X-Y\;\;Y-Z\;\;.\;\;X+Y+Z) \tag{13}$$

may be used to characterize a rotation. It follows from (5) that these symbols satisfy the normalization condition

$$\begin{aligned} &3C^2+s^2+(1-3\tau)(x^2+y^2+z^2) \\ &\quad =3C^2+s^2+2(1-3\tau)(x^2+xy+y^2)=3. \end{aligned} \tag{14}$$

The plane perpendicular to a direction with Weber indices $[x\,y\,z\,s]$ has *Miller–Bravais indices*

$$\left(x\;\;y\;\;z\;\;s\frac{2c^2}{3a^2}\right)=\left(x\;\;y\;\;z\frac{s}{1-3\tau}\right). \tag{15}$$

2.3. *Equivalent rotations, choice of a representative in each equivalence class*

Consider two neighbouring grains of the same rhombohedral phase. The relative orientation of their lattices can be described by different rotations. If R is a rotation that maps lattice 1 onto lattice 2 then any of the six symmetry rotations S_i of lattice 1 followed by R has the same effect. The symbols that correspond to the rotations RS_i, $i=1,\ldots,6$ are given in Table 2, where

Table 2. *The symbols corresponding to RS_i, where $R\sim(C\,x\,y\,z\,s)$ denotes an arbitrary rotation and S_i, $i=1,\ldots,6$ a symmetry rotation of the rhombohedral lattice*

S_i(°)	S_i	Five-term symbol for RS_i
0	(10000)	$(C\,x\,y\,z\,s)$
120[0001]	(10003)/2	$((C-s)/2\;\;-z\;\;-x\;\;-y\;\;(s+3C)/2)$
240[0001]	$(1000\bar{3})/2$	$((C+s)/2\;\;-y\;\;-z\;\;-x\;\;(s-3C)/2)$
$180[\bar{2}110]$	$(0\bar{2}110)\,.\,g$	$(xK\;\;-2C\;\;C-s\;\;C+s\;\;(y-z)K)\,.\,g$
$180[1\bar{2}10]$	$(01\bar{2}10)\,.\,g$	$(yK\;\;C+s\;\;-2C\;\;C-s\;\;(z-x)K)\,.\,g$
$180[11\bar{2}0]$	$(011\bar{2}0)\,.\,g$	$(zK\;\;C-s\;\;C+s\;\;-2C\;\;(x-y)K)\,.\,g$

$$K=1-3\tau \quad\text{and}\quad g=(2K)^{-1/2}. \tag{16}$$

A rotation mapping lattice 1 onto lattice 2 may be expressed using instead of the basis $E=(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3)$ a symmetry-equivalent basis ES_i. The rotation is then described by the matrix $R'=S_i^{-1}RS_i$, R' may be interpreted also as a rotation expressed in the original basis of lattice 1 with the same rotation angle as R and with a symmetry-equivalent rotation axis. Because either lattice may be taken as lattice 1, also $R^{-1}\sim(-C\,x\,y\,z\,s)$ is equivalent to R. Therefore one may define two rotations R and R' as (*rhombohedrally*) *equivalent* if

$$R'=S_iRS_j \quad\text{or}\quad R'=S_iR^{-1}S_j \tag{17}$$

where S_i and S_j denote rhombohedral symmetry rotations. The maximum number of different equivalent rotations is therefore $6\times6\times2=72$ and the maximum number of different equivalent symbols is 144 because the symbol is determined by the rotation only up to a sign.

If S is the 120° rotation about [0001] and T the 180° rotation about $[11\bar{2}0]$ then one obtains

$$R'=S^{-1}RS\sim(C\,y\,z\,x\,s) \tag{18}$$

and

$$R''=T^{-1}RT\sim(-C\;\;-y\;\;-x\;\;-z\;\;s). \tag{19}$$

It follows that the 144 equivalent five-term symbols are obtained from the six symbols in Table 2 by arbitrary combinations of the following operations:

(*a*) sign change of the first component or simultaneous sign change of the last four components;

(*b*) simultaneous sign change of the middle three components combined with interchanging two of them.

Symbols that are connected by one of these operations correspond to rotations with the same angle and with axes that are related by point symmetry operations of the rhombohedral lattice, *i.e.* by elements of $\bar{3}m$. Both operations (*a*) correspond to the

Table 3. *Some properties of equivalence classes of rotations determined by the form of their representative: $N = 6\omega$ is the number of different rotations in the class, N' the number of different* 180° *rotations*

ω	Representative	N'	Axes of 180° rotations in the SST
1	$\{100.0\}$	3	11.0
	$\{C00.C\}$	4	$00.1, 10.0, 01.0$
2	$\{C00.s\}, 0<s<C$	6	$C+s\ C-s.0,\ C-s\ C+s.0$
	$\{C0y.C\}, 0<y\leq 2gC$	6	$y0.2C,\ 0C.Ky$
3	$\{Cx0.C\}, 0<x<2gC$	6	$0x.2C,\ C0.Kx$
	$\{C\,gC\,gC.0\}$	0	
	$\{C0y.s\}, 0<y\leq 2gC, 0\leq s<C$	6	$C-s\ C+s.2Ky$
	$\{Cx0.s\}, 0<x<2gC, 0<s<C$	6	$C+s\ C-s.2Kx$
6	$\{Cxy.C\}, 0<x<x+y<2gC$	6	$yx.2C$
	$\{C\ x\ 2gC-x.\,C\}, 0<x<gC$	6	$2gC-x\ x.2C$
	$\{Cxx.0\}, 0<x<gC$	0	
12	All other representatives	0	

inversion, the reason being that simultaneous sign change of all five components corresponds to the identity. Each of the three operations (b) corresponds to a mirror reflection at one of the three mirror planes through the axis $\bar{3}$. The combination of (b) with (a) corresponds to a rotation about a twofold axis [see (19)]; the combination of two operations (b) yields a cyclic permutation of the middle three components and corresponds to a rotation about the axis $\bar{3}$ [see (18)].

The three mirror planes of $\bar{3}m$ and the plane containing the twofold axes divide the total solid angle into 12 congruent spherical triangles.

The connection between equivalent symbols shows that each class of such symbols contains exactly one symbol $(C\,x\,y\,.\,s)$ that satisfies the conditions

$$x\geq 0,\quad y\geq 0,\quad s\geq 0, \tag{20}$$

$$C\geq s,\quad 2gC\geq x+y, \tag{21}$$

$$\begin{aligned} &y\geq x \quad \text{if } s=0,\\ &y>x \quad \text{if } s>0 \quad \text{and} \quad 2gC=x+y. \end{aligned} \tag{22}$$

The inequalities (21) choose among equivalent rotations those with minimum angle; (20) those with axis in a particular one of the 12 spherical triangles, which will be called the 'standard spherical triangle' or SST. If there are several such rotations then (22) will make a unique choice. A symbol satisfying (20)–(22) will be called the *representative* $\{C\,x\,y\,.\,s\}$ of its equivalence class; the corresponding rotation is the representative of an equivalence class of rotations. A rotation that corresponds to a symbol satisfying (20, 21) is usually called a disorientation. Conditions on quaternions equivalent to (20)–(22) were given by Grimmer (1980).

The number N of different rotations in a rhombohedral equivalence class is always a factor of 72 and a multiple of 6, *i.e.* the integer $\omega = N/6$ is always a factor of 12. An example with $\omega = 1$ is the class consisting of the six symmetry rotations of the rhombohedral lattice.

Table 3 gives for all possible forms of the representative the corresponding value of ω and a characterization of the 180° rotations contained in the class.

3. Rotations of rhombohedral lattices that generate coincidence site lattices

3.1. *Coincidence rotations*

Attention will be restricted from now on to *coincidence rotations, i.e.* to rotations with the property that the original and the rotated lattice have translation vectors in common that do not all lie in one plane. The common translation vectors then form a three-dimensional lattice, called the *coincidence site lattice* or CSL. The volume V_c of its unit cell is a multiple of the volume V of the unit cell of the crystal lattice; the ratio V_c/V is called the *multiplicity* of the CSL.

Here and in the following section, rhombohedral coordinates and quadruples will be used as in § 2.2. The reasons for this are that the connection (3) between the rhombohedral quadruple and the rotation matrix expressed in rhombohedral crystal coordinates is particularly simple and, more important, that use will be made in the next section of a general result, which gives the multiplicity in terms of the rotation matrix if this matrix is expressed in a basis that defines a primitive cell of the lattice.

A rotation is a coincidence rotation if and only if its matrix R expressed in crystal coordinates is rational, *i.e.* has only rational matrix elements (Grimmer, 1976). It follows from the algorithm for matrix inversion that R^{-1} is rational if and only if R is rational. The matrix R^{-1} is obtained by replacing C by $-C$ in (3). The elements of R will be denoted by R_{ij}, the elements of R^{-1} by $R_{\bar{i}\bar{j}}$. It follows from (3) that

$$\begin{aligned}
&R_{33}-R_{\bar{3}\bar{3}}=4\tau C(X-Y)\\
&R_{33}-R_{\bar{3}\bar{3}}+R_{31}-R_{\bar{3}\bar{1}}+R_{32}-R_{\bar{3}\bar{2}}=4C(X-Y)\\
&R_{12}+R_{\bar{1}\bar{2}}-R_{21}-R_{\bar{2}\bar{1}}=4\tau(X+Y+Z)(X-Y)\\
&2(R_{11}-R_{\bar{2}\bar{2}}+R_{\bar{1}\bar{2}}-R_{21})+R_{13}+R_{\bar{1}\bar{3}}-R_{23}-R_{\bar{2}\bar{3}}\\
&\quad=4(X+Y+Z)(X-Y).
\end{aligned} \tag{23}$$

Because the left-hand sides of (23) are rational, the right-hand sides will be rational, too. If τ is irrational then it follows that $C(X-Y)=0$ and $(X+Y+Z)\times(X-Y)=0$. Similarly one obtains $C(Y-Z)=0$ and $(X+Y+Z)(Y-Z)=0$, *i.e.*

$$\begin{aligned} &X=Y=Z \\ \text{or}\quad &C=X+Y+Z=0 \end{aligned} \tag{24}$$

if τ is irrational. The case τ rational is equivalent to K rational because of (16), to c^2/a^2 rational because of (7), and to $\cos\alpha$ rational because of (2).

It follows from (3) and (5) that

$$4C^2=1+R_{11}+R_{22}+R_{33} \tag{25}$$

$$4KX^2=(1-\tau)(1+R_{11}-R_{22}-R_{33}) -2\tau(R_{12}+R_{13}) \tag{26}$$

$$4KY^2=(1-\tau)(1+R_{22}-R_{33}-R_{11}) -2\tau(R_{23}+R_{21}) \tag{27}$$

$$4KZ^2=(1-\tau)(1+R_{33}-R_{11}-R_{22}) -2\tau(R_{31}+R_{32}) \tag{28}$$

$$4KYZ=-\tau(1-R_{11}+R_{21}+R_{31}) +(1-\tau)(R_{32}+R_{23}) \tag{29}$$

$$4KZX=-\tau(1-R_{22}+R_{32}+R_{12}) +(1-\tau)(R_{13}+R_{31}) \tag{30}$$

$$4KXY=-\tau(1-R_{33}+R_{13}+R_{23}) +(1-\tau)(R_{21}+R_{12}) \tag{31}$$

$$4KCX=\tau(R_{22}-R_{33}+R_{12}-R_{13}) +(1-2\tau)(R_{32}-R_{23}) \tag{32}$$

$$4KCY=\tau(R_{33}-R_{11}+R_{23}-R_{21}) +(1-2\tau)(R_{13}-R_{31}) \tag{33}$$

$$4KCZ=\tau(R_{11}-R_{22}+R_{31}-R_{32}) +(1-2\tau)(R_{21}-R_{12}). \tag{34}$$

If τ is rational then the right-hand sides of (25)-(34) are rational and it follows from (25), (32)-(34) that there exists a number λ and four coprime integers m, U, V, W such that

$$C^2=\lambda m,\quad CX=\lambda U,\quad CY=\lambda V,\quad CZ=\lambda W. \tag{35}$$

'Coprime' means that the greatest common divisor of the integers equals 1, *i.e.*

$$\gcd(m, U, V, W)=1. \tag{36}$$

It follows from (35) and (5) that

$$\begin{aligned} \lambda m = C^2 &= C^2[C^2+(1-2\tau)(X^2+Y^2+Z^2) \\ &\quad +2\tau(YZ+ZX+XY)] \\ &=\lambda^2[m^2+(1-2\tau)(U^2+V^2+W^2) \\ &\quad +2\tau(VW+WU+UV)]=\lambda^2 D, \end{aligned}$$

where

$$D=m^2+(1-2\tau)(U^2+V^2+W^2) +2\tau(VW+WU+UV). \tag{37}$$

If $C\neq 0$ then $\lambda\neq 0$ and hence $\lambda=m/D$, *i.e.* $C^2=m^2/D$ and

$$C=m/D^{1/2},\quad X=U/D^{1/2},\quad Y=V/D^{1/2},\quad Z=W/D^{1/2}. \tag{38}$$

Equations (36)-(38) remain true also if $C=0$. This follows from (26), (30)-(32) if $X\neq 0$, from (27), (29), (31), (33) if $Y\neq 0$, from (28)-(30), (34) if $Z\neq 0$. $C=X=Y=Z=0$ is not possible because of (5). Substituting (38) into (3) one obtains

$$R=\frac{1}{D}\begin{pmatrix} m^2+(1-2\tau)(U^2-V^2-W^2)+2\tau(mV-mW-VW) & 2[\tau U(W+U-m)-(1-\tau)mW+(1-2\tau)UV] & 2[\tau U(U+V+m)+(1-\tau)mV+(1-2\tau)WU] \\ 2[\tau V(V+W+m)+(1-\tau)mW+(1-2\tau)UV] & m^2+(1-2\tau)(V^2-W^2-U^2)+2\tau(mW-mU-WU) & 2[\tau V(U+V-m)-(1-\tau)mU+(1-2\tau)VW] \\ 2[\tau W(V+W-m)-(1-\tau)mV+(1-2\tau)WU] & 2[\tau W(W+U+m)+(1-\tau)mU+(1-2\tau)VW] & m^2+(1-2\tau)(W^2-U^2-V^2)+2\tau(mU-mV-UV) \end{pmatrix}. \tag{39}$$

Equations (37) and (39) give for $U=V=W$

$$R=\frac{1}{m^2+3U^2}\times\begin{pmatrix} m^2-U^2 & 2U(U-m) & 2U(U+m) \\ 2U(U+m) & m^2-U^2 & 2U(U-m) \\ 2U(U-m) & 2U(U+m) & m^2-U^2 \end{pmatrix} \tag{40}$$

and for $m=U+V+W=0$

$$R=\frac{-1}{U^2+UV+V^2}\times\begin{pmatrix} V(U+V) & -UV & U(U+V) \\ -UV & U(U+V) & V(U+V) \\ U(U+V) & V(U+V) & -UV \end{pmatrix}. \tag{41}$$

If τ is irrational then one can show using (24) that a rational matrix R must have one of the forms (40), (41) with parameters satisfying (36). Conversely, it follows from (39), (37) and (36) that R is rational if τ is rational or if (24) is satisfied. Coincidence rotations can therefore be characterized for a given value of τ by quadruples (m, U, V, W) consisting of four coprime integers. Doing this one has replaced the normalization condition (5) by (36). The expression $[X, Y, Z]$ for the axis and $\cos\theta=C$ for the half-angle of the rotation become now $[U, V, W]$ and

$$\cos\theta = mD^{-1/2} \tag{42}$$

or

$$\tan\theta = (1/m)[(1-2\tau)(U^2+V^2+W^2) + 2\tau(VW+WU+UV)]^{1/2} = (n/m)[(1-2\tau)(\tilde{U}^2+\tilde{V}^2+\tilde{W}^2) + 2\tau(\tilde{V}\tilde{W}+\tilde{W}\tilde{U}+\tilde{U}\tilde{V})]^{1/2}, \quad (43)$$

where

$$n = \gcd(U, V, W), \quad \tilde{U} = U/n, \quad \tilde{V} = V/n, \quad \tilde{W} = W/n. \quad (44)$$

From (44) it follows that

$$\gcd(\tilde{U}, \tilde{V}, \tilde{W}) = 1 \quad (45)$$

and [owing to (36)] that

$$\gcd(m, n) = 1. \quad (46)$$

A coincidence rotation is therefore a rotation about a lattice vector $[\tilde{U}, \tilde{V}, \tilde{W}]$ by a half-angle θ, the tangent of which is the product of an arbitrary rational number n/m times a quantity that is proportional to the length of the vector $[\tilde{U}, \tilde{V}, \tilde{W}]$.

If τ is *irrational* then a coincidence rotation is either [*cf.* (40)] a rotation about $\bar{3}$ with a rational value of $\sqrt{3}\tan\theta$ $(=3\tilde{U}n/m)$ or [*cf.* (41)] a 180° rotation about a lattice vector $[\tilde{U}, \tilde{V}, -\tilde{U}-\tilde{V}]$ perpendicular to $\bar{3}$. The equations (40), (41) show that R is independent of τ in both cases. The coincidence rotations for irrational τ are therefore the same for each value of τ and they coincide with those coincidence rotations for rational values of τ that satisfy $U=V=W$ or $m=U+V+W=0$. They will be called '*common*' coincidence rotations, in contrast to the '*specific*' coincidence rotations, which do not satisfy $U=V=W$ or $m=U+V+W=0$ and which depend on the (rational) value of τ.

If τ is *rational* then there exist integers μ, ν satisfying

$$\nu/\mu = \tau \quad (47)$$

and

$$\gcd(\mu, \nu) = 1. \quad (48)$$

With

$$F = \mu D = \mu m^2 + (\mu-2\nu)(U^2+V^2+W^2) + 2\nu(VW+WU+UV), \quad (49)$$

(39) becomes

$$R = \frac{1}{F}\begin{pmatrix} \mu m^2+(\mu-2\nu)(U^2-V^2-W^2)+2\nu(mV-mW-VW) & 2[\nu U(W+U-m)-(\mu-\nu)mW+(\mu-2\nu)UV] & 2[\nu U(U+V+m)+(\mu-\nu)mV+(\mu-2\nu)UW] \\ 2[\nu V(V+W+m)+(\mu-\nu)mW+(\mu-2\nu)UV] & \mu m^2+(\mu-2\nu)(V^2-W^2-U^2)+2\nu(mW-mU-WU) & 2[\nu V(U+V-m)-(\mu-\nu)mU+(\mu-2\nu)VW] \\ 2[\nu W(V+W-m)-(\mu-\nu)mV+(\mu-2\nu)UW] & 2[\nu W(W+U+m)+(\mu-\nu)mU+(\mu-2\nu)VW] & \mu m^2+(\mu-2\nu)(W^2-U^2-V^2)+2\nu(mU-mV-UV) \end{pmatrix} \quad (50)$$

and (42)

$$\cos\theta = (\mu m^2/F)^{1/2}. \quad (51)$$

The variables μ, ν, U, V, W and $\pm m$ being integers, F and the elements $r_{ij}^{\pm}$ of the matrices

$$r^+ = F\,.\,R \quad \text{and} \quad r^- = F\,.\,R^{-1} \quad (52)$$

will be integers, too.

3.2. *The multiplicity Σ of the coincidence site lattice*

Let R denote the rotation matrix expressed in terms of a basis that defines a primitive cell of the crystal lattice. The multiplicity Σ has been defined as the volume ratio of primitive cells for the CSL and the crystal lattice. It can be computed as follows.

Theorem 1 (*Σ theorem*)

Σ is the least positive integer such that ΣR and ΣR^{-1} are integral matrices.

The Σ theorem is valid for lattices of arbitrary symmetry, not just for rhombohedral lattices (Grimmer, 1976).

Because $r^+ = FR$ and $r^- = FR^{-1}$ have integral matrix elements, it follows from the Σ theorem that

$$F = \delta\,.\,\Sigma, \quad (53)$$

where δ denotes the greatest common divisor of the matrix elements of r^+ and r^-.* Equation (53) shows that δ is a divisor also of F, *i.e.* $\delta|F$.† Multiplying both sides of (25) by $F=\mu D$ and of (26)-(28) by μF, one obtains, using (38), (16) and (47),

$$\begin{aligned} 4\mu m^2 &= F + r_{11}^+ + r_{22}^+ + r_{33}^+ \\ 4\mu(\mu-3\nu)U^2 &= (\mu-\nu)(F + r_{11}^+ - r_{22}^+ - r_{33}^+) - 2\nu(r_{12}^+ + r_{13}^+) \\ 4\mu(\mu-3\nu)V^2 &= (\mu-\nu)(F + r_{22}^+ - r_{33}^+ - r_{11}^+) - 2\nu(r_{23}^+ + r_{21}^+) \\ 4\mu(\mu-3\nu)W^2 &= (\mu-\nu)(F + r_{33}^+ - r_{11}^+ - r_{22}^+) - 2\nu(r_{31}^+ + r_{32}^+). \end{aligned} \quad (54)$$

Because δ divides the right-hand sides of the equations (54), it divides also the left-hand sides. It follows because of (36) that

$$\delta|4\mu(\mu-3\nu), \quad (55)$$

i.e. Σ is a divisor of F and a multiple of $F/[4\mu(\mu-3\nu)]$. A stronger statement can be made if μ is even: all $r_{ij}^{\pm}$ are even in this case. It follows that δ is even and that Σ is a divisor of $F/2$. Even stronger statements follow from the Σ-rhomb theorem. In

* In the case of cubic and hexagonal lattices the quantity corresponding to δ has been called α by several authors. This might lead to confusion in the case of rhombohedral lattices.

† $p|q$ where p and q are integers and $p \neq 0$ means that q is an integral multiple of p; $p \nmid q$ means that q is not an integral multiple of p.

Appendix *A*, this theorem will be derived from the Σ theorem by means of elementary methods in number theory. It states:

Theorem 2 (*Σ-rhomb theorem for quadruples*)

The rotation with quadruple (m, U, V, W) acting on a rhombohedral lattice with shape characterized by μ, ν [where the six parameters are integers satisfying $\gcd(m, U, V, W) = \gcd(\mu, \nu) = 1$] generates a CSL with multiplicity

$$\Sigma = F/(F_1F_2F_3F_4) \tag{56}$$

where

$$F = \mu m^2 + (\mu - 2\nu)(U^2 + V^2 + W^2) + 2\nu(VW + WU + UV),$$

$$F_1 = \gcd(2, m + U + V + W), \tag{57}$$

$$F_2 = \gcd(2, m + U + V + W, U - V, V - W), \tag{58}$$

$$F_3 = \gcd[\mu, 2F_1^{-1}(U - V), 2F_1^{-1}(V - W)], \tag{59}$$

$$F_4 = \gcd\{\mu - 3\nu, 2F_2^{-1}m, m + U + V + W, 2[\mu V + \nu(U - 2V + W)]F_3^{-1}\}. \tag{60}$$

Notice that the arguments in (57)-(60) are all integral. This follows for the last argument in the expression for F_4 from (59) and the identity

$$2[\mu V + \nu(U - 2V + W)] = 2V.\mu + F_1\nu[2F_1^{-1}(U - V) - 2F_1^{-1}(V - W)].$$

The four numbers m, U, V, W cannot all be even because of (36). If they are all odd then $F_1 = F_2 = 2$, if two of them are odd then $F_1 = 2$ and $F_2 = 1$, otherwise $F_1 = F_2 = 1$.

For a given lattice, *i.e.* for fixed values of μ and ν, the Σ-rhomb theorem takes a simpler form. Take as an example the special case of a *primitive cubic lattice* ($\mu = 1$, $\nu = 0$), where it states

$$\Sigma = (m^2 + U^2 + V^2 + W^2)/(F_1F_2). \tag{61}$$

The expressions $F = m^2 + U^2 + V^2 + W^2$ and $\delta = F_1 . F_2$ contain identical powers of 2, *i.e.* $\delta = 4$ if m, U, V, W are all odd, $\delta = 2$ if two among m, U, V, W are odd, $\delta = 1$ if one or three among m, U, V, W are odd. It follows that $\Sigma = F/\delta$ is equal to the largest odd divisor of $m^2 + U^2 + V^2 + W^2$.

It was shown in the preceding section that the matrix R is independent of τ and therefore of μ and ν for common coincidence rotations. The Σ theorem then shows that Σ is independent of μ and ν. This is confirmed by the Σ-rhomb theorem, which takes the following form for common coincidence rotations:

Corollary 1 (*for quadruples of common coincidence rotations*)

If $U = V = W$ then $\Sigma = (m^2 + 3U^2)/4$ if m and U are odd, $\Sigma = m^2 + 3U^2$ otherwise.

If $m = U + V + W = 0$ then $\Sigma = U^2 + UV + V^2$.

Compared with the Σ theorem the Σ-rhomb theorem has several advantages: it simplifies the computation of Σ; it shows the connection between Σ and the parameters of the lattice and of the rotation more directly; and it makes the change to rotation symbols advantageous, as will be shown in the next section.

3.3. *The Σ-rhomb theorem for rotation symbols and its applications*

The rotation symbol that corresponds to a coincidence rotation $(mUVW)$ will be denoted by $(muvtw)$ or $(muv.w)$ where

$$u = U - V, \quad v = V - W, \quad t = W - U, \quad w = U + V + W. \tag{62}$$

From (36) one obtains

$$3|2u + v + w \tag{63}$$

and

$$\gcd[m, u, v, (2u + v + w)/3] = 1. \tag{64}$$

Replacing ν by

$$\rho = \mu - 3\nu \tag{65}$$

one obtains from (48)

$$3|\mu - \rho \tag{66}$$

and

$$\gcd[\mu, (\mu - \rho)/3] = 1. \tag{67}$$

It follows from (47) and (16) that

$$\rho/\mu = (\mu - 3\nu)/\mu = 1 - 3\tau = K \tag{68}$$

and from (7) that

$$c/a = (3\mu/2\rho)^{1/2}. \tag{69}$$

Defining $f = 3F$ one obtains from (49)

$$f = \mu(3m^2 + w^2) + 2\rho(u^2 + uv + v^2) \tag{70}$$

and from (51)

$$\cos\theta = (3\mu m^2/f)^{1/2}, \tag{71}$$

i.e.

$$\tan\theta = \left(\frac{f - 3\mu m^2}{3\mu m^2}\right)^{1/2} = \left[\frac{\mu w^2 + 2\rho(u^2 + uv + v^2)}{3\mu m^2}\right]^{1/2}. \tag{72}$$

Expressing the Σ-rhomb theorem in terms of these notations one obtains:

Theorem 3 (*Σ-rhomb theorem for rotation symbols*)

Consider the rotation with symbol $(m\,u\,v.w)$ acting on the rhombohedral lattice with axial ratio $c/a = (3\mu/2\rho)^{1/2}$, where the six parameters m, u, v, w, μ, ρ are integers satisfying (63), (64), (66), (67). The rotation generates a CSL with multiplicity

$$\Sigma = f/(3f_1f_2f_3f_4), \tag{73}$$

where f is given by (70) and

$$f_1 = \gcd(2, m+w) \quad (74)$$

$$f_2 = \gcd(2, m+w, u, v) \quad (75)$$

$$f_3 = \gcd(\mu, 2f_1^{-1}u, 2f_1^{-1}v) \quad (76)$$

$$f_4 = \gcd\{\rho, 2f_2^{-1}m, m+w, 2[\mu w + \rho(v-u)](3f_3)^{-1}\}. \quad (77)$$

For a given lattice, *i.e.* for fixed values of μ and ρ, the factors f_3 and f_4 will take a simpler form. Examples are:

(1) If $2\nmid\mu$ then $f_3 = \gcd(\mu, u, v)$.

(2) If $2\nmid\rho$ then

$$f_4 = \gcd\{\rho, m, w, 2[\mu w + \rho(v-u)](3f_3)^{-1}\}.$$

(3) If $3\nmid\mu$ [which is equivalent to $3\nmid\rho$ because of (60)] then $f_4 = \gcd(\rho, 2f_2^{-1}m, m+w)$.

From (2) and (3) it follows that:

(4) If $\gcd(6, \rho) = 1$ then $f_4 = \gcd(\rho, m, w)$.

The quantity δ introduced in (53) satisfies

$$\delta = F/\Sigma = f/(3\Sigma) = f_1 f_2 f_3 f_4, \quad (78)$$

and is a divisor of $4\mu\rho$ according to (55). Theorem 3 makes it possible to put additional restrictions on i_2, the number of factors of 2 in δ, if $\mu\rho$ is even. The theorem excludes $i_2 = 0$ if μ is even, also $i_2 = 2$ if μ contains exactly one factor 2. If, on the other hand, ρ is even then it excludes $i_2 = 1$ and the possibility that δ contains two factors of 2 more than ρ.

In the special case of a *body-centred cubic* (*b.c.c.*) *lattice*, where $\mu = 1$ and $\rho = 4$, one has $f_3 = 1$ and $f_4 = \gcd(4, 2m/f_2, m+w)$. If $2|m$ and $4|m+w$ then $\delta = 8$. In the remaining cases, $\delta = 4$ if $2|m+w$ and $\delta = 1$ otherwise. The quantities $f = 3m^2 + w^2 + 8(u^2 + uv + v^2)$ and δ contain identical powers of 2.

For a *face-centred cubic* (*f.c.c.*) *lattice*, where $\mu = 4$ and $\rho = 1$, one has $f_3 = \gcd(4, 2u/f_1, 2v/f_1)$ and $f_4 = 1$. Four cases can be distinguished, where each case precludes all those above:*

$$\begin{aligned} &\delta = 16 && \text{if } 4|u, v \text{ and } 2|m+w,\\ \text{otherwise } &\delta = 8 && \text{if } 2|u, v, m+w,\\ \text{otherwise } &\delta = 4 && \text{if } 2|u, v,\\ \text{otherwise } &\delta = 2. \end{aligned}$$

The quantities $f = 4(3m^2 + w^2) + 2(u^2 + uv + v^2)$ and δ contain identical powers of 2.

It follows that for the b.c.c. and f.c.c. lattices the multiplicity Σ is always equal to the largest odd divisor of $F = f/3$. The same result has been proved in § 3.2 for the primitive cubic (p.c.) lattice. These results are closely related to the well known result from the theory of coincidence rotations for cubic lattices that centring the p.c. lattice does not change the value of Σ (Ranganathan, 1966). The results given above for b.c.c. and f.c.c. lattices show a way to derive results on coincidences in b.c.c. and f.c.c. lattices directly instead of obtaining them, as is more usual, from centring the p.c. lattice.

Common coincidence rotations satisfy either $u = v = 0$ or $m = w = 0$. The Σ-rhomb theorem takes the following form in these cases:

Corollary 2 (*for symbols of common coincidence rotations*)

If $u = v = 0$ then $\Sigma = (3m^2 + w^2)/12$ if m and w are odd, $\Sigma = (3m^2 + w^2)/3$ otherwise.

If $m = w = 0$ then $\Sigma = (u^2 + uv + v^2)/3$.

It has been shown in the *Introduction* that tables of all the classes of coincidence rotations with multiplicity up to a given value Σ_c and with c/a in an interval around its experimental value are an important aid for interpreting detailed microscopic examinations of grain boundaries.

The importance of the Σ-rhomb theorem becomes apparent in computing such tables. It will be shown in the following section that the theorem often simplifies the determination of the classes for a given value of c/a. Much more important is the fact that the theorem makes it possible to pick out among the infinitely many rational numbers in a finite interval of c^2/a^2 a finite number of them which may give rise to specific coincidence rotations with $\Sigma \le \Sigma_c$. It is shown in Appendix *B* how the following lower bounds $\Sigma_{\text{l.b.}}$ for the multiplicity of specific coincidence rotations can be derived from theorem 3:

Theorem 4

The multiplicity of specific coincidence rotations for a fixed axial ratio determined by μ and ρ cannot be smaller than

$$\Sigma_{\text{l.b.}} = (8\mu\rho)^{1/2}/3 \quad \text{if } \mu \text{ and } \rho \text{ are odd,} \quad (79)$$

$$\Sigma_{\text{l.b.}} = (2\mu\rho)^{1/2}/3 \quad \text{otherwise.} \quad (80)$$

Consider as an example the technically important ceramic material α-Al_2O_3. It has a rhombohedral lattice with $c/a = 2{\cdot}73$, *i.e.* $c^2/a^2 = 7{\cdot}45$. Table 4 gives all values of c^2/a^2 between 7·25 and 7·65 for which specific coincidence rotations with $\Sigma \le 35$ are possible according to theorem 4 as well as $\Sigma_{\min}$, the actual minimum value of the multiplicity, which was determined with a computer program.

The Σ-rhomb theorem makes it possible to determine also upper bounds for the minimum value of the multiplicity of specific coincidence rotations:

Lemma 1

Let p and q be integers satisfying $3|p+q$ and either $9\nmid p$ or $9\nmid q$. Write $P = 2\mu\rho$ if $\mu\rho$ is odd or $P = \mu\rho/2$ if $\mu\rho$ is even as a product $P = pq$ with $|p-q|$ as small as possible. Then $\Sigma_{\min} \le \Sigma_1 = (p+q)/3$.

* $n|p, q$ means $n|p$ and $n|q$.

Table 4. *The values of the axial ratio in the interval* $7{\cdot}25 \le c^2/a^2 \le 7{\cdot}65$ *for which specific coincidence rotations with* $\Sigma \le 35$ *are possible according to theorem* 4

$\Sigma_{\rm l.b.}$ has been rounded to the next higher integer, $\Sigma_{\min}$ is the actual minimum value of the multiplicity. The rows are arranged in the order of increasing values of $c^2/a^2 = 3\mu/2\rho$; the lattice parameter α is indicated in degrees

μ	ρ	c^2/a^2	c/a	$\alpha(°)$	$\Sigma_{\rm l.b.}$	$\Sigma_{\min}$
87	18	7·25	2·693	55·88	19	32
155	32	7·266	2·695	55·83	34	34
34	7	7·286	2·699	55·77	8	8
117	24	7·313	2·704	55·69	25	25
132	27	7·333	2·708	55·63	29	29
49	10	7·35	2·711	55·58	11	14
162	33	7·364	2·714	55·54	35	38
64	13	7·385	2·717	55·48	14	14
79	16	7·406	2·721	55·42	17	29
94	19	7·421	2·724	55·38	20	22
109	22	7·432	2·726	55·35	24	40
124	25	7·44	2·728	55·32	27	27
139	28	7·446	2·729	55·30	30	51
154	31	7·452	2·730	55·29	33	36
15	3	7·5	2·739	55·15	7	7
161	32	7·547	2·747	55·02	34	34
146	29	7·552	2·748	55·00	31	34
131	26	7·558	2·749	54·99	28	48
116	23	7·565	2·750	54·97	25	25
101	20	7·575	2·752	54·94	22	37
86	17	7·588	2·755	54·90	19	20
71	14	7·607	2·758	54·85	15	26
56	11	7·636	2·763	54·77	12	12
153	30	7·65	2·766	54·73	32	32

The following lemma may give a stronger upper bound if $\mu\rho$ is a multiple of 81.

Lemma 2

If $3|\mu(\Leftrightarrow 3|\rho)$ then write $P = 2\mu\rho/3$ if $\mu\rho$ is odd or $P = \mu\rho/6$ if $\mu\rho$ is even as a product of two integers p and q with $|p-q|$ as small as possible. Then $\Sigma_{\min} \le \Sigma_2 = p + q$.

The existence of specific coincidence rotations with multiplicities as given by the two lemmata is shown in Appendix *C*.

For all cases contained in Table 4 one has $\Sigma_{\min} = \Sigma_1$. An example where $\Sigma_2 < \Sigma_1$ is $\mu = 81$, $\rho = 6$, where $\Sigma_1 = 28$ and $\Sigma_2 = 18 = \Sigma_{\min}$. No cases are known to the author where the following rule does not hold:

$$\Sigma_{\min} = \Sigma_1 \qquad \text{if } 81 \nmid \mu\rho,$$

$$\Sigma_{\min} = \min(\Sigma_1, \Sigma_2) \quad \text{if } 81|\mu\rho.$$

A general proof of the rule is lacking; it would simplify the computation of specific coincidence rotations with $\Sigma \le \Sigma_c$ and c/a in a given interval by eliminating straight away certain pairs μ, ρ for which $\Sigma_{\rm l.b.} \le \Sigma_c$.

4. Application to corundum-type oxides

Corundum, *i.e.* α-alumina, has space group $R\bar{3}c$ and $c/a = 2{\cdot}730$. There exists a number of oxides with the same structure type and a similar ratio c/a, *e.g.* Fe_2O_3 ($c/a = 2{\cdot}732$) and Cr_2O_3 ($c/a = 2{\cdot}741$). Alumina is an important ceramic material. Its microstructure has been studied in detail with a view to optimizing its properties by appropriate production processes. Several authors have measured the relative orientation of neighbouring grains and analysed the dislocations in the grain boundaries. The interpretation of the results in terms of CSL models has been unsatisfactory owing to the lack of a systematic investigation of all possible CSL's, as will be shown at the end of this section.

Table 5. *The equivalence classes of common coincidence rotations with* $\Sigma \le 60$

The rotation symbols of the representatives have the form $(m\,0\,0\,.\,w)$

Σ	Representative $\Theta(°)$	m	w	Axes in the SST of 180° rotations	
3	60·00	3	3	0 0 . 1 1 0 . 0	0 1 . 0
7	38·21	5	3	4 1 . 0	1 4 . 0
13	27·80	7	3	5 2 . 0	2 5 . 0
19	46·83	4	3	7 1 . 0	1 7 . 0
21	21·79	9	3	2 1 . 0	1 2 . 0
31	17·90	11	3	7 4 . 0	4 7 . 0
37	50·57	11	9	10 1 . 0	1 10 . 0
39	32·20	6	3	3 1 . 0	1 3 . 0
43	15·18	13	3	8 5 . 0	5 8 . 0
49	43·57	13	9	11 2 . 0	2 11 . 0
57	13·17	15	3	3 2 . 0	2 3 . 0

It has been shown in the *Introduction* that coincidence rotations which serve to interpret grain boundary structures have a low value of Σ and are either independent of c/a or correspond to a c/a ratio close to the experimental value. Table 5 gives the classes of common coincidence rotations with $\Sigma \le 60$. The class in the first row contains six different rotations ($\omega = 1$), all other classes contain 12 rotations ($\omega = 2$). The Weber indices of the axes of 180° rotations in the common classes have the form $[uv.0]$ or $[00.w]$ and coincide according to (15) with the Miller-Bravais indices of the corresponding symmetry plane, *i.e.* the plane perpendicular to the axis.

Table 6 gives the classes of specific coincidence rotations with $\Sigma \le 28$ for $c^2/a^2 = 7{\cdot}5$, *i.e.* $c/a = 2{\cdot}739$, an axial ratio close to the experimental values for the three oxides mentioned above. Many specific classes with low values of Σ exist for this value of c/a. Table 7 gives the classes of specific coincidence rotations with $\Sigma \le 28$ that satisfy $7{\cdot}25 \le c^2/a^2 \le 7{\cdot}65$ with the exception of $c^2/a^2 = 7{\cdot}5$.

The Σ columns of Tables 6 and 7 also contain, in the cases where there are several classes with the same value of Σ, in addition to this value an index consisting of a letter $a, b, c, \ldots$ assigned in the order of increasing values of Θ and/or a number $1, 2, \ldots$ where there are several classes with the same value of Θ. The representative is given by its angle and rotation symbol; the 180° rotations in the class with axis in the SST are given by the Weber indices $[u'v'.w']$ of these axes; the corresponding symmetry

Table 6. *Specific coincidence rotations with $\Sigma \leq 28$ for $c/a = 2{\cdot}739$*

Σ	ω	Representative $\Theta(°)$	$m\ u\ v\,.\,w$	Axes in the SST of 180° rotations		Symmetry planes in the SST	
7_1	3	85·90	1 0 2 . 1	1 0 . 1	0 5 . 2	1 0 . 5	0 1 . 2
7_2	3	85·90	3 6 0 . 3	0 1 . 1	5 0 . 2	0 1 . 5	1 0 . 2
$11a_1$	3	68·68	1 1 0 . 1	0 1 . 2	5 0 . 1	0 1 .10	1 0 . 1
$11a_2$	3	68.68	3 0 3 . 3	1 0 . 2	0 5 . 1	1 0 .10	0 1 . 1
$11b$	6	95·22	1 0 3 . 0		5 5 . 6		1 1 . 6
$13a$	6	57·42	2 0 3 . 0		5 5 . 3		1 1 . 3
$13b_1$	3	94·41	6 0 15 . 6	5 0 . 4	0 2 . 1	1 0 . 4	0 2 . 5
$13b_2$	3	94·41	2 5 0 . 2	0 5 . 4	2 0 . 1	0 1 . 4	2 0 . 5
$17a$	6	71·12	3 2 2 . 3	1 1 . 3		1 1 .15	
$17b_1$	6	96·76	1 2 1 . 1	1 2 . 2		1 2 .10	
$17b_2$	6	96·76	3 3 6 . 3	2 1 . 2		2 1 .10	
$19a_1$	6	65·10	3 0 5 . 1		1 2 . 1		1 2 . 5
$19a_2$	6	65·10	9 15 0 . 3		2 1 . 1		2 1 . 5
$19b$	6	86·98	2 3 3 . 0				
21	6	64·62	1 1 1 . 0				
$23a$	6	55·58	6 5 5 . 0				
$23b_1$	6	87·51	2 0 5 . 1		1 3 . 2		1 3 .10
$23b_2$	6	87·51	6 15 0 . 3		3 1 . 2		3 1 .10
$23c$	6	91·25	3 4 4 . 3	2 2 . 3		2 2 .15	

Table 7. *Specific coincidence rotations with $\Sigma \leq 28$ and $7{\cdot}25 \leq c^2/a^2 \leq 7{\cdot}65$ (see Table 6 for $c/a = 2{\cdot}739$)*

Axial ratio	Σ	ω	Representative $\Theta(°)$	$m\ u\ v\,.\,w$	Axes in the SST of 180° rotations		Symmetry planes in the SST	
2·699	8	3	86·42	1 0 2 . 1	1 0 . 1	0 17 . 7	7 0 .34	0 1 . 2
	15	3	93·82	7 0 17 . 7	17 0 .14	0 2 . 1	1 0 . 4	0 7 .17
	22	6	64·42	21 34 0 . 7		2 1 . 1		14 7 .34
	24	6	65.38	1 1 1 . 0				
	25	3	68·90	1 1 0 . 1	0 1 . 2	34 0 . 7	0 7 .68	1 0 . 1
2·704	25	3	102·71	3 0 9 . 3	3 0 . 2	0 13 . 8	4 0 .13	0 1 . 3
2·711	14	3	75·52	5 0 7 . 5	7 0 .10	0 7 . 2	1 0 . 7	0 5 . 7
	18	3	68·83	1 1 0 . 1	0 1 . 2	49 0 .10	0 5 .49	1 0 . 1
	21	3	99·59	5 14 0 . 5	0 7 . 5	7 0 . 4	0 2 . 7	5 0 .14
	23	3	86·26	1 0 2 . 1	1 0 . 1	0 49 .20	10 0 .49	0 1 . 2
	$28a$	6	82.82	3 7 0 . 1		14 7 .10		2 1 . 7
	$28b$	6	97·18	1 2 1 . 1	1 2 . 2		5 10 .49	
2·717	14	3	94·10	13 0 32 .13	16 0 .13	0 2 . 1	1 0 . 4	0 13 .32
	15	3	86·18	1 0 2 . 1	1 0 . 1	0 32 .13	13 0 .64	0 1 . 2
	20	3	72·54	13 16 0 .13	0 8 .13	4 0 . 1	0 1 . 8	13 0 .16
2·724	22	3	86·09	1 0 2 . 1	1 0 . 1	0 47 .19	19 0 .94	0 1 . 2
2·728	27	3	94·25	25 0 62 .25	31 0 .25	0 2 . 1	1 0 . 4	0 25 .62
2·750	25	3	94·59	23 0 58 .23	29 0 .23	0 2 . 1	1 0 . 4	0 23 .58
	27	3	85·75	1 0 2 . 1	1 0 . 1	0 58 .23	23 0.116	0 1 . 2
2.755	20	3	85·70	1 0 2 . 1	1 0 . 1	0 43 .17	17 0 .86	0 1 . 2
2·758	26	3	68·57	1 1 0 . 1	0 1 . 2	71 0 .14	0 7 .71	1 0 . 1
2·763	12	3	94·78	11 0 28 .11	14 0 .11	0 2 . 1	1 0 . 4	0 11 .28
	13	3	85·59	1 0 2 . 1	1 0 . 1	0 28 .11	11 0 .56	0 1 . 2
	17	3	72·90	11 14 0 .11	0 7 .11	4 0 . 1	0 1 . 8	11 0 .14
	27	3	64·79	11 8 0 .11	0 4 .11	7 0 . 1	0 1 .14	11 0 . 8

planes are given by their Miller-Bravais indices $(hk.l) \sim (\rho u'\rho v'.\mu w')$. Either $[u'v'.w']$ or $(hk.l)$ will be independent of $K = \rho/\mu$ if they are expressed in terms of the parameters in the rotation symbol of the representative according to Table 3. Cases where $[u'v'.w']$ is independent of K have been written on the left side; cases where $(hk.l)$ is independent of K have been written on the right side.

Pairs of specific rotations with symmetry planes related as $(hk.l)$ and $(kh.l)$ have the same multiplicities for the axial ratio considered in Table 6. This is not the case for the axial ratios considered in Table 7. If h and k are interchanged in the symmetry planes appearing in this table then the corresponding multiplicities will be larger than 28. This implies that the table contains no symmetry planes of the form $(hh.l)$. If l and at least one of the numbers h and k are not divisible by 3 then the indices $(hk.l)$ of the symmetry planes in Table 7 satisfy $3|-h+k+l$.*

* *Note added in proof*

The author learned after the acceptance of the present article that Doni, Fanides & Bleris [*Cryst. Res. Technol.* (1986). **21**, 1469-1474] published a paper on the determination of coincidence rotations for rhombohedral lattices. They start with the assumption that Σ is the least positive integer such that ΣR is an integral matrix, which is not always true. A counterexample is the class with representative rotation $\{muv.w\} = \{15\ \ 7\ \ 14\ \ .\ \ 5\}$ of the rhombohedral lattice with $\mu = 49$ and $\rho = 10$, *i.e.* $c/a = 2{\cdot}711$, for which

$$R = \frac{1}{14}\begin{pmatrix} 18 & 9 & 8 \\ -8 & 1 & -14 \\ -4 & 6 & 12 \end{pmatrix} \quad \text{and} \quad R^{-1} = \frac{1}{98}\begin{pmatrix} 48 & -30 & -67 \\ 76 & 124 & 94 \\ -22 & -72 & 45 \end{pmatrix}.$$

Their assumption gives $\Sigma = 14$ whereas the true value of Σ is $7 \times 14 = 98$.

The symmetry planes appearing most frequently in Table 7 are

(01.2), 7 times

(10.4), 5 times

(10.1), 3 times.

The basal plane (00.1) and the planes of type {01.2}, {10.4} and {10.1} are exactly those mentioned by Morrissey & Carter (1984) as possible twin planes. The *basal twin* (c twin) with plane (00.1) corresponds to the common rotation with $\Sigma = 3$ (*cf.* Table 5). This twin and the *rhombohedral twin* (r twin) with twin plane of type {01.2} are the most common types of twins in corundum and haematite (Morrissey & Carter, 1984; Bursill & Withers, 1979). The planes {01.2} are the faces of the morphological rhombohedral cell, which has an axial ratio $c/2a$ as compared with c/a for the structural cell (Kronberg, 1957). The planes {10.1} are the faces of the structural rhombohedral cell defined by the vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$.

Morrissey & Carter (1984) investigate commercially available sintered alumina, determining the relative orientation of neighbouring grains and the Miller–Bravais indices of the boundary planes between them. The twin boundaries with planes {01.2} and {10.4} are described as coincidence boundaries with multiplicities $\Sigma = 8$ and $\Sigma = 14$, respectively. In the first case, they remark that 'the value $\Sigma = 7$ is actually closer to a perfect CSL'. They discuss boundaries corresponding to the common coincidence rotations with $\Sigma = 7$ and $\Sigma = 13$ but are not aware of the existence of specific coincidence rotations with the same multiplicities. The common rotations with $\Sigma = 7$ and $\Sigma = 13$ have symmetry planes of type $\{hk.0\}$ according to Table 5 and therefore cannot serve to describe the {01.2} and {10.4} twins. However, Tables 6 and 7 show that the smallest multiplicities of specific coincidence rotations with planes {01.2} and axial ratio in the interval $2{\cdot}693 \le c/a \le 2{\cdot}766$ are $\Sigma = 7$ ($c/a = 2{\cdot}739$) and $\Sigma = 8$ ($c/a = 2{\cdot}699$). The first solution has an axial ratio much closer to the experimental value 2·730 of corundum. Also Shiue & Phillips (1984), making use of a theorem by Grimmer (1974), found that the rhombohedral twin is better described as $\Sigma = 7$ than as $\Sigma = 8$. The situation is similar for the twin with plane of type {10.4}, for which Tables 6 and 7 give the following rotations with small values of Σ:

$$\Sigma = 12, \quad c/a = 2{\cdot}763,$$

$$\Sigma = 13, \quad c/a = 2{\cdot}739,$$

$$\Sigma = 14, \quad c/a = 2{\cdot}717.$$

The solution with axial ratio closest to the experimental value is $\Sigma = 13$, not $\Sigma = 14$.

Morrissey & Carter (1983) determined the Burgers vectors of dislocations in basal twin boundaries and found that they in fact coincide with vectors of short length of the DSC lattice for the common rotation with $\Sigma = 3$. This was confirmed by Shiue & Phillips (1984).

Lartigue & Priester (1984, 1985, 1986) have investigated grain boundaries in polycrystalline alumina. Lacking results on coincidence rotations for rhombohedral lattices, they interpret their observations in terms of the (common and specific) coincidence rotations for the primitive hexagonal lattice with $c^2/a^2 = 15/2$. These rotations had been determined first by Bonnet *et al.* (1981) for multiplicities $\Sigma_h \le 25$ and by Delavignette (1983) for $\Sigma_h \le 35$. In the rhombohedral lattice obtained by centring the primitive hexagonal lattice these rotations generate CSL's with multiplicity $\Sigma = \Sigma_h$ or $\Sigma = 3\Sigma_h$, as will be shown in § 5. The true multiplicity may therefore be three times larger than indicated by Lartigue & Priester (1984, 1985, 1986). Other shortcomings of an interpretation of boundaries in α-alumina in terms of the CSL's for primitive hexagonal lattices are:

(1) A primitive cell of the DSC lattice for the rhombohedral case can be obtained by centring the corresponding cell for the hexagonal case in such a way that the cell volume decreases by a factor of 3 if $\Sigma = \Sigma_h$ and by a factor of 9 if $\Sigma = 3\Sigma_h$. The Burgers vectors of dislocations in the boundary being vectors of short length of the DSC lattice, some of the Burgers vectors most likely to occur are lost in the hexagonal treatment.

(2) Table 7 shows that the c/a values with specific rotations of multiplicity $\Sigma \le 28$ that lie closest to the experimental value 2·730 for alumina are 2·728 and 2·724; the closest value for the hexagonal lattice is 2·739 instead.

It is possible in some cases to reinterpret the results of Lartigue & Priester (1984, 1985, 1986) immediately in terms of the results for rhombohedral lattices: basal twins correspond to the common coincidence rotation with $\Sigma = 3$. In general, however, additional information is needed for a reinterpretation because the relative orientation is described assuming hexagonal symmetry instead of the rhombohedral symmetry of α-alumina. This reinterpretation is carried out by Lartigue & Priester (1988) and by Grimmer, Bonnet, Lartigue & Priester (1989).

The experimental studies of the remaining corundum-type oxides are much less detailed: Bursill & Withers (1979) observe basal twins and twins with {01.2} and {10.2} planes in haematite iron ore (Fe_2O_3). The basal twins may again be interpreted in terms of the common rotation with $\Sigma = 3$, the other two twins in terms of specific rotations with $\Sigma = 7$ for $c/a = 2{\cdot}739$. The usual rhombohedral twin has a plane {01.2}; considerably stronger strain contrast was observed in the twin with {10.2}.

5. Comparison of the results for rhombohedral and hexagonal lattices

Consider a primitive hexagonal lattice and the rhombohedral lattice obtained from it by rhombohedral centring. The multiplicities Σ^h of the coincidence site lattice (CSL) generated by a given rotation in the hexagonal lattice and Σ of the CSL generated by the same rotation in the rhombohedral lattice are connected by:

Theorem 5

The coincidence site lattices generated by the same rotation in a primitive hexagonal lattice and in the rhombohedral lattice obtained by centring the hexagonal lattice have multiplicities differing by at most a factor of 3.

This can be shown as follows. Rhombohedral centring of the primitive hexagonal lattice leads to a rhombohedral lattice with a volume of the primitive cell 3 times smaller. By a further centring the rhombohedral lattice can be transformed into a primitive hexagonal lattice with values of c and a 3 times smaller than for the original lattice. The primitive cell of the finer hexagonal lattice has a volume 9 times smaller than the primitive cell of the rhombohedral lattice. A rotation generates in both hexagonal lattices CSL's with the same multiplicity Σ^h. The CSL for the rhombohedral lattice contains the CSL for the coarser hexagonal lattice and is contained in the CSL for the finer hexagonal lattice. Therefore Σ must be a divisor of $3\Sigma^h$ and a multiple of $\Sigma^h/9$, *i.e.* $\Sigma = 3\Sigma^h, \Sigma^h, \Sigma^h/3$ or $\Sigma^h/9$. If the rhombohedral centring does not give additional common translations then $\Sigma = 3\Sigma^h$.

It will be shown next that $\Sigma = \Sigma^h/9$ does not occur. Consider two congruent primitive hexagonal lattices, 1 and 2, with common translation vectors forming a three-dimensional CSL. The following considerations can be formulated more easily if the lattices are taken as point lattices with at least one point in common. The CSL consists then of all those points that are common to the two lattices. The rhombohedral centring is carried out on lattice 1 first. Two new net planes are inserted in this way between each pair of neighbouring net planes perpendicular to the sixfold axis of lattice 1. The old coincidence points lie in the old net planes. These will not receive additional points. If the centring produces additional coincidence sites, then these sites must lie in the new net planes; the distance between neighbouring net planes of the CSL decreases by a factor of 3 in this case. Analogous considerations hold if the rhombohedral centring is consecutively carried out on lattice 2. Because the density of lattice points is always the same for parallel net planes one obtains the following results: $\Sigma = \Sigma^h/3$, Σ^h or $3\Sigma^h$ according to whether both, one or none of the two centrings produces new net planes of CSL.

It is interesting to compare the minimum values of the multiplicities of specific coincidence rotations for the hexagonal and the rhombohedral lattice with the same value of c/a. This can be done by comparing the values in Table 4 (or in Table 7) with the results of Delavignette (1983), which give, for example,

$$\Sigma_{\min} = 8 < \Sigma^h_{\min} = 24 \quad \text{if } c/a = 2{\cdot}699$$

and

$$\Sigma_{\min} > 28 > \Sigma^h_{\min} = 17 \quad \text{if } c/a = 2{\cdot}708.$$

This result confirms that the cases $\Sigma = \Sigma^h/3$ and $\Sigma = 3\Sigma^h$ do occur.

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APPENDIX *A*
Proof of the Σ-rhomb theorem

A.1. *Introduction*

The Σ-rhomb theorem for rhombohedral quadruples, which will be proved in this Appendix, expresses the multiplicity Σ of a coincidence rotation in terms of the parameters m, U, V, W, which determine the rotation, and of μ, ν, which determine the axial ratio of the lattice.

If we define $\rho = \mu - 3\nu$, it follows from (49), (50) and (52) that

$$\begin{aligned}
4\mu m^2 &= F + r^+_{11} + r^+_{22} + r^+_{33}\\
4\mu m U &= r^+_{33} - r^-_{33} - r^+_{23} + r^-_{23}\\
4\mu m V &= r^+_{11} - r^-_{11} - r^+_{31} + r^-_{31}\\
4\mu m W &= r^+_{22} - r^-_{22} - r^+_{12} + r^-_{12}\\
4\mu m(U+V+W) &= r^+_{32} - r^-_{32} + r^+_{13} - r^-_{13} + r^+_{21} - r^-_{21}\\
4\mu U(U+V+W) &= F + r^+_{11} - r^-_{22} - r^-_{33}\\
&\quad + r^+_{12} + r^-_{12} + r^+_{13} + r^-_{13}\\
4\mu V(U+V+W) &= F + r^+_{22} - r^-_{33} - r^-_{11}\\
&\quad + r^+_{23} + r^-_{23} + r^+_{21} + r^-_{21}\\
4\mu W(U+V+W) &= F + r^+_{33} - r^-_{11} - r^-_{22} \qquad (81)\\
&\quad + r^+_{31} + r^-_{31} + r^+_{32} + r^-_{32}\\
4\rho m(U-V) &= r^+_{31} - r^-_{31} + r^+_{32} - r^-_{32} - 2r^+_{33} + 2r^-_{33}\\
4\rho U(U-V) &= F + r^+_{11} - r^-_{22} - r^-_{33} - r^+_{12} - r^-_{12}\\
4\rho V(U-V) &= -F + r^-_{33} + r^-_{11} - r^+_{22} + r^+_{21} + r^-_{21}\\
4\rho W(U-V) &= r^+_{31} + r^-_{31} - r^+_{32} - r^-_{32}\\
4\rho m(V-W) &= r^+_{12} - r^-_{12} + r^+_{13} - r^-_{13} - 2r^+_{11} + 2r^-_{11}\\
4\rho U(V-W) &= r^+_{12} + r^-_{12} - r^+_{13} - r^-_{13}\\
4\rho V(V-W) &= F + r^+_{22} - r^-_{33} - r^-_{11} - r^+_{23} - r^-_{23}\\
4\rho W(V-W) &= -F + r^-_{11} + r^-_{22} - r^+_{33} + r^+_{32} + r^-_{32}.
\end{aligned}$$

Σ will be determined by evaluating the factor $\delta = F/\Sigma$. δ is contained as a factor in each term on the right-hand sides of the 16 equations (81). Each group of four equations combined with (36) therefore gives one of the following results:

$$\delta | 4\mu m \tag{82}$$

$$\delta | 4\mu(U+V+W) \tag{83}$$

$$\delta | 4\rho(U-V) \tag{84}$$

$$\delta | 4\rho(V-W). \tag{85}$$

In order to derive the Σ-rhomb theorem from the Σ theorem it is useful to write the rotation matrix not only in the form (49), (50) but also as follows: Let $\bar{r}_{ij}^{\pm}$ be the elements of the matrices $\bar{r}^{+} = 3FR$, $\bar{r}^{-} = 3FR^{-1}$ respectively. Then one obtains

$$3F = \mu[3m^2 + (U+V+W)^2] + 2\rho[(U-V)^2 + (U-V)(V-W) + (V-W)^2] \tag{86}$$

and

$$\begin{aligned} 3r_{11}^{+} = \bar{r}_{11}^{+} = {} & \mu[3m^2 + 2m(V-W) \\ & + (U+V+W)(U-V-W)] \\ & + 2\rho[(U+V)(U-V) \\ & + (W-m)(V-W)] \\ 3r_{21}^{+} = \bar{r}_{21}^{+} = {} & 2\mu[m(V+2W) + (U+V+W)V] \\ & + 2\rho[2V(U-V) + (V-m)(V-W)]. \end{aligned} \tag{87}$$

Equation (50) shows that the remaining matrix elements of $\bar{r}^{+}$ and $\bar{r}^{-}$ are obtained as follows: $\bar{r}_{31}^{+}$ is obtained from $\bar{r}_{21}^{+}$ by exchanging $m \leftrightarrow -m$, $V \leftrightarrow W$; $\bar{r}_{i1}^{-}$ $(i = 1, 2, 3)$ is obtained from $\bar{r}_{i1}^{+}$ by exchanging $m \leftrightarrow -m$. The other elements are obtained from those in the first column by cyclic permutations: Making the replacement $U \to V \to W \to U$ in the expression for $\bar{r}_{ij}^{\pm}$, one obtains the matrix element with subscripts i, j replaced according to $1 \to 2 \to 3 \to 1$. It follows that the expressions for all the $\bar{r}_{ij}^{\pm}$ are obtained from (87) by the operations

$$m \to -m, \quad \text{permutations of } U, V, W. \tag{88}$$

Taking into account that $W - U = -(U-V) - (V-W)$, one recognizes that each term of $\bar{r}_{ij}^{\pm}$ contains one of the factors μ, $U-V$, $V-W$ and one of the factors 2ρ, m, $U+V+W$. Each term of $3F$ even contains one of the factors μ, $(U-V)^2$, $(U-V)(V-W)$, $(V-W)^2$ and one of the factors 2ρ, m^2, $(U+V+W)^2$.

With the definitions

$$\beta = \gcd(\mu, U-V, V-W) \tag{89}$$

and

$$\gamma = \gcd(\rho, m, U+V+W) \tag{90}$$

it follows from the remarks made above that $\beta\gamma | \text{all } \bar{r}_{ij}^{\pm}$ (*i.e.* $\beta\gamma$ is a factor of all $\bar{r}_{ij}^{+}$ and of all $\bar{r}_{ij}^{-}$, $i, j = 1, 2, 3$). $\beta\gamma$ is therefore a factor of $3F/\Sigma = 3\delta$, *i.e.*

$$\beta\gamma | 3\delta. \tag{91}$$

The quantity δ, being an integer, can be written uniquely as

$$\delta = d_1 2^{d_2} 3^{d_3}, \tag{92}$$

where the d_i are integers and

$$\gcd(6, d_1) = 1. \tag{93}$$

Similarly, one can write

$$\beta = b_1 2^{b_2} 3^{b_3}, \qquad \gamma = c_1 2^{c_2} 3^{c_3} \tag{94}$$

with integers b_i, c_i and

$$\gcd(6, b_1) = \gcd(6, c_1) = 1. \tag{95}$$

A.2. *Determination of d_1*

It will be shown that

$$d_1 = b_1 c_1. \tag{96}$$

It follows from (91) that $b_1 c_1 | d_1$ but it remains to be shown that $d_1 | b_1 c_1$. Equation (48) shows that

$$\gcd(\mu, \rho) | 3. \tag{97}$$

From (92), (93) it follows because of (55) that $d_1 = BC$, where $B = \gcd(d_1, \mu)$ and $C = \gcd(d_1, \rho)$. $\gcd(B, \rho) = \gcd(C, \mu) = 1$ because of (97). Equations (82)-(85) show therefore that $C|m$, $C|U+V+W$, $B|U-V$, $B|V-W$; *i.e.* $B|\beta$, $C|\gamma$. B and C do not contain factors 2 or 3 so that it follows from (94) that $B|b_1$, $C|c_1$, *i.e.* $d_1|b_1c_1$.

A.3. *Determination of d_2*

Let k be the number of factors of 2 in $\beta\gamma$,

$$k = b_2 + c_2.$$

If $b_2 > 0$ then $2|\mu \xrightarrow{(97)} 2\nmid\rho \to c_2 = 0$. Similarly, it follows from $c_2 > 0$ that $b_2 = 0$ so that either $b_2 = k$ or $c_2 = k$. Relation (91) shows that $2^k|\delta$, *i.e.* $d_2 \geq k$. It will be shown in the following that $d_2 \leq k+2$ and the conditions will be derived under which $d_2 = k+2$ and $d_2 = k+1$ respectively.

(1) Assume $d_2 > k+2$

(1.1) $2\nmid\mu \xrightarrow{(82)\text{-}(85)} 2^{k+1}|m, \quad U+V+W, \quad \rho(U-V), \rho(V-W)$.

It follows because of (90) that $2^k|\rho$, $2^{k+1}\nmid\rho$.

(1.2) $2|\mu \xrightarrow{(82)\text{-}(85)} 2^{k+1}|\mu m, \quad \mu(U+V+W), \quad U-V, V-W$.

It follows because of (89) that $2^k|\mu$, $2^{k+1}\nmid\mu$.

In both cases it follows that $2|m$, $U+V+W$, $U-V$, $V-W$. This is possible only if m, U, V, W are all even, contrary to (36).

(2) Assume $d_2 = k+2$.

(2.1) $2\nmid\rho \to 2\nmid\gamma \to 2^k|\beta \to 2^k|\mu, U-V, V-W$.

(2.1.1.) $k = 0$.

Assume μ even $\xrightarrow{(48)}$ ν odd. Equation (87) shows because $4|r_{21}^+$ that $(V-m)(V-W)$ is even and because $4|r_{23}^+$ that $(V-m)(U-V)$ is even. It follows that $V-m$ is even because μ, $U-V$ and $V-W$ cannot all be even if $k=0$. Using $W-U=-(U-V)-(V-W)$ one can show similarly that also $U-m$ and $W-m$ are even. It follows that $U-V$ and $V-W$ are even, contrary to $k=0$.

$$\Rightarrow \mu \text{ odd} \to \nu \text{ even because } \rho \text{ is odd.}$$

$$4|F \xrightarrow{(49)} 4|m^2+U^2+V^2+W^2$$
$$\xrightarrow{(36)} m,\ U,\ V,\ W \text{ are all odd}$$
$$\xrightarrow{(50)} 4|r_{11}^+, r_{21}^+.$$

(2.1.2) $k>0 \to 2|U-V$, $V-W \to U$, V, W are all even or all odd.

Assume U, V, W even $\xrightarrow{(36)}$ m odd $\xrightarrow{(86)}$ $2^{k+2}|\mu$. Equation (87) shows because $2^{k+2}|r_{21}^+$ that $2^{k+1}|V-W$ and because $2^{k+2}|r_{13}^+$ that $2^{k+1}|U-V$, contrary to the definition of k.

$$\Rightarrow U,\ V,\ W \text{ odd} \xrightarrow{(86)} m \text{ odd or } 2^{k+2}|\mu.$$

Assume m even $\to$ $2^{k+2}|\mu$. Equation (87) shows because $2^{k+2}|r_{21}^+$ that $2^{k+1}|V-W$ and because $2^{k+2}|r_{13}^+$ that $2^{k+1}|U-V$, contrary to the definition of k.

$$\Rightarrow m \text{ odd} \xrightarrow{(87)} 2^{k+2}|r_{11}^+, r_{21}^+.$$

It follows for $k\geq 0$ that

$$m,\ U,\ V,\ W \text{ are all odd.} \qquad (a)$$

Because condition (a) is invariant under the operations (88), it follows from $2^{k+2}|r_{11}^+, r_{21}^+$ that $2^{k+2}|$all $r_{ij}^\pm$, *i.e.* $2^{k+2}|\delta$.

(2.2) $2|\rho \xrightarrow{(48)} 2\nmid\mu$, $\nu \to 2\nmid\beta \to 2^k|\gamma \to 2^k|\rho$, m, $U+V+W$.

Equation (87) shows because $2^{k+2}|r_{21}^+$ that

$$2^{k+1}|\mu(m+U+V+W)V+\rho(V-W)V \quad (98)$$

and because $2^{k+2}|r_{32}^+, r_{13}^+$ that

$$2^{k+1}|\mu(m+U+V+W)W+\rho(W-U)W \quad (99)$$

and

$$2^{k+1}|\mu(m+U+V+W)U+\rho(U-V)U. \quad (100)$$

(2.2.1) $k=0$.

$$4|F \xrightarrow{(86),2|\rho} 4|3m^2+(U+V+W)^2$$
$$\to 2|m+U+V+W.$$

(2.2.2) $k>0$. Equation (36) shows that $2|m$, $U+V+W$ implies that exactly one of the numbers U, V, W is even.

Assume $2^{k+1}\nmid\rho$.

Assume $2^{k+1}\nmid m+U+V+W$.

If U is even then V, W are odd and (98) is not fulfilled. Similarly, it follows from V even that (99) is not fulfilled, from W even that (100) is not fulfilled.

$\Rightarrow 2^{k+1}|m+U+V+W$.

If U is even then V, W are odd and (99) is not fulfilled. Similarly, it follows from V even that (100) is not fulfilled, from W even that (98) is not fulfilled.

$\Rightarrow 2^{k+1}|\rho$. Because only one of the numbers U, V, W is even, it follows from (98)-(100) that $2^{k+1}|m+U+V+W$.

It follows for $k\geq 0$ that

$$2^{k+1}|\rho,\ m+U+V+W. \qquad (b)$$

If (b) holds in the case (2.2) then $2^{k+2}|r_{21}^+, r_{11}^+$. The former holds because (98) is satisfied, the latter because (87) shows that $2^{k+2}|r_{11}^+$ if

$$3m^2+2m(V-W)+(U+V+W)(U-V-W)$$
$$=4m(m+V)$$
$$+(m+U+V+W)(-m+U-V-W)$$

is a multiple of 2^{k+2}. This is fulfilled because it follows from $m+U+V+W$ even that $-m+U-V-W$ is even. Condition (b) being invariant under the operations (88), it follows from $2^{k+2}|r_{11}^+, r_{21}^+$ that $2^{k+2}|$all $r_{ij}^\pm$, *i.e.* $2^{k+2}|\delta$.

(3) Assume $d_2\geq k+1$. Equation (87) shows that $2^{k+1}|r_{21}^+$ is always satisfied.

(3.1) $2\nmid\gamma \to 2^k|\beta \to 2^k|\mu$, $U-V$, $V-W$. $2^{k+1}|F \xrightarrow{(86)} 2^{k+1}|\mu[m^2+(U+V+W)^2] \to 2^{k+1}|\mu$ or $2|m+U+V+W$. $2^{k+1}|r_{11}^+$ is satisfied in both cases.

(3.2) $2|\gamma \to k>0$, $2^k|\rho$, m, $U+V+W \xrightarrow{(87)} 2^{k+1}|r_{11}^+$. $2|m+U+V+W$ is always satisfied in this case.

Because the conditions

$$2|m+U+V+W \qquad (c)$$

and

$$2^{k+1}|\mu \qquad (d)$$

are invariant under the operations (88), it follows from $2^{k+1}|r_{11}^+, r_{21}^+$ that $2^{k+1}|$all $r_{ij}^\pm$, *i.e.* $2^{k+1}|\delta$.

In summary, $d_2=k+2$ holds if and only if one of the conditions (a), (b) is satisfied, $d_2\geq k+1$ holds if and only if one of the conditions (c), (d) is satisfied.

A.4. *Determination of* d_3

Redefine k to be the number of factors of 3 in $\beta\gamma$,

$$k=b_3+c_3.$$

It follows from (48) and $\rho=\mu-3\nu$ that each case belongs to one of three classes. (a) $3^2|\mu \to 3|\rho$, $3^2\nmid\rho$, (b) $3^2\nmid\mu$, $3|\mu \to 3|\rho$, (c) $3\nmid\mu \to 3\nmid\rho$. Two subclasses may be distinguished according to (89), (90) and (94) if (a) or (b) holds, *i.e.* each case belongs to one and only one of the following classes:

(1) $3^2|\mu$ $(\to 3|\rho, 3^2\nmid\rho)$, $b_3=k$, $c_3=0$

(2) $3^2|\mu$ $(\to 3|\rho, 3^2\nmid\rho)$, $b_3=k-1$, $c_3=1$, $k>0$

(3) $3^2\nmid\mu, 3|\mu\ (\to 3|\rho)$, $\quad b_3=0,\ c_3=k$

(4) $3^2\nmid\mu, 3|\mu\ (\to 3|\rho)$, $\quad b_3=1,\ c_3=k-1,\ k>0$

(5) $3\nmid\mu\ (\to 3\nmid\rho)$, $\quad b_3=c_3=0,\ k=0.$

If $d_3>0$, *i.e.* $3|\delta$, then it follows from (55) that $3|\mu\to 3|\rho$. Because $\delta|F$, it follows that $3|F\xrightarrow{(49)}3|(U+V+W)^2-3(VW+WU+UV)\to 3|U+V+W$, *i.e.*

$$\text{If } d_3>0 \text{ then } 3|\mu,\ \rho,\ U+V+W. \tag{101}$$

It follows that $d_3=k=0$ for the cases in class (5).

From (91) it follows that $3^{k-1}|\delta$, *i.e.* $d_3\geq k-1$. It will be shown in the following that $d_3\leq k$ for the cases in the classes (1)-(4) and the conditions will be derived under which $d_3=k$. $3\nmid\nu$ in the classes (1)-(4) because of (48). It follows from (50) that

$$r_{33}^{+}-r_{33}^{-}=4\nu m(U-V) \tag{102}$$

$$r_{11}^{+}-r_{11}^{-}=4\nu m(V-W) \tag{103}$$

$$r_{13}^{+}+r_{13}^{-}=4U[\nu(U+V+W)+\rho W] \tag{104}$$

$$r_{21}^{+}+r_{21}^{-}=4V[\nu(U+V+W)+\rho U] \tag{105}$$

$$r_{32}^{+}+r_{32}^{-}=4W[\nu(U+V+W)+\rho V] \tag{106}$$

$$=4W[\mu V+\nu\{(U-V)-(V-W)\}]. \tag{107}$$

(1) Assume $d_3>k$.

(1.1) $3^2|\mu\ (\to 3|\rho, 3^2\nmid\rho)$, $b_3=k$, $c_3=0$

$$c_3=0\xrightarrow{(90),(101)}3\nmid m\xrightarrow{(82),(102),(103)}3^{k+1}|\mu,$$
$$U-V,\ V-W \text{ contrary to } b_3=k.$$

(1.2) $3^2|\mu\ (\to 3|\rho, 3^2\nmid\rho)$, $b_3=k-1$, $c_3=1$, $k>0$

$$3^2\nmid\rho\xrightarrow{(84),(85)}3^k|U-V,\ V-W\xrightarrow{(89)}3^k\nmid\mu\xrightarrow{(82)}9|m$$

$$3^{k+1}|r_{32}^{+}+r_{32}^{-}\to 3^k|r_{32}^{+}+r_{32}^{-}\xrightarrow{(107)}3|VW$$
$$\xrightarrow{3|U-V,V-W}3|U,\ V,\ W.$$

It follows that $3|m$, U, V, W contrary to (36).

(1.3) $3^2\nmid\mu$, $3|\mu\ (\to 3|\rho)$, $b_3=0$, $c_3=k$
$b_3=0\xrightarrow{(89),(101)}3\nmid U-V$ or $3\nmid V-W$. It follows from (102), (103) that $3^{k+1}|m$ and from (84), (85) that $3^{k+1}|\rho\xrightarrow{(104)-(106)}3^{k+1}|U(U+V+W)$, $V(U+V+W)$, $W(U+V+W)\xrightarrow{(36)}3^{k+1}|U+V+W$ contrary to $c_3=k$.

(1.4) $3^2\nmid\mu$, $3|\mu\ (\to 3|\rho)$, $b_3=1$, $c_3=k-1$, $k>0$

$$3^2\nmid\mu\xrightarrow{(82),(83)}3^k|m,\ U+V+W\xrightarrow{(90)}3^k\nmid\rho$$
$$\xrightarrow{(84),(85)}9|U-V,\ V-W$$

$$3^{k+1}|r_{32}^{+}+r_{32}^{-}\to 3^k|r_{32}^{+}+r_{32}^{-}\xrightarrow{(106)}3|VW.$$

It follows that $3|m$, U, V, W contrary to (36).

(2) Assume $d_3=k$.

(2.1) $3^2|\mu\ (\to 3|\rho, 3^2\nmid\rho)$, $b_3=k$, $c_3=0\xrightarrow{(89)}3^k|\mu$, $U-V$, $V-W$

$$r_{11}^{+}=\underline{\mu}(m^2+U^2-V^2-W^2)$$
$$-2\nu(U+V)\underline{(U-V)}$$
$$-2\nu(W-m)\underline{(V-W)}\to 3^k|r_{11}^{+}$$

$$r_{21}^{+}/2=\underline{\mu}(UV+mW)-2\nu V\underline{(U-V)}$$
$$+\nu(m-V)\underline{(V-W)}\to 3^k|r_{21}^{+}.$$

The conditions $3^k|\mu$, $U-V$, $V-W$ being invariant under the operations (88) because $W-U=-(U-V)-(V-W)$, it follows that $3^k|$all $r_{ij}^{\pm}$, *i.e.* $d_3\geq k$.

(2.2) $3^2|\mu\ (\to 3|\rho, 3^2\nmid\rho)$, $b_3=k-1$, $c_3=1$, $k>0$

$$\xrightarrow{(89),(90)}3^{k-1}|\mu,\ U-V,\ V-W, 3|m,\ U+V+W,\ \rho$$

$$\left.\begin{aligned}&\xrightarrow{(104)\ 3^k|\rho(V-W)}3^k|U[\nu(U+V+W)+\rho V]\\&\xrightarrow{(105)\ 3^k|\rho(U-V)}3^k|V[\nu(U+V+W)+\rho V]\\&\xrightarrow{(106)}3^k|W[\nu(U+V+W)+\rho V]\end{aligned}\right\}$$

$$\xrightarrow{(36)}3^k|\nu(U+V+W)+\rho V$$

$$r_{11}^{+}=\mu m^2+\mu(U+V+W)(U-V-W)$$
$$-2\nu(U+V+W)(U-V)+2\nu m(V-W)$$
$$+2W[\nu(U+V+W)+\rho V] \tag{108}$$
$$r_{21}^{+}/2=m[\mu W+\nu(V-W)]$$
$$+V[\nu(U+V+W)+\rho U].$$

The conditions $3^k|\nu(U+V+W)+\rho V$, $3^{k-1}|\mu$, $U-V$, $V-W$, $3|m$, $U+V+W$, ρ guarantee $3^k|r_{11}^{+}$, r_{21}^{+}; they are invariant under the operations (88) because $\rho W=\rho V-\rho(V-W)$, $\rho U=\rho V+\rho(U-V)$, and $(W-U)=-(U-V)-(V-W)$. It follows that $3^k|$all $r_{ij}^{\pm}$, *i.e.* $d_3\geq k$.

(2.3) $3^2\nmid\mu$, $3|\mu\ (\to 3|\rho)$, $b_3=0$, $c_3=k\xrightarrow{(90)}3^k|\rho$, m, $U+V+W$

$$r_{11}^{+}=\underline{\rho}(U^2-V^2-W^2)+\underline{m}[\mu m+2\nu(V-W)]$$
$$+\nu\underline{(U+V+W)}(U-V-W)\to 3^k|r_{11}^{+}$$
$$r_{21}^{+}/2=\underline{\rho}UV+\underline{m}[\mu W+\nu(V-W)]$$
$$+\nu\underline{(U+V+W)}V\to 3^k|r_{21}^{+}.$$

The conditions $3^k|\rho$, m, $U+V+W$, being invariant under the operations (88), it follows that $3^k|$all $r_{ij}^{\pm}$, *i.e.* $d_3\geq k$.

(2.4) $3^2\nmid\mu$, $3|\mu\ (\to 3|\rho)$, $b_3=1$, $c_3=k-1$, $k>0$

$$\xrightarrow{(89),(90)}3^{k-1}|\rho,\ m,\ U+V+W, 3|\mu,\ U-V,\ V-W.$$

The condition $3^k|\nu(U+V+W)+\rho V$ is derived as in (2.2) if $k>1$; if $k=1$ the condition is satisfied because

$b_3=1$. The conditions $3^k|\nu(U+V+W)+\rho V$, $3^{k-1}|\rho$, m, $U+V+W$, $3|\mu$, $U-V$, $V-W$ guarantee $3^k|r_{11}^+$, r_{21}^+ because of (108); they are invariant under the operations (88). It follows that $3^k|$all $r_{ij}^\pm$, *i.e.* $d_3\geq k$.

$3^k|\nu(U+V+W)+\rho V$ is always satisfied in the case (2.3) and in (2.1) because $\nu(U+V+W)+\rho V=\mu V+\nu(U-V)-\nu(V-W)$. The results on d_3 can therefore be summarized as follows: $d_3=k$ if $3^k|\nu(U+V+W)+\rho V$, $d_3=k-1$ otherwise.

A.5. *The Σ-rhomb theorem*

It will be shown that the results obtained for d_1, d_2 and d_3 are equivalent to the Σ-rhomb theorem. Because of (53), the theorem may be stated as follows:

$$\delta=efgh,$$

where

$$\begin{aligned} e&=\gcd(2, m+U+V+W)\\ f&=\gcd(2, m+U+V+W, U-V, V-W)\\ g&=\gcd[\mu, 2e^{-1}(U-V), 2e^{-1}(V-W)] \qquad (109)\\ h&=\gcd\{\rho, 2f^{-1}m, m+U+V+W,\\ &\qquad 2[\nu(U+V+W)+\rho V]g^{-1}\}. \end{aligned}$$

Notice that all the arguments in the expressions for g and h are integral, in particular g is a factor of

$$\begin{aligned} &2[\nu(U+V+W)+\rho V]\\ &\quad=2V.\mu+e\nu.2e^{-1}(U-V)-e\nu.2e^{-1}(V-W). \end{aligned}$$

Proof of (109): *efgh* may be written uniquely as $\delta_1 2^{\delta_2}3^{\delta_3}$, where the δ_i are integers and $\gcd(6,\delta_1)=1$. It has to be shown that $\delta_i=d_i$ for $i=1,2,3$. Let $\gcd_1(a,b,\dots)$ denote the product of the factors other than 2 and 3 in $\gcd(a,b,\dots)$. Let $\gcd_i(a,b,\dots)$ for $i=2$ or 3 denote the number of the factors of 2 or 3 respectively in $\gcd(a,b,\dots)$.

(1) Equations (109) show that $\delta_1=g_1h_1$, where $g_1=\gcd_1(\mu, U-V, V-W)$ and $h_1=\gcd_1\{\rho, m, U+V+W, [\nu(U+V+W)+\rho V]g_1^{-1}\}$. Equations (89), (94) show $g_1=b_1$, (90), (94) show $c_1=\gcd_1(\rho, m, U+V+W)$, and (97) shows $\gcd(b_1,c_1)=1$. It follows that $h_1=c_1\to\delta_1=b_1.c_1=d_1$ according to (96).

(2) Equations (109) show that $\delta_2=e_2+f_2+g_2+h_2$, where

$$\begin{aligned} e_2&=\gcd_2(2, m+U+V+W)\\ f_2&=\gcd_2(2, m+U+V+W, U-V, V-W)\\ g_2&=\gcd_2[\mu, 2^{1-e_2}(U-V), 2^{1-e_2}(V-W)]\\ h_2&=\gcd_2\{\rho, 2^{1-f_2}m, m+U+V+W,\\ &\qquad 2^{1-g_2}[\nu(U+V+W)+\rho V]\}. \end{aligned}$$

If μ is odd then $g_2=0$. The fourth argument in the expression for h_2 is then a linear combination with integral coefficients of the first three arguments:

$$\begin{aligned} 2[\nu(U+V+W)+\rho V]&=2V\rho-2^{f_2}\nu.2^{1-f_2}m\\ &\quad+2\nu(m+U+V+W) \end{aligned}$$

and may therefore be omitted. If μ is even, then ρ is odd. Already the first argument in the expression for h_2 shows that $h_2=0$. It follows that $h_2=\gcd_2(\rho, 2^{1-f_2}m, m+U+V+W)$ is always true. The following cases may be distinguished:

$$\begin{aligned} &e_2=1\to g_2=b_2\to h_2=c_2+1 && \text{if } f_2=0 \text{ and}\\ & && 2^{c_2+1}|\rho, m+U+V+W,\\ &\qquad\qquad h=c_2 && \text{otherwise.}\\ &e_2=0\to f_2=0=h_2\to g_2=b_2+1 \text{ if } 2^{b_2+1}|\mu\\ &\qquad\qquad \text{and } g_2=b_2 && \text{otherwise.} \end{aligned}$$

It follows that $\delta_2=d_2$ in all the cases distinguished in the calculation of d_2.

(3) $\delta_3=g_3+h_3$, where $g_3=\gcd_3(\mu, U-V, V-W)$ and $h_3=\gcd_3\{\rho, m, U+V+W, 3^{-g_3}[\nu(U+V+W)+\rho V]\}$. Equations (89), (94) show $g_3=b_3$, (90), (94) show $c_3=\gcd_3(\rho, m, U+V+W)$. The five cases distinguished in the calculation of d_3 will be considered separately:

(1) $3^2|\mu$, $c_3=0$

$\to h_3=0$

(2) $3^2|\mu$, $c_3=1$

$\to h_3=1$ if $3^{b_3+1}|\nu(U+V+W)+\rho V$,

$h_3=0$ otherwise

(3) $3^2\nmid\mu$, $3|\mu$, $b_3=0$

$\to h_3=c_3$

(4) $3^2\nmid\mu$, $3|\mu$, $b_3=1$

$\to h_3=c_3$ if $3^{c_3+1}|\nu(U+V+W)+\rho V$,

$h_3=c_3-1$ otherwise

(5) $3\nmid\mu$, $3\nmid\rho$

$\to g_3=h_3=0$.

$\delta_3=d_3$ in all these cases.

APPENDIX *B*
A lower bound for the multiplicity of specific coincidence rotations

B.1. *Introduction*

Specific coincidence rotations exist if the square of the axial ratio is a rational number, *i.e.* $c^2/a^2=3\mu/2\rho$. A lower bound for the multiplicity of these rotations will be derived in terms of μ and ρ. Specific coincidence rotations satisfy

$$u\neq0 \quad\text{or}\quad v\neq0$$
$$\text{and} \qquad\qquad\qquad\qquad\qquad\qquad (110)$$
$$m\neq0 \quad\text{or}\quad w\neq0.$$

Because equivalent rotations have the same multiplicity, it suffices to give a lower bound for the multiplicity of disorientations, *i.e.* m, u, v, w may be restricted by

$$\begin{aligned} &u \geq 0,\ v \geq 0,\ w \geq 0 \\ &m \geq w,\ m \geq (\rho/2\mu)^{1/2}(u+v). \end{aligned} \tag{111}$$

Denote the maximum of u and v by a, $a = \max(u, v)$. Use will be made in the following of (110) and of a subset of (111), *i.e.*

$$\begin{aligned} &u \geq 0,\ v \geq 0,\ a > 0 \\ &m \geq w \geq 0,\ m > 0. \end{aligned} \tag{112}$$

It follows from the Σ-rhomb theorem for rotation symbols that

$$\Sigma \geq f/(3 f_1 f_2 f_3 f_4'),$$

where

$$\begin{aligned} f &= \mu(3m^2 + w^2) + 2\rho(u^2 + uv + v^2), \\ f_1 &= \gcd(2, m+w) \\ f_2 &= \gcd(2, m+w, u, v) \\ f_3 &= \gcd(\mu, 2f_1^{-1}u, 2f_1^{-1}v) \\ f_4' &= \gcd(\rho, 2f_2^{-1}m, m+w). \end{aligned}$$

B.2. Derivation of the bound

Because $\gcd(\mu, \nu) = 1$ and $\rho = \mu - 3\nu$ the following cases can be distinguished:

(a) $2|\nu, 2\nmid\mu \Rightarrow 2\nmid\rho$

(b) $2\nmid\nu, 2|\mu \Rightarrow 2\nmid\rho$

(c) $2\nmid\nu, 2\nmid\mu \Rightarrow 2|\rho$.

Case (a)

$$f_3 = \gcd(\mu, u, v),\ f_4' = \gcd(\rho, m, w).$$

A number of subcases may be distinguished:

(1.1) $m+w$ odd $\to f_1 = f_2 = 1$, $f_3 \leq a$, $f_4' \leq m$, $f \geq 3\mu m^2 + 2\rho a^2$.

(1.2) $m+w$ even, u, v not both even $\to f_1 = 2$, $f_2 = 1$, $f_3 \leq a$, $f_4' = \gcd(\rho, 2m, m+w)$.

(1.2.1) m odd ($\to w$ odd) and $w = m$ $\to f_4' \leq m, f \geq 4\mu m^2 + 2\rho a^2$.

(1.2.2) m odd ($\to w$ odd) and $w < m$ $\to f_4' \leq m/3, f > 3\mu m^2 + 2\rho a^2$.

(1.2.3) m even $\to f_4' \leq m/2, f \geq 3\mu m^2 + 2\rho a^2$.

(1.3) $m+w$, u, v even $\to f_1 = f_2 = 2$, $f_3 \leq a/2$. m and w are odd because of (64).

(1.3.1) $w = m \to f_4' \leq m, f \geq 4\mu m^2 + 2\rho a^2$

(1.3.2) $w < m \to f_4' \leq m/3, f > 3\mu m^2 + 2\rho a^2$.

The lowest bound on Σ follows from (1.2.1) and (1.3.1), *i.e.*

$$\Sigma \geq \frac{2\mu m^2 + \rho a^2}{3ma} = \frac{1}{3}\left(2\mu\frac{m}{a} + \rho\frac{a}{m}\right) = F(m/a).$$

The value of $x = m/a$ for which $F(x)$ becomes a minimum is obtained by setting $\mathrm{d}F/\mathrm{d}x = 0$, *i.e.*

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(2\mu x + \frac{\rho}{x}\right) = 2\mu - \frac{\rho}{x^2} = 0$$

$$\Rightarrow x = \left(\frac{\rho}{2\mu}\right)^{1/2}$$

$$\Rightarrow \Sigma \geq \frac{2\mu}{3}\left(\frac{\rho}{2\mu}\right)^{1/2} + \frac{\rho}{3}\left(\frac{2\mu}{\rho}\right)^{1/2} = \frac{(8\mu\rho)^{1/2}}{3}.$$

Case (b)

The only change with respect to case (a) concerns $f_3 = \gcd(\mu, 2f_1^{-1}u, 2f_1^{-1}v)$: $f_3 \leq 2a$ in (1.1), $f_3 \leq a$ in (1.2) and in (1.3).

The lowest bound on Σ follows therefore from (1.3.1), *i.e.*

$$\Sigma \geq \frac{2\mu m^2 + \rho a^2}{6ma} \Rightarrow \Sigma \geq \frac{(2\mu\rho)^{1/2}}{3}.$$

Case (c)

$$f_3 = \gcd(\mu, u, v),\ f_4' = \gcd(\rho, 2f_2^{-1}m, m+w).$$

(1.1) $m+w$ odd $\to f_1 = f_2 = 1$, $f_3 \leq a$, $f_4' = \gcd(\rho, m, w) \leq m$, $f \geq 3\mu m^2 + 2\rho a^2$.

(1.2) $m+w$ even, u, v not both even $\to f_1 = 2$, $f_2 = 1$, $f_3 \leq a$, $f_4' = \gcd(\rho, 2m, m+w)$.

(1.2.1) m odd ($\to w$ odd) and $w = m$ $\to f_4' \leq 2m, f \geq 4\mu m^2 + 2\rho a^2$.

(1.2.2) m odd ($\to w$ odd) and $w < m$ $\to f_4' \leq 2m/3, f > 3\mu m^2 + 2\rho a^2$.

(1.2.3) m even and $w = 0$ $\to f_4' \leq m, f \geq 3\mu m^2 + 2\rho a^2$.

(1.2.4) m even and $w = m$
$$\to \left\{\begin{matrix} f_4' \leq 2m \text{ if } 4|\rho \\ f_4' \leq m \text{ if } 4\nmid\rho \end{matrix}\right\}, f \geq 4\mu m^2 + 2\rho a^2.$$

(1.2.5) m even and $0 < w < m$ $\to f_4' \leq m/2, f > 3\mu m^2 + 2\rho a^2$.

(1.3) $m+w$, u, v even $\to f_1 = f_2 = 2$, $f_3 \leq a/2$, $f_4' = \gcd(\rho, m, w)$. This coincides with (1.3) in case (a).

The lowest bound on Σ follows from (1.2.1) [same bound from (1.2.4) if $4|\rho$], *i.e.*

$$\Sigma \geq \frac{2\mu m^2 + \rho a^2}{6ma} \Rightarrow \Sigma \geq \frac{(2\mu\rho)^{1/2}}{3}.$$

The results for cases (a)-(c) can be summarized as

$$\Sigma \geq (8\mu\rho)^{1/2}/3 \quad \text{if } \mu\rho \text{ is odd},$$

$$\Sigma \geq (2\mu\rho)^{1/2}/3 \quad \text{otherwise},$$

as stated in theorem 4.

APPENDIX C

Upper bounds for the minimum multiplicity of specific coincidence rotations

The existence of a specific coincidence rotation with multiplicity as given by lemma 1 can be shown as follows: Let μ_0 be a factor of μ, ρ_0 a factor of ρ such that $3\nmid\mu_0, \rho_0$. It follows that either $3|\mu_0 + \rho_0$ or $3|\mu_0 - \rho_0$. Equations (63) and (64) are satisfied in the first case by the rotation symbol $(0\,0\,\mu_0\,.\,\rho_0)$ and in the second case by the rotation symbol $(0\,\mu_0\,0\,.\,\rho_0)$. Choose for μ_0 a factor of $\mu/2$ if μ is even, choose ρ_0 even if ρ is even. The Σ-rhomb theorem gives then for these rotation symbols

$$f = \mu\rho_0^2 + 2\rho\mu_0^2$$

$$f_1 = \gcd(2, \rho_0) = \begin{cases} 1 & \text{if } \rho \text{ is odd} \\ 2 & \text{if } \rho \text{ is even} \end{cases}$$

$$f_2 = 1$$

$$f_3 = \gcd(\mu, \mu_0\,.\,2/f_1) = \begin{cases} \mu_0 & \text{if } \mu \text{ is odd} \\ 2\mu_0 & \text{if } \mu \text{ is even} \end{cases}$$

$$f_4 = \gcd(\rho, \rho_0) = \rho_0,$$

and $\Sigma = f/(3f_1f_2f_3f_4)$ becomes

$$\begin{aligned} \Sigma &= (\mu\rho_0/\mu_0 + 2\rho\mu_0/\rho_0)/3 && \text{if } \mu\rho \text{ is odd,} \\ \Sigma &= (\mu\rho_0/2\mu_0 + \rho\mu_0/\rho_0)/3 && \text{if } \mu\rho \text{ is even.} \end{aligned} \tag{113}$$

If $\mu\rho$ is odd then every integral factor of $2\mu\rho$ with the same number of factors of 3 as ρ is of the form $2\rho\mu_0/\rho_0$. If $\mu\rho$ is even then every integral factor of $\mu\rho/2$ with the same number of factors of 3 as ρ is of the form $\rho\mu_0/\rho_0$ with $2\mu_0|\mu$ if μ is even, ρ_0 even if ρ is even. Equation (113) shows that Σ has the form given in lemma 1.

The existence of a specific coincidence rotation with multiplicity as given by lemma 2 can be shown as follows: Let ρ_0 be a factor of $\rho/3$, μ_0 a factor of μ such that $3|\mu_0$. Equations (63), (64) are satisfied by the rotation symbol $(\rho_0\,0\,\mu_0\,.\,0)$. Choose for μ_0 a factor of $\mu/2$ if μ is even, choose ρ_0 even if ρ is even. The Σ-rhomb theorem gives then for these rotation symbols

$$f = 3\mu\rho_0^2 + 2\rho\mu_0^2,$$

f_1, f_2 and f_3 as in the proof of lemma 1 and

$$f_4 = \gcd(\rho_0, \rho/3) = \rho_0.$$

The multiplicity becomes

$$\begin{aligned} \Sigma &= \mu\rho_0/\mu_0 + (2\rho/3)\mu_0/\rho_0 && \text{if } \mu\rho \text{ is odd,} \\ \Sigma &= \mu\rho_0/2\mu_0 + (\rho/3)\mu_0/\rho_0 && \text{if } \mu\rho \text{ is even.} \end{aligned}$$

If $\mu\rho$ is even then (at least) one of the factors p, q of $\mu\rho/6$ is a multiple of 3. This factor can be written in the form $(\rho\mu_0)/(3\rho_0)$, the other in the form $(\mu\rho_0)/(2\mu_0)$.

If $\mu\rho$ is odd then one has either that one of the factors p, q of $2\mu\rho/3$ is a multiple of 6 or that one is not a multiple of 2 and the other not a multiple of 3. In the first case the factor which is a multiple of 6 can be written as $(2\rho\mu_0)/(3\rho_0)$ and the other factor as $\mu\rho_0/\mu_0$. In the second case consider the rotation symbol $(2\rho_0\,0\,\mu_0\,.\,0)$ with ρ_0, μ_0 as above. The Σ-rhomb theorem gives $f_1 = 2$, $f_2 = 1$, $f_3 = \mu_0$, $f_4 = \rho_0$ and

$$\Sigma = 2\mu\rho_0/\mu_0 + (\rho/3)\mu_0/\rho_0$$

for this symbol. The factor which is not a multiple of 3 can be written as $2\mu\rho_0/\mu_0$, the other as $(\rho\mu_0)/(3\rho_0)$. This completes the proof of lemma 2.

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