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Twinning by reticular pseudo-merohedry in trigonal, tetragonal and hexagonal crystals

Hans Grimmer[a]* and Karsten Kunze[b]

[a]Laboratory for Neutron Scattering, ETHZ and PSI, CH-5232 Villigen PSI, Switzerland, and [b]Geologisches Institut, ETH Zürich, CH-8092 Zürich, Switzerland. Correspondence e-mail: hans.grimmer@psi.ch

Twin laws for trigonal, tetragonal and hexagonal crystals describing twins with principal axes inclined by an angle $\Phi > 0$ are analysed. Twins by reticular merohedry (*i.e.* obliquity $\delta = 0$) are possible only for certain values s of the axial ratio c/a. For any other axial ratio r, the laws describe twinning by reticular pseudo-merohedry, *i.e.* with obliquity $\delta > 0$. It is shown that (a) $\tan\delta$ is a product of two factors, one of which is $\sin\Phi$, the other depends only on the relative deviation of r from s; (b) $\tan\delta \simeq \varepsilon$, where ε denotes the deformation parameter introduced by Bonnet & Durand [*Philos. Mag.* (1975), **32**, 997–1006]. The angle Φ is listed for all cases of reticular merohedry of trigonal, tetragonal and hexagonal (*i.e.* optically uniaxial) crystals with twin index $\Sigma \leq 5$. Mallard's criterion requires that twin laws by (reticular) pseudo-merohedry have $\Sigma \leq 5$ and $\delta \leq 6^\circ$. Le Page [*J. Appl. Cryst.* (2002), **35**, 175–181] has written a program determining laws with twin index $\Sigma \leq \Sigma_{\max}$ and obliquity $\delta \leq \delta_{\max}$ for any given lattice geometry. Here those solutions are analysed and completed for optically uniaxial crystals. Their lattices are characterized by the Bravais class (tP, tI, hP or hR) and the axial ratio $c/a = r$. For small $\delta_{\max}$, most solutions are related to (reticular) merohedry for an appropriate value $s \simeq r$ of the axial ratio. It is argued that other solutions, which are not related to (reticular) merohedry, are not needed to explain observed laws of growth twinning but may be important to interpret observed laws of deformation twinning.

1. Introduction

A twin consists of two adjacent crystal individuals of the same phase, the orientations of which are related by a so-called twin law. The corresponding lattices, 1 and 2, are obviously congruent. We restrict our attention to optically uniaxial crystals, *i.e.* to lattices of Bravais types tP, tI, hP and hR, which have a principal four-, six- or threefold symmetry axis, respectively, and which can be characterized (up to similarity) by the axial ratio c/a. The rotation $\mathbf{R}$ that maps lattice 1 onto lattice 2 can be decomposed as $\mathbf{R} = \mathbf{R}_\perp \mathbf{R}_\parallel$, where $\mathbf{R}_\perp$ and $\mathbf{R}_\parallel$ are rotations with axes perpendicular and parallel to the principal axis of lattice 1, respectively; $\mathbf{R}_\parallel$ is performed first. Owing to the tetragonal, hexagonal or trigonal holohedry of the lattice, the angle and axis of the rotation $\mathbf{R}$ are not uniquely determined. Let Θ be the smallest rotation angle that maps lattice 1 onto 2. Then the angles Φ of $\mathbf{R}_\perp$ and Ψ of $\mathbf{R}_\parallel$ may be chosen such that $0 \leq \Phi \leq \Theta$, $0 \leq \Psi \leq \Theta$ and $\cos(\Phi/2)\cos(\Psi/2) = \cos(\Theta/2)$ (Grimmer & Bonnet, 1990). Because $\mathbf{R}_\parallel$ leaves the principal symmetry axis invariant and $\mathbf{R}_\perp$ rotates it by Φ, it follows from $\mathbf{R} = \mathbf{R}_\perp \mathbf{R}_\parallel$ that Φ is the angle between the principal symmetry axes of the two individuals.

If the rotation is such that lattices 1 and 2 have a fraction $1/\Sigma$ of translation vectors in common, then Σ is always an integer, called twin index or multiplicity. We speak of twinning by merohedry ($\Sigma = 1$) or by reticular merohedry ($\Sigma > 1$), respectively. If $\mathbf{R} = \mathbf{R}_\parallel$, *i.e.* $\Phi = 0$ and $\Psi = \Theta$, then Σ is independent of c/a and $\mathbf{R}$ is called a common coincidence misorientation. If $\Phi > 0$, then Σ depends also on the axial ratio and assumes finite values only for specific ratios $c/a = s$, for which c^2/a^2 is rational, *i.e.* $c^2/a^2 = \mu/\nu$, where μ and ν are integers without common divisor. We then speak of a specific coincidence misorientation.

All common and most specific coincidence misorientations with a low value of Σ can be described also by a 180° rotation about an appropriate lattice direction [uvw]. If this is the case then the plane (hkl) normal to [uvw] is a lattice plane (*i.e.* all six components h, k, l and u, v, w are integers). Both the 180° rotation with axis [uvw] and the mirror reflection in (hkl) then describe the same misorientation of the two lattices. We shall indicate the cases in which the misorientation can be described also by a 60, 90 or 120° rotation. If the point group of the crystal structure is a subgroup of the lattice holohedry, then different descriptions of the same lattice misorientation may correspond to different twin laws by reticular merohedry, *i.e.*

to different relations between the orientations and handedness (if applicable) of the two crystal structures.

If the axial ratio $c/a = r$ slightly deviates from the value s, for which exact coincidence occurs as considered above, then the normal to the twin mirror plane (hkl) no longer coincides with the 180° rotation axis [uvw] but deviates from it by a small angle δ, called the obliquity. One then speaks of twinning by reticular (for $\Sigma > 1$) pseudo-merohedry (Friedel, 1926). Notice that for $\delta > 0$ the mirror reflection in (hkl) and the 180° rotation about [uvw] no longer describe exactly the same misorientation of the two lattices.

Whereas for reticular merohedry the two lattices possess coincident cells M1 and M2 with volumes Σ times larger than the volume of a primitive cell, the two cells are only approximately coincident in the case of reticular pseudo-merohedry. Bonnet & Durand (1975) described the mapping $\mathbf{A}$ that maps M1 onto M2 as a product $\mathbf{A} = \mathbf{R}_o\mathbf{D}$, where $\mathbf{R}_o$ is a rotation and $\mathbf{D}$ a pure deformation, which can be characterized by its principal strains $\varepsilon_1 \le \varepsilon_2 \le \varepsilon_3$. Bonnet & Cousineau (1977) found for hexagonal twins that the principal strains have the form $\varepsilon_1 = -\varepsilon$, $\varepsilon_2 = 0$, $\varepsilon_3 = \varepsilon$ (pure shear) if $\varepsilon << 1$. Grimmer & Bonnet (1990) showed that, considering terms up to first order in ε,

(i) $\mathbf{R}_o$ is the identity,

(ii) the relations $\varepsilon_1 = -\varepsilon$, $\varepsilon_2 = 0$, $\varepsilon_3 = \varepsilon$ are true for all optically uniaxial crystals,

(iii) ε is a product of two factors; one is determined by the misorientation of the two lattices, the other by the relative deviation of the axial ratio r from s,

$$\varepsilon = \frac{|s - r|}{r} \sin \Phi.$$

In this paper, it will be shown that the obliquity δ satisfies

$$\tan \delta = \frac{|s^2 - r^2|}{2rs} \sin \Phi,$$

and thus is related to the deformation parameter ε by

$$\tan \delta = \frac{s + r}{2s} \varepsilon.$$

If r is close to s, then the factor $(s + r)/2s$ is close to 1, so that $\tan\delta \simeq \varepsilon$. The expressions for ε and $\tan\delta$ in terms of $\sin\Phi$ are of importance if one wants to extend all twin laws by reticular merohedry to reticular pseudo-merohedry with ε or δ less than a given upper limit, because the value of $\sin\Phi$ determines how far s may deviate from the axial ratio r of the crystal under consideration.

In many instances, the angle Φ is equal to the rotation angle Θ of the representative rotation $\mathbf{R}$. More specifically, this is the case if $\mathbf{R} = \mathbf{R}_\perp$ is a rotation about an axis perpendicular to the principal axis, *i.e.* the representative integer quadruple (m, U, V, W) has $W = 0$ [for definition see below equation (8)]. This applies to all specific misorientations of hexagonal lattices with $\Sigma \le 7$ and to most specific misorientations of tetragonal lattices with $\Sigma \le 5$, for which the angle Θ has been listed by Grimmer (1989*b*, 2003). The tetragonal cases with $\Phi \ne \Theta$ and all rhombohedral ones with $\Sigma \le 5$ will be listed in this paper.

In §2, the above relations for δ will be derived and illustrated with the example of the (301) twin in metallic tin. In the subsequent three sections, the situation will be reviewed for hexagonal, rhombohedral and tetragonal lattices, respectively.

2. Connection between the obliquity δ and the deformation parameter ε

The angle between the normal to the crystal plane (hkl) and the crystal direction [uvw] is called the obliquity δ. Friedel (1926) gave a formula for δ valid for an arbitrary basis a, b, c, α, β, γ, which was reproduced by Donnay & Donnay (1972). If $\alpha = \beta = 90°$ and $a = b$ (which includes conventional tetragonal and hexagonal bases), it reads

$$\cos^2 \delta = \frac{(uh + vk + wl)^2}{(uh' + vk' + wl')(u'h + v'k + w'l)} \frac{h'(u' + v' \cos \gamma)}{h(u + v \cos \gamma)}. \tag{1a}$$

Here the primed indices are given by

$$(h'k'l') = (u + v \cos \gamma \quad v + u \cos \gamma \quad wc^2/a^2) \tag{1b}$$

and

$$[u'v'w'] = [h - k \cos \gamma \quad k - h \cos \gamma \quad l \sin^2 \gamma a^2/c^2]. \tag{1c}$$

Note that ($h'k'l'$) is the plane normal to [uvw], and [$u'v'w'$] is the direction normal to (hkl). In the tetragonal case ($\gamma = 90°$), equation (1) simplifies to

$$\cos^2 \delta = \frac{(uh + vk + wl)^2}{(u^2 + v^2 + \frac{c^2}{a^2} w^2)(h^2 + k^2 + \frac{a^2}{c^2} l^2)}, \tag{2}$$

and, in the hexagonal case ($\gamma = 120°$), to

$$\cos^2 \delta = \frac{(uh + vk + wl)^2}{(u^2 - uv + v^2 + \frac{c^2}{a^2} w^2)[\frac{4}{3}(h^2 + hk + k^2) + \frac{a^2}{c^2} l^2]}. \tag{3}$$

Consider a case of reticular merohedry with axial ratio $c/a = s$ such that s^2 is a rational number, where the two individuals of the twin are related by a specific coincidence misorientation. This may be described by the twin mirror plane (hkl) or, alternatively, by the 180° rotation with axis [uvw] perpendicular to (hkl), where all six components h, k, l and u, v, w are integers. Per definition, the obliquity is zero between (hkl) and [uvw] for the axial ratio s.

With the indices h, k, l and u, v, w fixed, the obliquity will deviate from zero if the axial ratio $c/a = r$ is different from s. With indices [uvw] set equal to $[u'v'w'] = [hkl/s^2]$ for a tetragonal or $[u'v'w'] = [2h + k \; h + 2k \; 3l/(2s^2)]$ for a hexagonal basis, respectively, the obliquity between (hkl) and [uvw] for an arbitrary aspect ratio $c/a = r$ results from

$$\cos^2 \delta = \frac{(H^2 + l^2/s^2)^2}{(H^2 + l^2 r^2/s^4)(H^2 + l^2/r^2)} \tag{4}$$

with $H^2 = h^2 + k^2$ in the tetragonal and $H^2 = 4/3(h^2 + hk + k^2)$ in the hexagonal case. Equivalently, it is given by

$$\tan\delta = \left[\frac{1-\cos^2\delta}{\cos^2\delta}\right]^{1/2} = \left|\frac{s}{r}-\frac{r}{s}\right|\frac{Hls}{H^2s^2+l^2} = \frac{|s^2-r^2|}{2rs}\sin\varphi, \tag{5}$$

where $\varphi/2 = \arctan(Hs/l)$ is the angle between the normal $[u'v'w']$ of the plane (hkl) and the principal crystal axis of either twin individual for the specific axial ratio $c/a = s$. Since the lattices of both twin individuals are transferred into each other by a mirror operation on the twinning plane (hkl), their principal axes include the angle φ in total.

Let $\mathbf{R}$ be the reduced rotation representing twinning at the plane (hkl), *i.e.* $\mathbf{R}$ is symmetrically equivalent to a 180° rotation about the direction $[u'v'w']$ normal to the twinning plane (hkl). The decomposition $\mathbf{R}(\Theta) = \mathbf{R}_\perp(\Phi)\mathbf{R}_\parallel(\Psi)$ from §1, where $\Phi \le 90°$ is the angle between the principal symmetry axes of the two individuals, shows that the angle φ of (5) is equal to either Φ or $180° - \Phi$. It follows that $\sin\varphi$ may be replaced by $\sin\Phi$ in (5) and that

$$\tan\delta = \frac{s+r}{2s}\frac{|s-r|}{r}\sin\Phi = \frac{s+r}{2s}\varepsilon, \tag{6}$$

where

$$\varepsilon = \frac{|s-r|}{r}\sin\Phi \tag{7}$$

is the deformation parameter as defined by Grimmer & Bonnet (1990).

In other words, by changing the axial ratio from s to r, the angle $\Phi/2$ of the principal axis to the normal of (hkl) [or to (hkl) if $\varphi > 90°$] becomes α with $\tan\alpha = (s/r)\tan(\Phi/2)$, and the angle $\Phi/2$ of the direction $[uvw]$ to the principal axis [or the plane (001) if $\varphi > 90°$] becomes β with $\tan\beta = (r/s)\tan(\Phi/2)$, so that

$$\tan\delta = \tan|\alpha-\beta| = \frac{\left|\frac{s}{r}-\frac{r}{s}\right|\tan\frac{\Phi}{2}}{1+\tan^2\frac{\Phi}{2}} = \frac{1}{2}\left|\frac{s}{r}-\frac{r}{s}\right|\sin\Phi,$$

which is equivalent to (6).

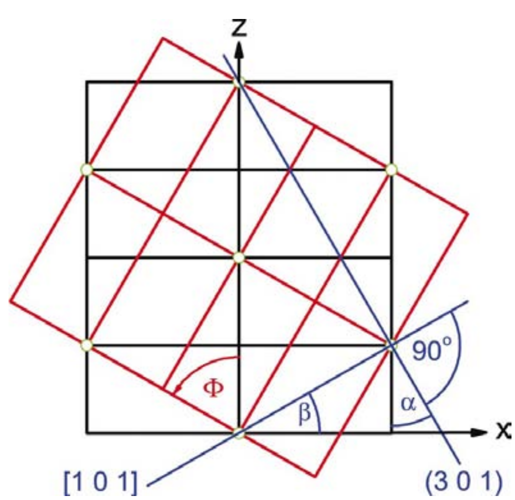

Figure 1
Example of twinning by reticular merohedry with $\Sigma = 2$ of a tetragonal lattice with $c/a = 1/\sqrt{3}$. The 60° rotation Φ maps the black lattice 1 onto the red lattice 2; $\alpha = \beta = \Phi/2$. The twin mirror plane is (301), its normal is [101].

Consider as an example the tetragonal lattice with axial ratio $s = c/a = 1/\sqrt{3}$. The rotation $\mathbf{R}$ by $\Theta = 60°$ about the b axis defines a twin law by reticular merohedry with $\Sigma = 2$ (and $\delta = 0$). Because b is perpendicular to the principal axis c, we have $\mathbf{R}_\perp = \mathbf{R}$ and $\Phi = \Theta = 60°$ (see Fig. 1). The twin law is usually expressed by the twin mirror plane (301) or the 180° rotation with axis [101]. It follows that $\tan(\varphi/2) = Hs/l = \sqrt{3}$, whence $\varphi = 120° = 180° - \Phi$.

Metallic tin (β-Sn) has a body-centred tetragonal lattice with axial ratio $r = 0.5477 \simeq \sqrt{0.3}$, which is close to $s = 1/\sqrt{3} = 0.5774$. For the axial ratio r, the axis [101] is no longer exactly perpendicular to the plane (301), *i.e.* the obliquity no longer vanishes, as shown in Fig. 2.

Fig. 2 shows that the obliquity can be expressed as $\delta = |\alpha - \beta|$; with $\tan\alpha = 1/3r = 1/\sqrt{2.7}$ and $\tan\beta = r = \sqrt{0.3}$, it gives

$$\tan\delta = \tan(t|\alpha-\beta|) = \frac{\tan\alpha - \tan\beta}{1+\tan\alpha\tan\beta} = \frac{1}{4\sqrt{30}}.$$

The same result is obtained using (2) with $(hkl) = (301)$, $[uvw] = [101]$ and $r^2 = c^2/a^2 = 0.3$,

$$\cos^2\delta = \frac{480}{481} \Rightarrow \tan\delta = \left[\frac{1-\cos^2\delta}{\cos^2\delta}\right]^{1/2} = \frac{1}{4\sqrt{30}}, \quad \delta = 2.613°.$$

3. Hexagonal lattices

Given a conventional hexagonal coordinate system with axes c and a, we denote by the quadruple (m, U, V, W) of coprime integers (*i.e.* integers without a common divisor) a rotation with axis $[UVW]$ and angle

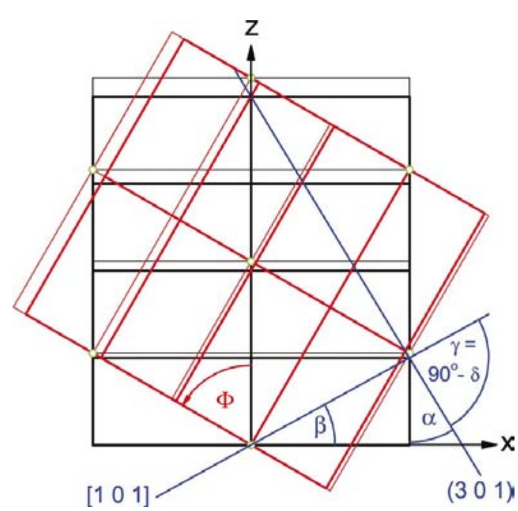

Figure 2
The (301) twin in β-Sn provides an example of twinning by reticular pseudo-merohedry. The 60° rotation Φ maps the black lattices onto the red ones. The lattices of the twin in β-Sn are shown by bold lines; the thin lines repeat the lattices of Fig. 1. The angle γ between [101] and the twin mirror plane (301) in β-Sn is $\gamma = 90° - \delta = 90° + \beta - \alpha$.

Table 1
Specific misorientations of hexagonal lattices with $\Sigma \leq 5$.

		$s^2 = \mu/\nu$			Representative			Twin mirror plane 1		Twin mirror plane 2		Descriptions by rotations with angle		
Σ	$s = c/a$	μ	ν	ω	(m, U, V, W)	$\cos\Theta = \cos\Phi$	$\Theta = \Phi$ (°)	(hkl)	$[uvw]$	(hkl)	$[uvw]$	60°	90°	120°
2	0.5	1	4	3	2 2 1 0	0	90	1 1 1	1 1 2	1 1 $\bar{1}$	1 1 $\bar{2}$		×	
	0.8660	3	4	3	2 3 0 0	0	90	1 0 1	2 1 2	1 0 $\bar{1}$	2 1 $\bar{2}$		×	
	1	1	1	3	1 2 1 0	0	90	1 1 2	1 1 1	1 1 $\bar{2}$	1 1 $\bar{1}$		×	
	1.7321	3	1	3	1 3 0 0	0	90	1 0 2	2 1 1	1 0 $\bar{2}$	2 1 $\bar{1}$		×	
3	0.3536	1	8	6	4 2 1 0	1/3	70.5288	1 1 1	1 1 4	2 2 $\bar{1}$	1 1 $\bar{2}$		×	×
	0.6124	3	8	6	4 3 0 0	1/3	70.5288	1 0 1	2 1 4	2 0 $\bar{1}$	2 1 $\bar{2}$		×	×
	0.7071	1	2	6	2 2 1 0	1/3	70.5288	1 1 2	1 1 2	1 1 $\bar{1}$	1 1 $\bar{1}$		×	×
	1.2247	3	2	6	2 3 0 0	1/3	70.5288	1 0 2	2 1 2	1 0 $\bar{1}$	2 1 $\bar{1}$		×	×
	1.4142	2	1	6	1 2 1 0	1/3	70.5288	1 1 2	2 2 1	1 1 $\bar{4}$	1 1 $\bar{1}$		×	×
	2.4495	6	1	6	1 3 0 0	1/3	70.5288	1 0 2	4 2 1	1 0 $\bar{4}$	2 1 $\bar{1}$		×	×
4	0.25	1	16	3	4 2 1 0	0	90	2 2 1	1 1 4	2 2 $\bar{1}$	1 1 $\bar{4}$		×	
	0.2887	1	12	6	6 2 1 0	1/2	60	1 1 1	1 1 6	3 3 $\bar{1}$	1 1 $\bar{2}$	×		×
	0.4330	3	16	3	4 3 0 0	0	90	2 0 1	2 1 4	2 0 $\bar{1}$	2 1 $\bar{4}$		×	
	0.5	1	4	6	2 1 0 0	1/2	60	1 0 1	2 1 6	3 0 $\bar{1}$	2 1 $\bar{2}$	×		×
	0.5774	1	3	6	3 2 1 0	1/2	60	1 1 2	1 1 3	3 3 $\bar{2}$	1 1 $\bar{1}$	×		×
	0.8660	3	4	6	2 2 1 0	1/2	60	1 1 1	3 3 2	1 1 $\bar{3}$	1 1 $\bar{2}$	×		×
	1	1	1	6	1 1 0 0	1/2	60	1 0 2	2 1 3	3 0 $\bar{2}$	2 1 $\bar{1}$	×		×
	1.5	9	4	6	2 3 0 0	1/2	60	1 0 1	6 3 2	1 0 $\bar{3}$	2 1 $\bar{2}$	×		×
	1.7321	3	1	6	1 2 1 0	1/2	60	1 1 2	3 3 1	1 1 $\bar{6}$	1 1 $\bar{1}$	×		×
	2	4	1	3	1 4 2 0	0	90	1 1 4	2 2 1	1 1 $\bar{4}$	2 2 $\bar{1}$		×	
	3	9	1	6	1 3 0 0	1/2	60	1 0 2	6 3 1	1 0 $\bar{6}$	2 1 $\bar{1}$	×		×
	3.4641	12	1	3	1 6 0 0	0	90	1 0 4	4 2 1	1 0 $\bar{4}$	4 2 $\bar{1}$		×	
5	0.2041	1	24	6	6 2 1 0	1/5	78.4630	2 2 1	1 1 6	3 3 $\bar{1}$	1 1 $\bar{4}$			
	0.25	1	16	6	8 2 1 0	3/5	53.1301	1 1 1	1 1 8	4 4 $\bar{1}$	1 1 $\bar{2}$			
	0.3536	1	8	6	2 1 0 0	1/5	78.4630	2 0 1	2 1 6	3 0 $\bar{1}$	2 1 $\bar{4}$			
	0.4082	1	6	6	3 2 1 0	1/5	78.4630	1 1 1	1 1 3	3 3 $\bar{2}$	1 1 $\bar{2}$			
	0.4330	3	16	6	8 3 0 0	3/5	53.1301	1 0 1	2 1 8	4 0 $\bar{1}$	2 1 $\bar{2}$			
	0.5	1	4	6	4 2 1 0	3/5	53.1301	1 1 2	1 1 4	2 2 $\bar{1}$	1 1 $\bar{1}$			
	0.6124	3	8	6	2 2 1 0	1/5	78.4630	1 1 1	3 3 4	2 2 $\bar{3}$	1 1 $\bar{2}$			
	0.7071	1	2	6	1 1 0 0	1/5	78.4630	1 0 1	2 1 3	3 0 $\bar{2}$	2 1 $\bar{2}$			
	0.8165	2	3	6	3 4 2 0	1/5	78.4630	1 1 2	2 2 3	3 3 $\bar{4}$	1 1 $\bar{1}$			
	0.8660	3	4	6	4 3 0 0	3/5	53.1301	1 0 2	2 1 4	2 0 $\bar{1}$	2 1 $\bar{1}$			
	1	1	1	6	2 2 1 0	3/5	53.1301	1 1 1	2 2 1	1 1 $\bar{4}$	1 1 $\bar{2}$			
	1.0607	9	8	6	2 3 0 0	1/5	78.4630	1 0 1	6 3 4	2 0 $\bar{3}$	2 1 $\bar{2}$			
	1.2247	3	2	6	1 2 1 0	1/5	78.4630	1 1 2	3 3 2	1 1 $\bar{3}$	1 1 $\bar{1}$			
	1.4142	2	1	6	1 2 0 0	1/5	78.4630	1 0 2	4 2 3	3 0 $\bar{4}$	2 1 $\bar{1}$			
	1.7321	3	1	6	2 3 0 0	3/5	53.1301	1 0 1	4 2 1	1 0 $\bar{4}$	2 1 $\bar{2}$			
	2	4	1	6	1 2 1 0	3/5	53.1301	1 1 2	4 4 1	1 1 $\bar{8}$	1 1 $\bar{1}$			
	2.1213	9	2	6	1 3 0 0	1/5	78.4630	1 0 2	6 3 2	1 0 $\bar{3}$	2 1 $\bar{1}$			
	2.4495	6	1	6	1 4 2 0	1/5	78.4630	1 1 4	3 3 1	1 1 $\bar{6}$	2 2 $\bar{1}$			
	3.4641	12	1	6	1 3 0 0	3/5	53.1301	1 0 2	8 4 1	1 0 $\bar{8}$	2 1 $\bar{1}$			
	4.2426	18	1	6	1 6 0 0	1/5	78.4630	1 0 4	6 3 1	1 0 $\bar{6}$	4 2 $\bar{1}$			

$$\Theta = 2\arctan\left\{\frac{1}{m}\left[\frac{a^2(U^2 - UV + V^2) + c^2W^2}{3c^2}\right]^{1/2}\right\}. \qquad (8)$$

The angle Θ has the same sign as m; the rotation is anticlockwise for $m > 0$ and clockwise for $m < 0$. In general, there are 12×24 rotations that describe the same misorientation of two congruent hexagonal lattices. The number of actually different rotations can be written as 12ω, where ω is a divisor of 24 (Grimmer, 1980; Grimmer & Warrington, 1987). Because $\pm(m, U, V, W)$ describe the same rotation (both axis and angle change sign), there are 24ω different quadruples.

Grimmer (1989*b*) determined for primitive hexagonal lattices all the twin laws by reticular merohedry with $\Sigma \leq 7$ that correspond to specific misorientations. We list in Table 1 the cases with $\Sigma \leq 5$ in a form better suited to compute the obliquity according to equation (3). The misorientations appear in the order of increasing Σ values and, for fixed Σ, in the order of increasing $s = c/a$. The rational value of s^2 is given as μ/ν. The number of different quadruples of coprime integers describing the misorientation is 24ω, of which only one is listed: the representative quadruple, which describes a rotation with minimum rotation angle and satisfies $m > 0$, $U \geq 2V \geq 0$, $W \geq 0$ (Grimmer & Warrington, 1987). Table 1 shows that $W = 0$ holds for all the representative quadruples with $\Sigma \leq 5$, whence $\Phi = \Theta$.[1] From among the rotations that describe the same misorientation, we listed two 180° rotations with mutually perpendicular axes $[uvw]$ satisfying $2v \geq u \geq v \geq 0$ and $w > 0$ in the first, $w < 0$ in the second case. The planes normal to $[uvw]$ are called twin mirror planes and have Miller indices (hkl) satisfying $h \geq k \geq 0$ and $l > 0$ in the first, $l < 0$ in

[1] Note that the quadruple $\{M\ u\ v\ .\ w\}$ used in Grimmer (1989*b*) is based on 4-index Weber notation and is proportional to $\{3m\ U{+}V\ U{-}2V.\ 3W\}$. Those quadruple components uvw are not identical to the indices $[uvw]$ used here for the axis normal to the twin mirror plane.

Table 2
Obliquities $\delta < 6^\circ$ for twin laws with $\Sigma \le 8$ in quartz.

For the twin laws within parentheses, the twin plane/twin axis pairs 1 and 2 must be exchanged and the signs of all four third components (l_1, w_1, l_2, w_2) reversed. Rows marked A in the last column were discussed by Friedel (1923) on page 90; those marked B were mentioned on page 92 as giving previous solutions with a larger twin index Σ; the one marked 0 was not discussed at all.

			Twin mirror plane 1		Twin mirror plane 2					
s	s^2	Σ	(hkl)	$[uvw]$	(hkl)	$[uvw]$	$\Theta = \Phi$ (°)	δ (°)	Twin laws	F
1	1	2	1 1 2	1 1 1	$1\,1\,\bar{2}$	$1\,1\,\bar{1}$	90	5.4526	Japan	A
		4	1 0 2	2 1 3	$3\,0\,\bar{2}$	$2\,1\,\bar{1}$	60	4.7257	Sardinian (Belowda)	B
		5	1 1 1	2 2 1	$1\,1\,\bar{4}$	$1\,1\,\bar{2}$	53.1301	4.3668	Breithaupt	A
		7	1 0 1	4 2 3	$3\,0\,\bar{4}$	$2\,1\,\bar{2}$	81.7868	5.3970	Esterel	B
		8	4 1 2	3 2 1			Φ = 41.4096	3.6127		A
							Θ = 46.5674			
1.0607	9/8	5	1 0 1	6 3 4	$2\,0\,\bar{3}$	$2\,1\,\bar{2}$	78.4630	2.0441	Esterel	B
		7	2 0 1	6 3 2	$1\,0\,\bar{3}$	$2\,1\,\bar{4}$	44.4153	1.4603	Cornish	A
1.0954	6/5	7	1 0 2	4 2 5	$5\,0\,\bar{4}$	$2\,1\,\bar{1}$	64.6231	0.2148	Sardinian	B
1.1180	5/4	6	1 1 1	5 5 2	$1\,1\,\bar{5}$	$1\,1\,\bar{2}$	48.1897	0.6945	Breithaupt	B
		8	1 0 1	10 5 6	$3\,0\,\bar{5}$	$2\,1\,\bar{2}$	75.5225	0.9021	Esterel	B
1.1547	4/3	7	1 1 2	4 4 3	$3\,3\,\bar{8}$	$1\,1\,\bar{1}$	81.7868	2.7511	Japan	B
		8	1 1 4	2 2 3	$3\,3\,\bar{4}$	$2\,2\,\bar{1}$	60	2.4076		B
1.2247	3/2	3	1 0 1	2 1 1	$1\,0\,\bar{2}$	$2\,1\,\bar{2}$	70.5288	5.7942	Esterel (Sardinian)	A
		7	1 1 1	3 3 1	$1\,1\,\bar{6}$	$1\,1\,\bar{2}$	44.4153	4.3077		0

the second case. This choice guarantees that $[uvw]_1$ lies in the plane $(hkl)_2$ and $[uvw]_2$ in $(hkl)_1$. Neither the integers h, k, l nor the integers u, v, w have a common divisor. If we define $S = hu + kv + lw$, the multiplicity (twin index) becomes $\Sigma = S$ if S is odd, $\Sigma = S/2$ if S is even (Friedel, 1926; Donnay & Donnay, 1972).

Certain twin laws are usually expressed by rotations of (approximately) 60, 90 or 120° about a crystallographic axis (see *e.g.* Friedel, 1926). The last columns in Table 1 show which specific misorientations with $\Sigma \le 5$ have such (exact) descriptions: 90° descriptions exist in all cases with $\cos\Theta = 0$. (Note that one of these is also the representative rotation with axis either [100] or [210].) 90 and 120° descriptions exist in all cases with $\cos\Theta = 1/3$; 60 and 120° descriptions in all cases with $\cos\Theta = 1/2$. (The representative rotations for the latter give 60° descriptions with axis either [100] or [210].) Note that all misorientations listed in Table 1 can be described also by 180° rotations about the directions $[uvw]$.

Two hexagonal lattices with axial ratios s_1 and s_2 satisfying $(s_1 s_2)^2 = 3/4$ will be called pseudo-reciprocal because primitive bases $\mathbf{e}_i$ in lattice 1 and $\mathbf{f}_i$ in lattice 2, $i = 1, 2, 3$, can be defined that satisfy $\mathbf{e}_i \cdot \mathbf{f}_j = k\delta_{ij}$, where k is a constant of dimension length squared. Table 1 shows that to each misorientation of a hexagonal lattice with a given value of Σ there corresponds a related misorientation of its pseudo-reciprocal lattice with the same Σ value. This is illustrated in Fig. 3.

Consider quartz as an example. It has a hexagonal lattice with axial ratio $r = 1.1$ at ambient temperature and pressure. Friedel (1923) discussed twin laws in quartz satisfying $\Sigma \le 8$ and $\delta < 6^\circ$. From Table 1 extended to $\Sigma \le 8$ the possibilities listed in Table 2 are obtained.

Several of the twin mirror planes (hkl) given in Table 2 have been observed in high-quartz by Drugman (1927, 1930). These are the Japan (Verespatak) (112), Esterel (101), Sardinian (102), Belowda (302), Cornish (201) and Breithaupt (111) laws. Mallard's criterion ($\Sigma \le 5$, $\delta < 6^\circ$) associates particularly low twin indices $\Sigma = 3$ to the Esterel law and $\Sigma = 2$ to the Japan (Verespatak) law, most common in high-quartz (Frondel, 1962), and explains in addition to these and the Sardinian law also the Belowda and Breithaupt laws (which were actually observed in high-quartz only after 1923). The conclusion by Friedel (1923) that $\Sigma \le 5$, $\delta < 6^\circ$ is sufficient to explain the twin laws observed in high-quartz seems questionable in view of further laws observed by Drugman (1927), *i.e.* Cornish (201), Wheal Coates (211), Pierre-Levée (213) and Zinnwald, of which only the Cornish law ($\mu/\nu = 9/8$, $\Sigma = 7$, $\delta = 1.4603^\circ$) appears in Table 2. The lowest twin indices with $\delta < 6^\circ$ are $\Sigma = 15$ ($\mu/\nu = 3/2$, $\delta = 3.0735^\circ$) for Wheal Coates and $\Sigma = 13$ ($\mu/\nu = 9/8$, $\delta = 2.0800^\circ$) for Pierre-Levée. Friedel (1933) mentioned the additional twin laws found by Drugman (1927, 1930) but did not examine them from the point of view of Mallard's criterion. He only discussed the Zinnwald law in

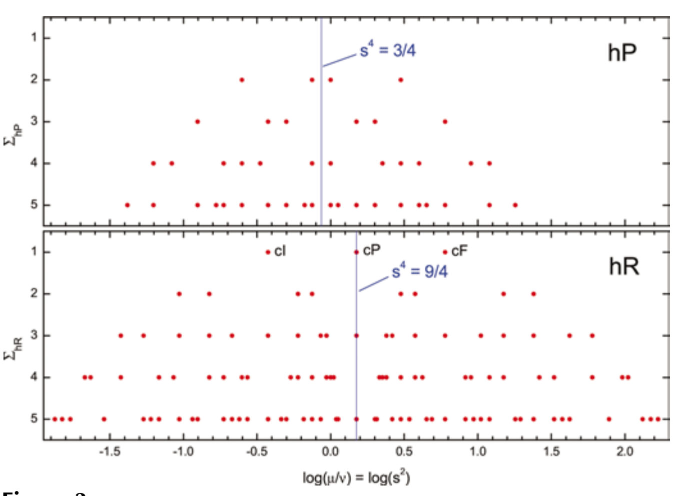

Figure 3
Specific misorientations of primitive (hP) and rhombohedrally centred (hR) hexagonal lattices with multiplicity (twin index) $\Sigma \le 5$ as a function of the axial ratio s.

detail and concluded that this law cannot be explained by Mallard's criterion. We shall come back to this in §6.

The output from the program *OBLIQUE* (available at http://ylp.icpet.nrc.ca/oblique/) by Le Page (2002), carried out for *hP* with $c/a = 1.1$, $\Sigma \leq 8$ and $\delta < 6°$, contains the following solutions: (*a*) the trivial solution corresponding to the symmetry operations of *hP*, (*b*) the common coincidence misorientation with $\Sigma = 7$, (*c*) all the 14 solutions in Table 2 with $\delta < 6°$, (*d*) 17 additional solutions that do not correspond to $[uvw] \perp (hkl)$ in an *hP* lattice with an appropriate value of c/a (collected in Table 3).

Table 3
Additional solutions obtained with program *OBLIQUE* of Le Page (2002) for *hP* with axial ratio $r = 1.1$ (quartz) that satisfy $\Sigma \leq 8$ and $\delta < 6°$.

Only the solution in bold was discussed by Friedel (1923). Further solutions, which are missed by *OBLIQUE*, are given with indices $l' \leq 0$ and $w' \leq 0$.

Additional solutions from *OBLIQUE*				Further solutions	
Σ	(*hkl*)	[*uvw*]	δ (°)	($h'k'l'$)	[$u'v'w'$]
4	1 0 1	5 3 3	5.3241		
5	5 5 1	1 1 0	5.1944	$0\,0\,\bar{1}$	$1\,1\,\overline{10}$
6	**2 1 1**	**4 3 1**	**2.9037**		
6	6 6 1	1 1 0	4.3323	$0\,0\,\bar{1}$	$1\,1\,\overline{12}$
6			5.3126	$1\,0\,\bar{1}$	$7\,4\,\bar{5}$
6	7 5 0	1 1 0	5.4964		
6			5.4964	1 0 0	12 7 0
6	3 2 7	1 1 1	5.7938		
7	7 7 1	1 1 0	3.7153	$0\,0\,\bar{1}$	$1\,1\,\overline{14}$
7			4.2451	$1\,0\,\bar{1}$	$9\,5\,\bar{5}$
7	4 3 0	1 1 0	4.7150		
7			4.7150	1 0 0	7 4 0
7	1 0 14	0 0 1	5.1841	1 0 0	$14\,7\,\bar{1}$
7	8 6 1	1 1 0	5.9926		
8	8 8 1	1 1 0	3.2519	$0\,0\,\bar{1}$	$1\,1\,\overline{16}$
8	4 3 9	1 1 1	3.5203		
8	9 7 0	1 1 0	4.1278		
8			4.1278	1 0 0	16 9 0
8	1 0 16	0 0 1	4.5389	1 0 0	$16\,8\,\bar{1}$
8			4.6930	$2\,0\,\bar{1}$	$7\,4\,\bar{2}$
8	3 1 1	4 3 1	5.1142		
8	9 7 1	1 1 0	5.2480		
8	8 0 1	2 1 0	5.6205	$0\,0\,\bar{1}$	$2\,1\,\overline{16}$

The further solutions listed in Table 3 were obtained by examining the output of *OBLIQUE* for the pseudo-reciprocal lattice. These solutions show that *OBLIQUE* generally does not give all solutions up to the chosen maximum values of Σ and δ. The main reason why *OBLIQUE* misses some solutions seems to be the circumstance that it does not treat [*uvw*] and (*hkl*) on an equal footing in contrast to their entries in the formulas for Σ and δ, which is compensated here by considering also the solutions for the pseudo-reciprocal lattice. We did not investigate whether this suffices for obtaining all solutions in cases that are not related to reticular merohedry.

In 12 of the 17 solutions from *OBLIQUE* listed in Table 3 (all those with [*uvw*] = [110], [210] or [001]), [*uvw*] describes the rotation axis of a twofold symmetry of high-quartz, whereas the corresponding (*hkl*) is a mirror plane slightly inclined to a symmetry plane of the *hP* lattice. Those mirror planes have large indices and were hardly ever observed in high-quartz twins. Among the mirror planes (*hkl*) in the five remaining solutions from *OBLIQUE*, (101) corresponds to Esterel twins and (211) to Wheal Coates twins. The former appears already in Table 2 with $\Sigma = 3$. Similarly, in ten of the 13 further solutions [all those with ($h'k'l'$) = (100) or (001)] ($h'k'l'$) gives $\Sigma > 1$ descriptions of the $\Sigma = 1$ merohedral twin, two others describe the Esterel twin and one the Cornish twin, all with larger values of Σ than the descriptions with lowest Σ value given in Table 2. The axes [$u'v'w'$] of 180° rotations have large indices in all 13 cases and were never observed in high-quartz twins. The additional solutions given in Table 3 were all but one neglected also by Friedel (1923). Whereas it seems doubtful whether they play a role in the description of growth twins from twinned nuclei, it will be shown that such solutions may be important to describe deformation twins.

Consider deformation twins in the h.c.p. metals Be, Ti, Zr, Re, Mg and Co as an example. According to Rosenbaum (1964) and Hagège (1989), the twin mirror planes listed in Table 4 have been observed.

Table 4
Twin mirror planes observed in deformation twins of h.c.p. metals.

r is the experimentally determined value of the axial ratio.

Element	Be	Ti	Zr	Re	Mg	Co
Axial ratio, *r*	1.568	1.587	1.593	1.615	1.623	1.623
(101)					×	
(102)	×	×	×	×	×	×
(103)					×	
(111)		×	×	×		×
(112)		×	×			
(113)			×			

Table 5 gives the obliquities obtained for those twin laws from Table 1 that have c/a close to the values *r* of Table 4.

Table 5
Obliquities $\delta < 6°$ for twin laws with $\Sigma \leq 5$ in h.c.p. metals (Mallard's criterion).

The solutions corresponding to observed twin laws are in bold.

		Twin mirror plane 1		Twin mirror plane 2			Obliquity δ (°) for r =					
							1.568	1.587	1.593	1.615	1.623	1.623
s	Σ	(*hkl*)	[*uvw*]	(*hkl*)	[*uvw*]	$\Theta = \Phi$ (°)	Be	Ti	Zr	Re	Mg	Co
1.4142	3	1 1 2	2 2 1	$1\,1\,\bar{4}$	$1\,1\,\bar{1}$	70.5288	5.569					
	5	1 0 2	4 2 3	$3\,0\,\bar{4}$	$2\,1\,\bar{1}$	78.4630	**5.786**					
1.5	4	1 0 1	6 3 2	$1\,0\,\bar{3}$	$2\,1\,\bar{2}$	60	2.200	2.797	2.984	3.664	**3.909**	3.909
1.7321	2	1 0 2	2 1 1	$1\,0\,\bar{2}$	$2\,1\,\bar{1}$	90	**5.692**	**5.005**	**4.789**	**4.006**	**3.723**	**3.723**
	4	1 1 2	3 3 1	$1\,1\,\bar{6}$	$1\,1\,\bar{1}$	60	4.933	**4.337**	**4.150**	3.471	3.226	3.226
	5	1 0 1	4 2 1	$1\,0\,\bar{4}$	$2\,1\,\bar{2}$	53.1301	4.559	4.007	3.835	3.207	**2.980**	2.980

Table 6
Additional solutions obtained with program *OBLIQUE* of Le Page (2002) for hP with r = 1.593 that satisfy either $\Sigma = 1$, $\delta < 18°$ or Mallard's criterion $\Sigma \leq 5$, $\delta < 6°$.

The quasi-normal pair 2 is missing in the output of *OBLIQUE*.

	Quasi-normal pair 1		Quasi-normal pair 2		Obliquity δ (°)
Σ	$(hkl)_1$	$[uvw]_1$	$(hkl)_2$	$[uvw]_2$	for r = 1.593
1	1 1 1	1 1 0	0 0 $\bar{1}$	1 1 $\bar{2}$	17.426
3	3 3 1	1 1 0	0 0 $\bar{1}$	1 1 $\bar{6}$	5.973
4	4 4 1	1 1 0	0 0 $\bar{1}$	1 1 $\bar{8}$	4.487
5	5 5 1	1 1 0	0 0 $\bar{1}$	1 1 $\overline{10}$	3.592

Table 4 shows that twins with mirror plane (102) have been observed in all the h.c.p. metals considered. This law satisfies Mallard's criterion with a low twin index $\Sigma = 2$ and obliquities $3.7 < \delta < 5.7°$. It has the particular property that twin laws 1 and 2 are symmetrically equivalent formulations. In the case of Be, Table 5 contains a second description satisfying the Mallard limits; it confirms (102) and [211] as possible twin laws and suggests (304) and [423] as less likely ones because Σ and δ are larger in this description than in the first one.

Twins with mirror plane (111) were observed in four of the six metals listed in Table 4. They do not satisfy the Mallard criterion according to Table 5. Also the (113) twin reported in Zr does not satisfy the Mallard criterion.

The output of the program *OBLIQUE* by Le Page (2002), carried out for hP with c/a = 1.593 (axial ratio of Zr), $\Sigma \leq 5$ and $\delta < 6°$, contains the following solutions: (*a*) the trivial solution corresponding to the symmetry operations of hP, (*b*) all the solutions for Zr in Table 5, (*c*) three additional solutions that do not correspond to $[uvw] \perp (hkl)$ in an hP lattice with an appropriate value of c/a (collected in Table 6).

Note that, in all four cases in Table 6, $[uvw]_1$ = [110] is the axis of a 180° symmetry rotation of the hP lattice, which is perpendicular to its symmetry plane (110), similarly $(hkl)_2$ = $(00\bar{1})$ is a symmetry plane of the hP lattice, which is perpendicular to the axis $[00\bar{1}]$ of one of its 180° symmetry rotations.

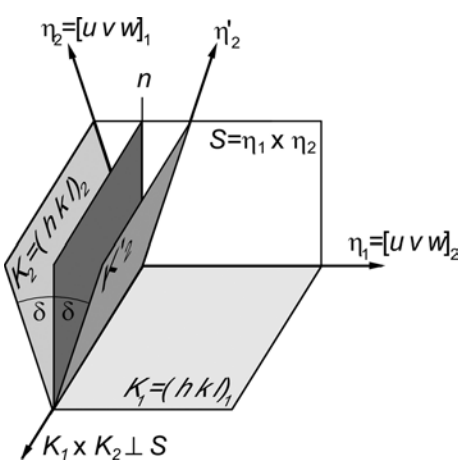

Figure 4
Definition of planes and directions for deformation twins. K_1 is the twin habit plane, K_2 the second plane that is not distorted by the twinning shear; n is normal to K_1; S is normal to K_1 and K_2 and is called the plane of shear. The twinning shear $g = 2\tan\delta$ is in the direction of η_1 and maps η_2 onto η_2'.

Table 7
Obliquities for some common deformation twins in h.c.p. metals calculated for the observed twinning shear.

					Obliquity δ (°) for	
Σ	K_1	η_2	K_2	η_1	Ti (r = 1.587)	Zr (r = 1.593)
2	1 0 2	2 1 1	1 0 $\bar{2}$	2 1 $\bar{1}$	5.005	4.789
1	1 1 1	1 1 0	0 0 $\bar{1}$	1 1 $\bar{2}$	17.488	17.426
3	1 1 2	2 2 1	1 1 $\bar{4}$	1 1 $\bar{1}$	6.216	6.419

The solutions with the lowest Σ values for each of the three values of s (*i.e.* the first, third and fourth rows in Table 5) correspond to deformation twin systems as described by Yoo (1981) (the third, second and first system, respectively, in his Table 4), when the following entities are identified (see also Fig. 4):

$$\begin{array}{rcll} (hkl)_1 & \leftrightarrow & K_1 & \text{(twin habit plane)} \\ (hkl)_2 & \leftrightarrow & K_2 & \text{(second undistorted plane)} \\ [uvw]_2 & \leftrightarrow & \eta_1 & \text{(glide direction)} \\ [uvw]_1 & \leftrightarrow & \eta_2 & \\ \Sigma & \leftrightarrow & q/2 & (\Sigma = \text{twin index}) \\ \delta & \leftrightarrow & \arctan(g/2) & (g = \text{twinning shear}) \\ r & \leftrightarrow & \gamma & \text{(axial ratio)} \end{array} \qquad (9)$$

These correspondences show that the twin system with K_1 = (111) in Yoo's Table 4 corresponds to the solution in our Table 6 with $\Sigma = 1$ and $\delta = 17.426°$. We note that deformation twins always correspond to pseudo-merohedry because the twinning shear $g = 2\tan\delta$, which is responsible for strain relief, vanishes if $\delta = 0$. Even values of δ much larger than allowed by Mallard's criterion may occur for deformation twins, which are commonly characterized by a very low index Σ. Examples are shown in Table 7, where the obliquities for Ti and Zr are listed for the most common deformation twins in h.c.p. metals (*cf.* Table 4 and Fig. 4 in Yoo, 1981).

4. Rhombohedral lattices

In contrast to primitive hexagonal lattices (hP), where $\Phi = \Theta$ in all cases with $\Sigma \leq 7$, we have $\Phi < \Theta$ in most cases of rhombohedral lattices (hR), even for low values of Σ. The cases with $\Sigma \leq 5$ are listed in Tables 8 and 9. There are in general 6×12 rotations that describe a given misorientation of two congruent hR lattices, of which 6ω are actually different (Grimmer, 1980, 1989*a*). Whereas in Grimmer (1989*a*) the quadruple (m, U, V, W) referred to rhombohedral axes, we use in the present paper the same conventional hexagonal coordinate system with three coordinate axes for hP and hR lattices and write $c^2/a^2 = \mu/\nu$ (as for primitive hexagonal lattices) instead of $c^2/a^2 = 3\mu/(2\mu - 6\nu)$. The representative quadruple (m, U, V, W) describes a rotation with minimum rotation angle given by equation (8) and satisfies $m > 0$, $2U \geq V \geq \frac{1}{2}U \geq 0$, $W \geq 0$. It is listed in Tables 8 and 9 together with $\cos\Theta$, $\cos\Phi$ and Φ. From among the rotations that describe the same misorientation, we list two 180° rotations with

Table 8
Specific misorientations of rhombohedral lattices with $\Sigma \leq 4$.

		$s^2 = \mu/\nu$			Representative				Twin mirror plane 1		Twin mirror plane 2		Descriptions by rotations with angle		
Σ	$s = c/a$	μ	ν	ω	(m, U, V, W)	$\cos\Theta$	$\cos\Phi$	Φ (°)	(hkl)	$[uvw]$	(hkl)	$[uvw]$	60°	90°	120°
1	0.6124	3	8	3	2 1 2 2	0	1/3	70.5288	1 0 1	2 1 4	2 0 $\bar{1}$	2 1 $\bar{2}$		×	×
	1.2247	3	2	3	1 2 1 1	0	1/3	70.5288	0 1 2	1 2 2	0 1 $\bar{1}$	1 2 $\bar{1}$		×	×
	2.4495	6	1	3	1 2 4 1	0	1/3	70.5288	0 1 2	2 4 1	0 1 $\bar{4}$	1 2 $\bar{1}$		×	×
2	0.3062	3	32	3	4 2 1 4	0	1/3	70.5288	0 2 1	1 2 8	0 4 $\bar{1}$	1 2 $\bar{4}$		×	×
	0.3873	3	20	3	5 1 2 5	1/4	2/3	48.1897	1 0 1	2 1 10	5 0 $\bar{1}$	2 1 $\bar{2}$			
	0.7746	3	5	3	5 4 2 5	1/4	2/3	48.1897	0 1 2	1 2 5	0 5 $\bar{2}$	1 2 $\bar{1}$			
	0.8660	3	4	3	1 1 2 1	−1/4	0	90	1 0 1	6 3 6	3 0 $\bar{3}$	2 1 $\bar{2}$			
	1.7321	3	1	3	1 2 4 1	−1/4	0	90	0 1 2	3 6 3	0 3 $\bar{6}$	1 2 $\bar{1}$			
	1.9365	15	4	3	1 2 1 1	1/4	2/3	48.1897	1 0 1	10 5 2	1 0 $\bar{5}$	2 1 $\bar{2}$			
	3.8730	15	1	3	1 2 4 1	1/4	2/3	48.1897	0 1 2	5 10 1	0 1 $\overline{10}$	1 2 $\bar{1}$			
	4.8990	24	1	3	1 8 4 1	0	1/3	70.5288	1 0 4	8 4 1	1 0 $\bar{8}$	4 2 $\bar{1}$		×	×
3	0.1936	3	80	3	5 1 2 5	−1/6	1/9	83.6206	4 0 1	2 1 10	5 0 $\bar{1}$	2 1 $\bar{8}$			
	0.2315	3	56	3	7 2 1 7	1/6	5/9	56.2510	0 2 1	1 2 14	0 7 $\bar{1}$	1 2 $\bar{4}$			
	0.3062	3	32	3	8 1 2 8	2/6	7/9	38.9424	1 0 1	2 1 16	8 0 $\bar{1}$	2 1 $\bar{2}$			
	0.3873	3	20	3	5 4 2 5	−1/6	1/9	83.6206	0 2 1	1 2 5	0 5 $\bar{2}$	1 2 $\bar{4}$			
	0.4629	3	14	3	7 2 4 7	1/6	5/9	56.2510	1 0 1	2 1 7	7 0 $\bar{2}$	2 1 $\bar{2}$			
	0.6124	3	8	6	3 2 1 1	3/6	5/9	56.2510	2 1 1	5 4 4			×		
				3	4 2 1 4	2/6	7/9	38.9424	0 1 2	1 2 8	0 4 $\bar{1}$	1 2 $\bar{1}$			
				6	4 3 3 0	2/6	3/9	70.5288							
	0.7746	3	5	3	5 4 8 5	−1/6	1/9	83.6206	1 0 1	4 2 5	5 0 $\bar{4}$	2 1 $\bar{2}$			
	0.9258	6	7	3	7 8 4 7	1/6	5/9	56.2510	0 1 2	2 4 7	0 7 $\bar{4}$	1 2 $\bar{1}$			
	0.9682	15	16	3	1 2 1 1	−1/6	1/9	83.6206	1 0 1	10 5 8	4 0 $\bar{5}$	2 1 $\bar{2}$			
	1.2247	3	2	6	3 2 4 1	3/6	5/9	56.2510	1 2 2	4 5 2			×		
				3	2 1 2 2	2/6	7/9	38.9424	0 2 1	2 4 1	0 1 $\bar{4}$	1 2 $\bar{4}$			
				6	2 3 3 0	2/6	3/9	70.5288							
	1.5492	12	5	3	5 16 8 5	−1/6	1/9	83.6206	0 1 2	4 8 5	0 5 $\bar{8}$	1 2 $\bar{1}$			
	1.6202	21	8	3	1 2 1 1	1/6	5/9	56.2510	1 0 1	14 7 4	2 0 $\bar{7}$	2 1 $\bar{2}$			
	1.9365	15	4	3	1 2 4 1	−1/6	1/9	83.6206	0 1 2	5 10 4	0 2 $\bar{5}$	1 2 $\bar{1}$			
	2.4495	6	1	6	3 8 4 1	3/6	5/9	56.2510	2 1 4	5 4 1			×		
				3	1 2 1 1	2/6	7/9	38.9424	1 0 1	8 4 1	1 0 $\bar{8}$	2 1 $\bar{2}$			
				6	1 3 3 0	2/6	3/9	70.5288							
	3.2404	21	2	3	1 2 4 1	1/6	5/9	56.2510	0 1 2	7 14 2	0 1 $\bar{7}$	1 2 $\bar{1}$			
	3.8730	15	1	3	1 8 4 1	−1/6	1/9	83.6206	1 0 4	10 5 2	1 0 $\bar{5}$	4 2 $\bar{1}$			
	4.8990	24	1	3	1 2 4 1	2/6	7/9	38.9424	0 1 2	8 16 1	0 1 $\overline{16}$	1 2 $\bar{1}$			
	6.4807	42	1	3	1 8 4 1	1/6	5/9	56.2510	1 0 4	14 7 1	1 0 $\overline{14}$	4 2 $\bar{1}$			
	7.7460	60	1	3	1 8 16 1	−1/6	1/9	83.6206	0 1 8	5 10 1	0 1 $\overline{10}$	4 8 $\bar{1}$			
4	0.1464	3	140	3	7 2 1 7	−1/8	1/6	80.4059	0 5 1	1 2 14	0 7 $\bar{1}$	1 2 $\overline{10}$			
	0.1531	3	128	3	8 1 2 8	0	2/6	70.5288	4 0 1	2 1 16	8 0 $\bar{1}$	2 1 $\bar{8}$		×	×
	0.1936	3	80	3	10 2 1 10	2/8	4/6	48.1897	0 2 1	1 2 20	0 10 $\bar{1}$	1 2 $\bar{4}$			
	0.2611	3	44	3	11 1 2 11	3/8	5/6	33.5573	1 0 1	2 1 22	11 0 $\bar{1}$	2 1 $\bar{2}$			
	0.2928	3	35	3	7 2 4 7	−1/8	1/6	80.4059	5 0 2	2 1 7	7 0 $\bar{2}$	2 1 $\bar{5}$			
	0.3873	3	20	6	3 2 1 1	1/8	1/6	80.4059	2 1 1	5 4 10					×
	0.4330	3	16	3	2 1 2 2	−2/8	0	90	0 2 1	3 6 12	0 6 $\bar{3}$	1 2 $\bar{4}$			
	0.5	1	4	3	3 1 2 3	1/8	3/6	60	1 0 1	6 3 18	9 0 $\bar{3}$	2 1 $\bar{2}$			
	0.5222	3	11	3	11 4 2 11	3/8	5/6	33.5573	0 1 2	1 2 11	0 11 $\bar{2}$	1 2 $\bar{1}$			
	0.7319	15	28	3	7 5 10 7	−1/8	1/6	80.4059	1 0 1	10 5 14	7 0 $\bar{5}$	2 1 $\bar{2}$			
	0.7746	3	5	6	3 2 4 1	1/8	1/6	80.4059	1 2 2	4 5 5					×
	0.8660	3	4	6	1 1 1 1	1/8	3/6	60	1 1 3	3 3 6					×
	0.9682	15	16	3	2 1 2 2	2/8	4/6	48.1897	0 2 1	5 10 4	0 2 $\bar{5}$	1 2 $\bar{4}$			
	1	1	1	3	3 4 2 3	1/8	3/6	60	0 1 2	3 6 9	0 9 $\bar{6}$	1 2 $\bar{1}$			
	1.0247	21	20	3	1 2 1 1	−1/8	1/6	80.4059	1 0 1	14 7 10	5 0 $\bar{7}$	2 1 $\bar{2}$			
	1.4639	15	7	3	7 20 10 7	−1/8	1/6	80.4059	0 1 2	5 10 7	0 7 $\overline{10}$	1 2 $\bar{1}$			
	1.5	9	4	3	1 2 1 1	1/8	3/6	60	1 0 1	18 9 6	3 0 $\bar{9}$	2 1 $\bar{2}$			
	1.5492	12	5	3	5 4 8 5	2/8	4/6	48.1897	1 0 4	4 2 5	5 0 $\bar{4}$	4 2 $\bar{1}$			
	1.7321	3	1	6	1 2 2 1	1/8	3/6	60	1 1 6	3 3 3					×
	1.9365	15	4	6	3 5 10 1	1/8	1/6	80.4059	1 2 5	4 5 2					×
	2.0494	21	5	3	1 2 4 1	−1/8	1/6	80.4059	0 1 2	7 14 5	0 5 $\overline{14}$	1 2 $\bar{1}$			
	2.8723	33	4	3	1 2 1 1	3/8	5/6	33.5573	1 0 1	22 11 2	1 0 $\overline{11}$	2 1 $\bar{2}$			
	3	9	1	3	1 2 4 1	1/8	3/6	60	0 1 2	9 18 3	0 3 $\overline{18}$	1 2 $\bar{1}$			
	3.4641	12	1	3	1 4 8 1	−2/8	0	90	1 0 4	12 6 3	3 0 $\overline{12}$	4 2 $\bar{1}$			
	3.8730	15	1	6	3 20 10 1	1/8	1/6	80.4059	2 1 10	5 4 1					×
	5.1235	105	4	3	1 5 10 1	−1/8	1/6	80.4059	0 1 5	7 14 2	0 1 $\bar{7}$	5 10 $\bar{2}$			
	5.7446	33	1	3	1 2 4 1	3/8	5/6	33.5573	0 1 2	11 22 1	0 1 $\overline{22}$	1 2 $\bar{1}$			
	7.7460	60	1	3	1 8 4 1	2/8	4/6	48.1897	1 0 4	20 10 1	1 0 $\overline{20}$	4 2 $\bar{1}$			
	9.7980	96	1	3	1 8 16 1	0	2/6	70.5288	0 1 8	8 16 1	0 1 $\overline{16}$	4 8 $\bar{1}$		×	×
	10.247	105	1	3	1 20 10 1	−1/8	1/6	80.4059	1 0 10	14 7 1	1 0 $\overline{14}$	10 5 $\bar{1}$			

Table 9
Specific misorientations of rhombohedral lattices with $\Sigma = 5$.

	$s^2 = \mu/\nu$			Representative				Twin mirror plane 1		Twin mirror plane 2		Descriptions by rotations	
$s = c/a$	μ	ν	ω	(m, U, V, W)	$\cos\Theta$	$\cos\Phi$	Φ (°)	(hkl)	$[uvw]$	(hkl)	$[uvw]$	90°	120°
0.1157	3	224	3	8 1 2 8	−2/10	1/15	86.1774	7 0 1	2 1 16	8 0 $\bar{1}$	2 1 $\overline{14}$		
0.1225	3	200	3	10 2 1 10	0	5/15	70.5288	0 5 1	1 2 20	0 10 $\bar{1}$	1 2 $\overline{10}$	×	×
0.1306	3	176	3	11 1 2 11	1/10	7/15	62.1819	4 0 1	2 1 22	11 0 $\bar{1}$	2 1 $\bar{8}$		
0.1698	3	104	3	13 2 1 13	3/10	11/15	42.8334	0 2 1	1 2 26	0 13 $\bar{1}$	1 2 $\bar{4}$		
0.2315	3	56	3	14 1 2 14	4/10	13/15	29.9265	1 0 1	2 1 28	14 0 $\bar{1}$	2 1 $\bar{2}$		
			3	4 2 1 4	−2/10	1/15	86.1774	4 0 1	2 1 7	7 0 $\bar{2}$	2 1 $\bar{8}$		
0.2449	3	50	3	5 1 2 5	0	5/15	70.5288	5 0 2	2 1 10	5 0 $\bar{1}$	2 1 $\bar{5}$	×	×
0.2611	3	44	3	11 4 2 11	1/10	7/15	62.1819	0 2 1	1 2 11	0 11 $\bar{2}$	1 2 $\bar{4}$		
0.3062	3	32	6	3 2 1 1	−1/10	−1/15	93.8226	2 1 1	5 4 16				
0.3397	3	26	3	13 2 4 13	3/10	11/15	42.8334	1 0 1	2 1 13	13 0 $\bar{2}$	2 1 $\bar{2}$		
0.3536	1	8	3	3 2 1 3	−1/10	3/15	78.4630	0 2 1	3 6 18	0 9 $\bar{3}$	1 2 $\bar{4}$		
0.4330	3	16	3	4 2 1 4	2/10	9/15	53.1301	0 3 3	1 2 8	0 4 $\bar{1}$	3 6 $\bar{6}$		
			3	4 1 2 4	2/10	9/15	53.1301	1 0 1	6 3 24	12 0 $\bar{3}$	2 1 $\bar{2}$		
0.4629	3	14	3	7 2 1 7	4/10	13/15	29.9265	0 1 2	1 2 14	0 7 $\bar{1}$	1 2 $\bar{1}$		
			3	2 1 2 2	−2/10	1/15	86.1774	0 2 1	2 4 7	0 7 $\bar{4}$	1 2 $\bar{4}$		
0.4899	6	25	3	5 4 2 5	0	5/15	70.5288	5 0 2	4 2 5	5 0 $\bar{4}$	2 1 $\bar{5}$	×	×
0.5222	3	11	3	11 4 8 11	1/10	7/15	62.1819	1 0 1	4 2 11	11 0 $\bar{4}$	2 1 $\bar{2}$		
0.6124	3	8	6	6 1 2 2	8/10	13/15	29.9265	2 4 1	4 5 2				
			6	4 1 2 2	6/10	11/15	42.8334	1 3 1	5 7 4				
			6	1 1 1 1	−1/10	3/15	78.4630	2 2 3	3 3 6				
			6	3 2 4 1	−1/10	−1/15	93.8226	1 2 2	4 5 8				
0.6794	6	13	3	13 8 4 13	3/10	11/15	42.8334	0 1 2	2 4 13	0 13 $\bar{4}$	1 2 $\bar{1}$		
0.7071	1	2	3	3 2 4 3	−1/10	3/15	78.4630	1 0 1	6 3 9	9 0 $\bar{6}$	2 1 $\bar{2}$		
0.8101	21	32	3	8 7 14 8	−2/10	1/15	86.1774	1 0 1	14 7 16	8 0 $\bar{7}$	2 1 $\bar{2}$		
0.8660	3	4	3	2 1 2 2	2/10	9/15	53.1301	3 0 6	2 1 4	2 0 $\bar{1}$	6 3 $\bar{3}$		
			3	2 2 1 2	2/10	9/15	53.1301	0 1 2	3 6 12	0 6 $\bar{3}$	1 2 $\bar{1}$		
0.9258	6	7	3	7 2 4 7	4/10	13/15	29.9265	1 0 4	2 1 7	7 0 $\bar{2}$	4 2 $\bar{1}$		
			3	1 2 1 1	−2/10	1/15	86.1774	1 0 1	8 4 7	7 0 $\bar{8}$	2 1 $\bar{2}$		
1.0445	12	11	3	11 16 8 11	1/10	7/15	62.1819	0 1 2	4 8 11	0 11 $\bar{8}$	1 2 $\bar{1}$		
1.0607	9	8	3	1 2 1 1	−1/10	3/15	78.4630	1 0 1	18 9 12	6 0 $\bar{9}$	2 1 $\bar{2}$		
1.2247	3	2	6	3 2 1 1	8/10	13/15	29.9265	2 1 1	5 4 1				
			6	2 2 1 1	6/10	11/15	42.8334	3 1 2	7 5 2				
			6	1 2 2 1	−1/10	3/15	78.4630	1 1 3	3 3 3				
			6	3 8 4 1	−1/10	−1/15	93.8226	2 1 4	5 4 4				
1.4142	2	1	3	3 8 4 3	−1/10	3/15	78.4630	0 1 2	6 12 9	0 9 $\overline{12}$	1 2 $\bar{1}$		
1.4361	33	16	3	1 2 1 1	1/10	7/15	62.1819	1 0 1	22 11 8	4 0 $\overline{11}$	2 1 $\bar{2}$		
1.6202	21	8	3	2 1 2 2	4/10	13/15	29.9265	0 2 1	7 14 2	0 1 $\bar{7}$	1 2 $\bar{4}$		
			3	4 14 7 4	−2/10	1/15	86.1774	0 1 2	7 14 8	0 4 $\bar{7}$	1 2 $\bar{1}$		
1.7321	3	1	3	1 2 1 1	2/10	9/15	53.1301	1 0 1	12 6 3	3 0 $\overline{12}$	2 1 $\bar{2}$		
			3	1 1 2 1	2/10	9/15	53.1301	0 3 3	2 4 1	0 1 $\bar{4}$	3 6 $\bar{6}$		
1.8516	24	7	3	1 2 4 1	−2/10	1/15	86.1774	0 1 2	8 16 7	0 7 $\overline{16}$	1 2 $\bar{1}$		
2.1213	9	2	3	1 2 4 1	−1/10	3/15	78.4630	0 1 2	9 18 6	0 3 $\bar{9}$	1 2 $\bar{1}$		
2.2079	39	8	3	1 2 1 1	3/10	11/15	42.83	1 0 1	26 13 4	2 0 $\overline{13}$	2 1 $\bar{2}$		
2.4495	6	1	6	3 2 4 1	8/10	13/15	29.9265	1 2 2	8 10 1				
			6	2 2 4 1	6/10	11/15	42.8334	1 3 4	5 7 1				
			6	1 4 4 1	−1/10	3/15	78.4630	1 1 6	6 6 3				
			6	3 8 16 1	−1/10	−1/15	93.8226	1 2 8	4 5 2				
2.8723	33	4	3	1 2 4 1	1/10	7/15	62.1819	0 1 2	11 22 4	0 2 $\overline{11}$	1 2 $\bar{1}$		
3.0619	75	8	3	2 10 5 2	0	5/15	70.5288	0 1 5	5 10 4	0 2 $\bar{5}$	5 10 $\bar{2}$	×	×
3.2404	21	2	3	1 2 1 1	4/10	13/15	29.9265	1 0 1	14 7 1	1 0 $\overline{14}$	2 1 $\bar{2}$		
			3	2 7 14 2	−2/10	1/15	86.1774	1 0 4	14 7 4	2 0 $\bar{7}$	4 2 $\bar{1}$		
3.4641	12	1	3	1 2 4 1	2/10	9/15	53.1301	0 1 2	12 24 3	0 3 $\overline{24}$	1 2 $\bar{1}$		
			3	1 4 2 1	2/10	9/15	53.1301	3 0 6	8 4 1	1 0 $\bar{8}$	6 3 $\bar{3}$		
4.2426	18	1	3	1 8 4 1	−1/10	3/15	78.4630	1 0 4	18 9 3	3 0 $\overline{18}$	4 2 $\bar{1}$		
4.4159	39	2	3	1 2 4 1	3/10	11/15	42.8334	0 1 2	13 26 2	0 1 $\overline{13}$	1 2 $\bar{1}$		
4.8990	24	1	6	3 32 16 1	−1/10	−1/15	93.8226	2 1 16	5 4 1				
5.7446	33	1	3	1 8 4 1	1/10	7/15	62.1819	1 0 4	22 11 2	1 0 $\overline{11}$	4 2 $\bar{1}$		
6.1237	75	2	3	1 5 10 1	0	5/15	70.5288	0 1 5	5 10 1	0 1 $\overline{10}$	5 10 $\bar{2}$	×	×
6.4807	42	1	3	1 2 4 1	4/10	13/15	29.9265	0 1 2	14 28 1	0 1 $\overline{28}$	1 2 $\bar{1}$		
			3	1 14 7 1	−2/10	1/15	86.1774	0 1 8	7 14 2	0 1 $\bar{7}$	4 8 $\bar{1}$		
8.8318	78	1	3	1 8 4 1	3/10	11/15	42.8334	1 0 4	26 13 1	1 0 $\overline{26}$	4 2 $\bar{1}$		
11.489	132	1	3	1 8 16 1	1/10	7/15	62.1819	0 1 8	11 22 1	0 1 $\overline{22}$	4 8 $\bar{1}$		
12.247	150	1	3	1 20 10 1	0	5/15	70.5288	1 0 10	20 10 1	1 0 $\overline{20}$	10 5 $\bar{1}$	×	×
12.961	168	1	3	1 14 28 1	-2/10	1/15	86.1774	0 1 14	8 16 1	0 1 $\overline{16}$	7 14 $\bar{1}$		

Table 10
Obliquities $\delta < 6^\circ$ for twin laws with $\Sigma \le 5$ in corundum and hematite.

The first solution describes basal twins; solutions describing rhombohedral twins are in bold. The row with $s^2 = 15/2$ refers to Grimmer (1989*a*).

			Twin mirror plane 1		Twin mirror plane 2				Obliquity δ (°)	
$s = c/a$	s^2	Σ	(hkl)	$[uvw]$	(hkl)	$[uvw]$	$\cos\Phi$	Φ (°)	Corundum	Hematite
Any	Any	3	0 0 3	0 0 3	$0\,3\,\bar{0}$	$3\,6\,\bar{0}$	1/2	60	0	0
2.4495	6	**1**	**0 1 2**	**2 4 1**	$\mathbf{0\,1\,\bar{4}}$	$\mathbf{1\,2\,\bar{1}}$	**1/3**	**70.5288**	**5.8479**	**5.8873**
		3	2 1 4	5 4 1			5/9	56.2510	5.1614	5.1962
		3	1 0 1	8 4 1	$1\,0\,\bar{8}$	$2\,1\,\bar{2}$	7/9	38.9424	3.9062	3.9326
		5	1 2 2	8 10 1			13/15	29.9265	3.1022	3.1232
		5	1 3 4	5 7 1			11/15	42.8334	4.2240	4.2526
2.7386	15/2	**7**	**0 1 2**	**15 30 6**	$\mathbf{0\,3\,\overline{15}}$	$\mathbf{1\,2\,\bar{1}}$	**3/7**	**64.6231**	**0.1631**	**0.1252**
2.8723	33/4	4	1 0 1	22 11 2	$1\,0\,\overline{11}$	$2\,1\,\bar{2}$	5/6	33.5573	1.6093	1.5861
		5	**0 1 2**	**11 22 4**	$\mathbf{0\,2\,\overline{11}}$	$\mathbf{1\,2\,\bar{1}}$	**7/15**	**62.1819**	**2.5739**	**2.5368**
3	9	**4**	**0 1 2**	**9 18 3**	$\mathbf{0\,3\,\overline{18}}$	$\mathbf{1\,2\,\bar{1}}$	**3/6**	**60**	**4.6762**	**4.6399**
3.2404	21/2	5	1 0 1	14 7 1	$1\,0\,\overline{14}$	$2\,1\,\bar{2}$	13/15	29.9265	4.9109	4.8898

mutually perpendicular axes $[uvw]$ satisfying $2u \ge v \ge \frac{1}{2}u \ge 0$ and $w > 0$ in the first, $w < 0$ in the second case. The planes (hkl) normal to $[uvw]$ are called twin mirror planes. Two such 180° rotations with mutually perpendicular axes exist in all cases with $\omega = 3$, one 180° rotation[2] occurs in most cases with $\omega = 6$, none in three exceptional cases where $W = 0$ (*i.e.* $\Phi = \Theta$). The triplets (hkl) are normalized such that h, k, l are smallest integers satisfying $-h + k + l = 3M$, M integer; u, v, w are smallest integers satisfying $-u + v + w = 3N$ and $v - w = 3P$, N and P integers. These conditions guarantee that $\frac{1}{3}[uvw]$ is a smallest vector of the obversely centred hR lattice and (hkl) a smallest vector of its reciprocal lattice. With $S = \frac{1}{3}(hu + kv + lw)$, the multiplicity (twin index) equals $\Sigma = S$ if S is odd, $\Sigma = S/2$ if S is even (see Koch, 1999). The last columns in Tables 8 and 9 show which specific misorientations with $\Sigma \le 5$ can be described exactly by 60, 90 or 120° rotations: 90 and 120° descriptions exist in all cases with $\cos\Theta = 0$; 60° descriptions in all cases with $\cos\Theta = 1/2$; 120° descriptions in all cases with $\omega = 6$ and $\cos\Theta = 1/8$. The three exceptions ($W = 0$) can be described neither by 60, 90, 120° nor by 180° rotations; thus they do not correspond to twins.

Rhombohedral lattices with axial ratios s_1 and s_2 satisfying $s_1 s_2 = 3/2$ will be called pseudo-reciprocal because they possess primitive bases $\mathbf{e}_i$ and $\mathbf{f}_i$, $i = 1, 2, 3$, satisfying $\mathbf{e}_i \cdot \mathbf{f}_j = k\delta_{ij}$, where k is a constant of dimension length squared. Tables 8 and 9 show that to each misorientation of a rhombohedral lattice with a given value of Σ there corresponds a related misorientation of its pseudo-reciprocal lattice with the same value of Σ. The three entries with $\Sigma = 1$ in Table 8 correspond to the special cases of cubic lattices: the rhombohedral lattice is identical to cI for $s^2 = 0.375$, to cP for $s^2 = 1.5$, and to cF for $s^2 = 6$. The lattices cI and cF are pseudo-reciprocal to each other, cP is pseudo-reciprocal to itself. This is illustrated in Fig. 3.

Consider as examples corundum (α-Al_2O_3) and hematite (α-Fe_2O_3), which both have space group $R\bar{3}c$ with axial ratio $c/a = 2.730$ and 2.732, respectively. In both cases, the most common twin besides the basal twin [twin mirror plane (001)] is the rhombohedral twin [twin mirror plane (012)] (Bursill & Withers, 1979). Table 10 gives the obliquities $\delta < 6^\circ$ for twin laws of corundum and hematite corresponding to misorientations with $\Sigma \le 5$.

The first solution in Table 10 gives the common misorientation with $\Sigma = 3$, which describes basal twins. The table also gives possible descriptions of rhombohedral twins with $\Sigma = 1$, 4, 5 and 7 (in bold). As s approaches the c/a ratio of the two minerals, δ decreases and Σ increases. Twins in corundum and hematite were discussed from the coincidence site lattice point of view by Grimmer (1989*a*), where a description with $\Sigma = 7$ (row with $s^2 = 15/2$ in Table 10) was proposed, which has particularly low obliquity.

The output from the program *OBLIQUE* by Le Page (2002), carried out for hR with $c/a = 2.73$, $\Sigma \le 5$ and $\delta < 6^\circ$, contains the following solutions: (*a*) the trivial solution corresponding to the symmetry operations of hR, (*b*) the solutions with $\Sigma \le 5$ for corundum of Table 10, (*c*) three additional solutions that do not correspond to $[uvw] \perp (hkl)$ in an hR lattice with an appropriate value of c/a (collected in Table 11).

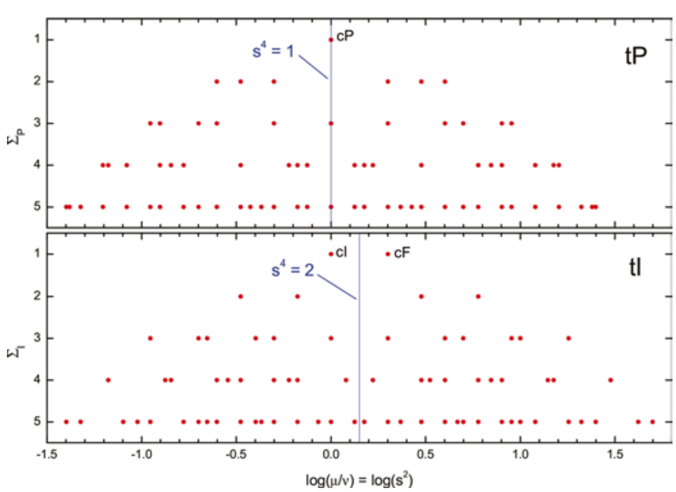

Figure 5
Specific misorientations of primitive (tP) and body-centred (tI) tetragonal lattices with multiplicity (twin index) $\Sigma \le 5$ as a function of the axial ratio s.

[2] A similar situation occurs in Table 2, where the misorientation in the case of $s = 1$ with $\Sigma = 8$ cannot be described by a second 180° rotation with perpendicular axis.

Table 11
Additional solutions obtained with program *OBLIQUE* for *hR* lattices with $r = 2.73$ (corundum) and $r = 2.732$ (hematite) satisfying either $\Sigma = 1$, $\delta < 18^\circ$ or Mallard's criterion $\Sigma \leq 5$, $\delta < 6^\circ$.

Further solutions, which are missed by *OBLIQUE*, are given with indices $l' \leq 0$ and $w' \leq 0$.

Additional solutions from *OBLIQUE*			Further solutions		Obliquity δ (°)	
Σ	(hkl)	[uvw]	($h'k'l'$)	[$u'v'w'$]	Corundum	Hematite
1	0 0 3	1 2 2	0 1 $\bar{1}$	3 6 0	17.6004	17.5883
4	4 0 1	6 3 0	0 0 $\bar{3}$	2 1 $\bar{8}$	4.5344	4.5311
5	0 5 1	3 6 0	0 0 $\bar{3}$	1 2 $\overline{10}$	3.6303	3.6276
5			0 1 $\bar{1}$	15 27 $\overline{30}$	3.8601	3.8710
5	3 2 7	5 4 1			5.3436	5.3687

Table 12
The specific misorientations of *tP* and *tI* lattices with $\Sigma \leq 5$ that can be described by 60, 90 or 120° rotations.

$i = 2\Sigma \cos \Theta$	ω	60°	90°	120°
$i = 0$, *i.e.* $\cos \Theta = 0$	Any		×	×
$i = \Sigma/4$, *i.e.* $\cos \Theta = 1/8$	Any		×	
$i = \Sigma$, *i.e.* $\cos \Theta = 1/2$	Not 8	×		×
	8	×		

Whereas the solutions in Table 10 suffice to describe growth twins in corundum and hematite, this is not the case for deformation twins. Those are described in structural coordinates by

basal twin:

$$K_1 = (003),\ \eta_2 = [122],\ K_2 = (01\bar{1}),\ \eta_1 = [360], \quad (10)$$

rhombohedral twin:

$$K_1 = (012),\ \eta_2 = [241],\ K_2 = (01\bar{4}),\ \eta_1 = [12\bar{1}] \quad (11)$$

(*cf.* Shiue & Phillips, 1984).

Relations (9) show that these descriptions correspond to the first solution in Table 11 for basal twins and to the second solution in Table 10 for rhombohedral ones.

5. Tetragonal lattices

In the tetragonal case, the specific misorientations with $\Sigma \leq 5$ have been given by Grimmer (2003) in his Tables 4 and 5 for primitive tetragonal (*tP*) lattices and in his Tables 9 and 10 for body-centred tetragonal (*tI*) lattices. The results are illustrated in Fig. 5.

The three cubic lattices appear in Fig. 5 as special cases of tetragonal lattices: *cP* and *cI* are the special cases of *tP* and *tI* with $s = 1$; *cF* is the special case of *tI* with $s^2 = 2$.

Table 12 indicates which of the specific misorientations listed in Tables 4, 5, 9 and 10 of Grimmer (2003) can be described not only by 180° rotations but also by 60, 90 or 120° rotations.[3]

In the tetragonal case, Θ is obtained from the integer i given in Tables 4, 5, 9 and 10 of Grimmer (2003) by $\Theta = \arccos(i/2\Sigma)$. (The multiplicity Σ is called Σ_P in Tables 4 and 5 and Σ_I in Tables 9 and 10, referring to *tP* and *tI* lattices, respectively.) The cases with $W \neq 0$ (*i.e.* $\Phi \neq \Theta$) in these four tables are listed in our Table 13.

[3] Correction: in Table 10 of Grimmer (2003), the representative (m, U, V, W) in the row with $c/a = 1.2247$ is (1100), not (2110).

Table 13
Specific misorientations of tetragonal lattices with $\Sigma \leq 5$ and $\Phi \neq \Theta$.

Σ	$s = c/a$	Representative (m, U, V, W)	$\cos \Theta$	$\cos \Phi$	Θ (°)	Φ (°)
$\Sigma_P = \Sigma_I = 3$	1	3 1 1 1	3/6	4/6	60	48.1897
$\Sigma_I = 3$	1.4142	3 2 0 1	3/6	4/6	60	48.1897
$\Sigma_P = \Sigma_I = 4$	0.5774	3 1 1 1	1/8	2/8	82.8192	75.5225
$\Sigma_I = 4$	0.8165	3 2 0 1	1/8	2/8	82.8192	75.5225
$\Sigma_P = \Sigma_I = 4$	1.7321	3 3 3 1	1/8	2/8	82.8192	75.5225
$\Sigma_I = 4$	2.4495	3 6 0 1	1/8	2/8	82.8192	75.5225
$\Sigma_P = \Sigma_I = 5$	1	3 3 1 1	−1/10	0	95.7392	90
$\Sigma_I = 5$	1.4142	3 4 2 1	−1/10	0	95.7392	90

It is observed in Table 13 and the four tables in Grimmer (2003) mentioned above that $\cos \Phi \leq 0.8$ ($\Phi \geq 36.87^\circ$) for *tP* and *tI* lattices with $\Sigma \leq 5$. It follows that $\sin \Phi \geq 0.6$, *i.e.* $\delta \geq \arctan[0.6|s^2 - r^2|/(2rs)]$, holds. This bound restricts, for a given value of r, the range of s values that may give rise to twins with $\Sigma \leq 5$ and obliquities smaller than a specified limit.

6. Discussion and conclusions

Early work on coincidence site lattices (CSL) of the French school (Bonnet & Durand, 1975) has started as a generalization of twin laws with twin index > 1; the notion of the CSL multiplicity Σ is a straightforward generalization of the twin index to those coincidence misorientations that cannot be described by any 180° rotation. However, new notions have been introduced in CSL theory, where the connections with notions from the field of twinning are not always evident. Specifically, the connection between the CSL deformation parameter ε and the obliquity δ in optically uniaxial crystals has been unknown before and is now established in this paper.

Our comparison of observed laws of growth twinning in quartz, corundum and hematite with the solutions satisfying the Mallard criterion leads us to propose the following modification of this criterion in the case of growth twins: only those pairs of a lattice plane (hkl) and a lattice direction [uvw] that become normal for an appropriate value s of the axial ratio c/a should be considered as candidates for twin laws. All possible twin laws of *hP* and *hR* lattices satisfying the modified Mallard criterion are then obtained from Tables 1, 8 and 9. The graphical representation of these tables in Fig. 3 shows their symmetry with respect to pseudo-reciprocity. The varying density of points as a function of s illustrates that the number of available twin laws satisfying the modified Mallard criterion depends on the axial ratio r of the crystal under consideration. Analogous results were obtained for tetragonal lattices.

We suggest to extend the proposed modification of Mallard's criterion for growth twins as follows to all crystal families: only those pairs of a lattice plane (hkl) and a lattice direction [uvw] that become normal for appropriate lattice parameters should be considered as candidates for twin laws of growth twins. Table 14 gives the corresponding restrictions on (hkl) and [uvw] explicitly.

Note that all the solutions selected in Table 3.3.8.2 of Hahn & Klapper (2003) satisfy these restrictions. In our Tables 2 and 3, it was shown that Friedel (1923) missed one of the solutions related to reticular merohedry and all but one of the 30 solutions not related to reticular merohedry. This makes us wonder whether he intuitively applied the restrictions proposed in Table 14.

In the case of reticular merohedry, *i.e.* in particular in all the cases given in Tables 1, 8 and 9, the twin index Σ gives the volume ratio between primitive cells of the CSL generated by a mirror reflection in (hkl) or alternatively by a 180° rotation about [uvw]. But what is the relation between the twin index and either the mirror reflection in (hkl) or the 180° rotation about [uvw] in those cases not related to reticular merohedry? Consider the row with $\Sigma = 5$ in Table 3 as an example. The parallelohedron defined by [110] and a smallest mesh in (551) has a volume that is ten times the volume of a primitive cell. The twin index 5 is assigned to it because this parallelohedron has points of the hexagonal lattice also in the centres of a pair of opposite faces (Donnay & Donnay, 1972). The 180° rotation about [110] is a symmetry rotation; the corresponding twin index is 1 (not 5); a mirror reflection in (551) generates a CSL with twin index 610 if $c/a = 1.1$. Also, the density of lattice points in the plane (551) is 11.18 times smaller than in the basal plane. We conclude that a small twin index does not indicate a probable twin law in the cases not related to reticular merohedry.

To illustrate the difference in the formulation of twin laws for growth and deformation twins, it is instructive to consider the spinel law and its analogue for deformation twins. Spinel growth twins can be described by a reflection in (111) or a 180° rotation about [111], corresponding to $\Sigma = 3$ and $\delta = 0$ and satisfying the restrictions given in Table 14. Deformation twins with $\Sigma = 3$ of f.c.c. metals also obey the spinel law (see *e.g.* Hahn & Klapper, 2003) and are described by

$$K_1 = (111), \eta_2 = \tfrac{1}{2}[112], K_2 = (11\bar{1}), \eta_1 = \tfrac{1}{2}[11\bar{2}] \qquad (12)$$

(see *e.g.* Kelly *et al.*, 2000). Using the correspondences (9) for K_1 and η_2, one obtains $\Sigma = 1$ and $\delta = 19.47°$ according to the formulas for cF lattices given by Donnay & Donnay (1972).[4] Note that the deformation shear determines Σ and δ uniquely and that neither Mallard's criterion nor the restrictions of Table 14 are satisfied, similarly as for (111) twins in h.c.p. metals and for basal twins in corundum and hematite.

The criterion for possible twin laws therefore depends on the type of twinning. If the relations (9) are used to describe deformation twins, also solutions that are not related to reticular merohedry play a role; the Mallard limit may have to be tightened for the twin index but considerably widened for the obliquity.

For twins grown from twinned nuclei, all the descriptions in the literature of which the authors are aware satisfy the restrictions proposed in Table 14; on the other hand, a number of twin laws firmly established in high-quartz suggest that the Mallard limit on the twin index should be relaxed.

Finally, aggregates formed when macroscopic crystals meet in a fluid may show misorientations that are best described by considering lattices with parameters within the experimental range (*i.e.* $\delta \simeq 0$) and allowing for large values of the twin index. An example is the Zinnwald twin described by Drugman (1930), which has been discussed in detail by Friedel (1933). In this case, a {101} rhombohedral face of each individual is parallel to a prism face {100} of the other, one set being in contact. The misorientation can be described by a rotation about [100] by an angle which is theoretically 38.21° for $c/a = 1.1$, in excellent agreement with the mean of the experimental values, which was 38°14′, *i.e.* 38.23° according to Friedel (1933). Both Drugman and Friedel concluded on the basis of experimental evidence that this twin originates from the coalescence of two single crystals floating in the magma. Friedel (1933) interprets the Zinnwald twin as one of the very few examples where the lattice coincidence is only one-dimensional, namely along [100]. Grimmer & Kunze (2003) showed that also interpretations with two- or three-dimensional coincidence are possible. These coincidences are approximate but become perfect for $c/a = 1.1$, a good approximation to the axial ratio of high-quartz at the elevated temperature and pressure at which the two crystals may have coalesced ($c/a \simeq 1.092$), and an excellent approximation to the axial ratio of α-quartz at ambient conditions, *i.e.* the present state of the twin ($c/a = 1.10000 \pm 0.00005$). The coincident cell in the contact plane is rectangular with lattice parameters a and $28c = 30.8a$. Its area is 28 times bigger than the smallest mesh in the prism face and 22 times bigger than the smallest mesh in the rhombohedral face. There exists also a three-dimensional coincident cell with volume 308 times the volume of a primitive cell of the hP lattice. It contains coincident points in every 11th prism face and in every 14th rhombohedral face.

Other examples of aggregates with large values of Σ have been discussed by Mykura *et al.* (1980) and by Nespolo *et al.* (1999).

Table 14
Proposed restrictions on (hkl) and [uvw] for twin laws of growth twins.

(hkl) and [uvw] refer to the conventional choice of the crystal coordinate system. (Note that the hexagonal family comprises hR as well as hP.)

Crystal family	Restrictions†
Cubic	$h:k:l = u:v:w$ (*i.e.* $\delta = 0$)
Tetragonal	$h:k = u:v$, $l = 0 \leftrightarrow w = 0$
Hexagonal	$h:k = (2u - v):(2v - u)$, $l = 0 \leftrightarrow w = 0$
Orthorhombic	$h = 0 \leftrightarrow u = 0$, $k = 0 \leftrightarrow v = 0$, $l = 0 \leftrightarrow w = 0$
Monoclinic	$k = 0 \leftrightarrow v = 0$, $h = l = 0 \leftrightarrow u = w = 0$
Triclinic (= anorthic)	No restrictions

† Key: $\leftrightarrow$ means 'if and only if', comma means logical AND.

[4] The spinel law is nothing but the basal twin law of hR lattices in the special case $c/a = \sqrt{6}$, in which the hR lattice becomes cF. This is true not only for the formulation as a twin with $\Sigma = 3$ and $\delta = 0$ but also for the description of the deformation mechanism with $\Sigma = 1$ and $\delta = 19.47°$. Note that relation (10) is formulated in hexagonal and (12) in cubic coordinates.

It has been shown here that all coincidence misorientations with $\Sigma \leq 5$ of tP, tI, hP and hR lattices can be expressed by 180° rotations about appropriate crystallographic axes with six exceptions. These exceptional cases cannot be described by 60, 90 or 120° rotations either; thus they do not correspond to twins. The exceptions relate to the special cases in which a trigonal or tetragonal crystal has a cP, cI or cF lattice.

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