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Near-Coincidence Orientations in Hexagonal Materials: from a Unified Twin Approach to a Quasiperiodic Description

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Abstract

In materials belonging to the hexagonal crystal family (hexagonal or trigonal crystal systems), for which the irrationality arises primarily from the lattice parameters, the concept of near-coincidence orientation has to be introduced in order to characterize experimental grain boundaries. The practical use of this concept can be simplified if a twin approach is introduced: high-Σ specific coincidence orientations are described as a deviation from very low-Σ twin orientations defined among a unique set of limiting Σ. Consequently, for real hexagonal or trigonal materials, each orientation relationship defined by a quaternion (m, u, v, w), all relatively prime integers, can be described, for any c/a, uniquely by a quasiperiodic arrangement of elementary 'twin' coincidences. Experimental cases of interfaces in hexagonal and rhombohedral crystals (h.c.p. metals, tungsten carbide, alumina) are analysed.

Introduction

In the past few years great interest has been dedicated to the study of grain boundaries in materials described in the hexagonal crystal family. Both theoretical and experimental results presented have outlined an emerging field of research where, for instance, mathematical calculation of coincidence orientations [Bleris, Nouet, Hagège & Delavignette (1982), Grimmer & Warrington (1987), Hagège & Nouet (1989) for hexagonal; Doni, Fanides & Bleris (1986), Grimmer (1989*a*) for rhombohedral], relaxation of the structure at the interface (Serra, Bacon & Pond, 1988; Hagège, Mori & Ishida, 1990), grain-boundary dislocation analysis (Antonopoulos, Karakostas, Komninou & Delavignette, 1988; Chen & King, 1988;

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Hagège, Chermant & Nouet, 1988) and statistical determination of the ratio of coincidence orientations (Grimmer, Bonnet, Lartigue & Priester, 1990) can interact for a better knowledge of the properties of a material.

The concept of coincidence orientation is only related to the mutual rotation of the lattices of the crystals defining an interface (Bollmann, 1982). This approach, if meant only as an approach, has been acknowledged as a sound base for interface studies. Moreover, in the case of coincidence, the projection of the periodicity of the common lattice on the boundary plane is a simple physical parameter which can be associated with the stability of the interface. The three-dimensional periodicity of a coincidence orientation is restricted by the principle of rationality of the nine elements of the rotation matrix (Grimmer, 1976) and consequently of the parameters defining the interface operation: nature of the lattice for each crystal (lattice parameters), mutual orientation of the lattices (rotation axis and angle). For relevant information on the atomic structure at the interface, additional parameters have also to be taken into account: rigid-body translation relating the two crystals, boundary-plane orientation and position, relaxation of the structure at the interface.

In hexagonal lattices (*hP*, *hR*), three-dimensional exact coincidence orientations occur only for very particular values of the rotation (generic or so-called common coincidences) or if the square of the axial ratio is a rational number (specific coincidences). Therefore, in materials belonging to the hexagonal crystal family (hexagonal or trigonal crystal systems), for which the irrationality arises primarily from the crystal parameters, the concept of near-coincidence orientation has to be introduced in order to characterize experimental grain boundaries. The practical use of this concept can be simplified if a twin approach is introduced as in the first part of this paper: high Σ specific coincidence orientations will be described as a deviation from low-Σ twin orientations defined among a unique set of limiting Σ. Firstly, the set of all the coincidence orientations can be classified, and therefore simplified, by using a 'twin-plane' description. In every subset, one for each twin plane, an infinite succession of limiting coincidence orientations envelops all the elements of the subset. Secondly, every element of the subset is deduced by a unique linear combination of the two nearest (with reference to c/a) limiting coincidence orientations. Every element of the subset can then be described by a periodic arrangement of two limiting cases. Every arrangement is unique and therefore characteristic of the exact coincidence orientation.

Since the discovery of quasicrystals (Shechtman, Blech, Gratias & Cahn, 1984) and the revival of quasiperiodicity, the effect of the irrationality of certain parameters on the grain-boundary structure has been the subject of a large number of studies (Gratias & Thalal, 1988; Rivier & Lawrence, 1988; Benderski, Cahn & Gratias, 1989; Sutton, 1988). The irrationality of the rotation angle, the rotation axis or the boundary plane were their main concern. Furthermore, as in the field of quasicrystals, the representation of the bicrystal in a hyperspace has revealed the crucial duality between order and periodicity at the boundary (Gratias & Thalal, 1988; Duneau & Oguey, 1989).

Following the same approach for hexagonal materials (*hP*, *hR*), the most obvious example of irrational symmetry, we would like to demonstrate, in the second part of this paper, that the concept of near-coincidence orientation can be better understood from the point of view of quasiperiodicity: each orientation relationship defined by a quaternion (m, u, v, w), all relatively prime integers, is described, for any c/a (therefore irrational), uniquely by a quasiperiodic arrangement of elementary 'twin' coincidences.

As a proof of the simplicity and applicability of this approach we shall, finally, analyse some real cases of interfaces in hexagonal and rhombohedral crystals: h.c.p. metals, tungsten carbide, alumina. In each case the experimental orientation is described as a quasiperiodic arrangement of elementary twin coincidences of low energy (typically $\Sigma = 1, 2$ or 3).

Exact coincidence orientations

For hexagonal materials the irrationality of the orientation relationship arises primarily from the crystal parameters and especially from the value of $(c/a)^2$. As demonstrated before, an exact three-dimensional coincidence orientation* arises for a given quaternion (m, u, v, w), all integers without common divisor, and a rational value of $(c/a)^2$ (Grimmer & Warrington, 1987; Hagège & Nouet, 1989; Grimmer, 1989*a*). The index of coincidence Σ is given for hexagonal and rhombohedral lattices respectively by

$$hP:\quad \Sigma = [(u^2+v^2-uv)\nu + (3m^2+w^2)\mu]/\alpha \quad \text{for } (c/a)^2 = \mu/\nu$$

$$hR:\quad \Sigma = [(u^2+v^2+uv)2\rho + (3m^2+w^2)\mu]/\delta \quad \text{for } (c/a)^2 = 3\mu/2\rho.$$

α and δ are unambiguously defined by specific selection rules.

If one considers all the proper symmetry operations which can be applied on each crystal defining an interface, twelve (*hP*) or six (*hR*) equivalent descriptions describe the orientation relationship. To every

* The common coincidence orientations, independent of c/a, are not included in this study.

equivalent description corresponds a rotation axis and a rotation angle. It has been found useful to consider also the plane perpendicular to each rotation axis (Delavignette, 1983). In the case of twins (mechanical, growth) the habit plane of the boundary is often normal to the equivalent rotation axis associated with a 180° rotation (twin description). For this work, this 180° description, and the corresponding axis and normal plane, will be chosen as representative of the orientation. If no 180° description is available, the largest angle of the twelve (or six) descriptions will be chosen; by extension the normal plane will still be noted 'twin' plane in quotation marks.

Hexagonal Bravais lattices

For the hP lattice the function $\Sigma = Fh(c/a)$,

$$\Sigma = [(u^2+v^2-uv)\nu+(3m^2+w^2)\mu]/\alpha$$

$$\text{for } (c/a)^2=\mu/\nu \text{ and g.c.d.}(\mu,\nu)=1,$$

$(c/a)^2$ being a rational number, can be plotted for every representative quaternion (m, u, v, w), such as g.d.c.$(m, u, v, w) = 1$. Then a unique minimum value $\Sigma^{\rm lim}_{\rm min}$ appears in a single envelope of $\Sigma^{\rm lim}$. This envelope is made of two parts, respectively ascending and descending monotonically, each with its own periodicity: $P_{\rm low}$ and $P_{\rm high}$.

$P_{\rm low}$ is a divisor of (u^2+v^2-uv) and $P_{\rm high}$ is a divisor of $(3m^2+w^2)$ with the remarkable property $\Sigma^{\rm lim}_{\rm min} = P_{\rm low}+P_{\rm high}$.

Every other Σ case, inside the envelope, is a simple linear combination of two consecutive $\Sigma^{\rm lim}$ with a very simple rule based on the same linear combination connecting all the relevant characteristics of the coincidence rule: Σ, μ/ν and all the parameters of the equivalent rotations.

Fig. 1 represents the plot of Fh for the quaternion (0, 2, 1, 1) which describes the $(10\bar{1}2)$ mechanical twin for h.c.p. metals:

$$\Sigma = (3\nu+\mu)/\alpha, \quad \alpha = 1 \text{ or } 3, \quad P_{\rm low} = P_{\rm high} = 1.$$

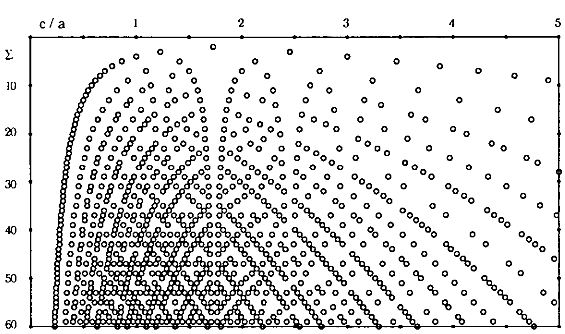

Fig. 1. Plot of Fh for the $(10\bar{1}2)$ mechanical twin: $m, u, v, w = 0, 2, 1, 1$; $0 < c/a < 5$ and Σ up to 60. $\Sigma^* = \Sigma^{\rm lim}_{\rm min} = 2$ appears for $(c/a)^2 = 3$.

and

$$\Sigma^{\rm lim}_{\rm min} = P_{\rm low}+P_{\rm high} = 2.$$

An infinite series of values $\Sigma^{\rm lim}$ with periodicity 1 on both sides of $\Sigma^{\rm lim}_{\rm min}$ contains all the other values of Σ.

As $(c/a)^2=\mu/\nu$ and g.c.d. $(\mu, \nu)=1$, there is only one possible value of Σ for each axial ratio; therefore two successive $\Sigma^{\rm lim}$ define a domain of Fh in which a particular value of Σ is defined as a linear combination of these two successive $\Sigma^{\rm lim}$.

As an example, one possible representation of the $(10\bar{1}2)$ mechanical twin for a metal such as zinc (Hagège, 1989) is the exact three-dimensional coincidence case $\Sigma = 28$ and $\mu/\nu = 45/13$ or $c/a = 1{\cdot}860_5$. This case is found in Fig. 1 by the following linear decomposition:

As $c/a = 1{\cdot}860_5$ is in between $\Sigma = 2$, $\mu/\nu = 3/1$, $c/a = 1{\cdot}732_1$ and $\Sigma = 3$, $\mu/\nu = 6/1$, $c/a = 2{\cdot}449_5$,

$2+3=5$	then $\Sigma = 5$
$3+6=9,\ 1+1=2$	then $\mu/\nu = 9/2$
	and $c/a = 2{\cdot}121_3$;

As $c/a = 1{\cdot}860_5$ is in between $\Sigma = 2$, $\mu/\nu = 3/1$, $c/a = 1{\cdot}732_1$ and $\Sigma = 5$, $\mu/\nu = 9/2$, $c/a = 2{\cdot}121_3$,

$2+5=7$	then $\Sigma = 7$
$3+9=12,\ 1+2=3$	then $\mu/\nu = 12/3$
	and $c/a = 2{\cdot}000_0$
$2+7=9$	then $\Sigma = 9$
$3+12=15,\ 1+3=4$	then $\mu/\nu = 15/4$
	and $c/a = 1{\cdot}936_5$
$2+9=11$	then $\Sigma = 11$
$3+15=18,\ 1+4=5$	then $\mu/\nu = 18/5$
	and $c/a = 1{\cdot}897_4$
$2+11=13$	then $\Sigma = 13$
$3+18=21,\ 1+5=6$	then $\mu/\nu = 21/6$
	and $c/a = 1{\cdot}870_1$
$2+13=15$	then $\Sigma = 15$
$3+21=24,\ 1+6=7$	then $\mu/\nu = 24/7$
	and $c/a = 1{\cdot}851_6$;

As $c/a = 1{\cdot}860_5$ is in between $\Sigma = 13$, $\mu/\nu = 21/6$, $c/a = 1{\cdot}870_1$ and $\Sigma = 15$, $\mu/\nu = 24/7$, $c/a = 1{\cdot}851_6$,

$15+13=28$	then $\Sigma = 28$
$24+21=45,\ 7+6=13$	then $\mu/\nu = 45/13$
	and $c/a = 1{\cdot}860_5$.

Table 1. *Typical cases of twin orientations for an hP lattice and for* $\Sigma^{lim}_{min}=2$: $(10\bar{1}1)$, $(11\bar{2}1)$ *twin planes, for* $\Sigma^{lim}_{min}=3$: $(10\bar{1}4)$, $(22\bar{4}1)$ *twin planes, for* $\Sigma^{lim}_{min}=4$: $(10\bar{1}3)$, $(30\bar{3}1)$ *twin planes and the corresponding sets of* Σ^{lim}

$(10\bar{1}1)$ twin plane											
$\Sigma=(3\nu+4\mu)/\alpha$	7	6	5	4	3	2	3	4	5	6	7
μ/ν	1/8	3/20	3/16	1/4	3/8	3/4	3/2	9/4	3/1	15/4	9/2
or	3/24	3/20	3/16	3/12	3/8	3/4	6/4	9/4	12/4	15/4	18/4
$(11\bar{2}1)$ twin plane											
$\Sigma=(\nu+4\mu)/\alpha$	7	6	5	4	3	2	3	4	5	6	7
μ/ν	1/24	1/20	1/16	1/12	1/8	1/4	1/2	3/4	1/1	5/4	3/2
or	1/24	1/20	1/16	1/12	1/8	1/4	2/4	3/4	4/4	5/4	6/4
$(10\bar{1}4)$ twin plane											
$\Sigma=(12\nu+\mu)/\alpha$		7		5		3	4	5	6	7	
μ/ν		2/1		3/1		6/1	12/1	18/1	24/1	30/1	
or		6/3		6/2		6/1	12/1	18/1	24/1	30/1	
$(22\bar{4}1)$ twin plane											
$\Sigma=(\nu+12\mu)/\alpha$		7	6	5	4	3		5		7	
μ/ν		1/40	1/32	1/24	1/16	1/8		1/4		3/8	
or		1/40	1/32	1/24	1/16	1/8		2/8		3/8	
$(10\bar{1}3)$ twin plane											
$\Sigma=(27\nu+4\mu)/\alpha$			7			4	5	6	7		
μ/ν			9/8			9/4	9/2	27/4	9/1		
or			9/8			9/4	18/4	27/4	36/4		
$(30\bar{3}1)$ twin plane											
$\Sigma=(3\nu+36\mu)/\alpha$			7	6	5	4			7		
μ/ν			1/16	1/12	1/8	1/4			1/2		
or			1/16	1/12	1/8	1/4			2/4		

Therefore, $\Sigma=28$, $\mu/\nu=45/13$, $c/a=1{\cdot}860_5$ is equivalent to

$$6\times(\Sigma=2,\ \mu/\nu=3/1)+1\times(\Sigma=3,\ \mu/\nu=6/1)$$
$$+5\times(\Sigma=2,\ \mu/\nu=3/1)+1\times(\Sigma=3,\ \mu/\nu=6/1)$$

with the simple rule $\Sigma=\Sigma'+\Sigma''$, $\mu=\mu'+\mu''$, $\nu=\nu'+\nu''$, keeping the two neighbouring cases $'$ and $''$ as the two closest (regarding c/a) of the final case.

More generally, the series of Σ^{lim} for $q=\ldots -3,-2,-1,0,1,2,3\ldots$ is written as:

$$\begin{array}{ccccc} -q\ \ldots & q=-3 & q=-2 & q=-1 & q=0\\ \Sigma^*+|q|P_l & \Sigma^*+3P_l & \Sigma^*+2P_l & \Sigma^*+P_l & \Sigma^*\\ \mu/(|q|+1)\nu & \mu/4\nu & \mu/3\nu & \mu/2\nu & \mu/\nu \end{array}$$

$$\begin{array}{ccccc} q=1 & q=2 & q=3 & \ldots & q\\ \Sigma^*+P_h & \Sigma^*+2P_h & \Sigma^*3P_h & & \Sigma^*|q|P_h\\ 2\mu/\nu & 3\mu/\nu & 4\mu/\nu & & (|q|+1)\mu/\nu.\dagger \end{array}$$

With the above formulation, typical cases of twin orientations for $\Sigma^{\rm lim}_{\rm min}=2,3$ and 4 are detailed in Table 1 with the formulation of Σ, the main part of the sequence of $\Sigma^{\rm lim}$'s and $\Sigma^{\rm lim}_{\rm min}$ and the corresponding axial ratio.

We can conclude at this stage that the knowledge, for one subset, of the twin plane indices and consequently the quaternion ($m=0$ for a 180° rotation), $\Sigma^*=\Sigma^{\rm lim}_{\rm min}$ and $P_{\rm low}$, $P_{\rm high}$ is sufficient to recover all the relevant parameters of one particular twin orientation for any c/a. It should be noted that only the indices of the twin plane are in fact necessary, the quaternion, Σ^*, $P_{\rm low}$ and $P_{\rm high}$ being derived from them. Table 2 is a summary of all the relevant information covering the field $\Sigma^*\leq 7$ and contains 42 different twin boundaries. The values of this table are fully consistent with those published in Tables 1 and 2 of Grimmer (1989*b*).

† $|q|$ is the absolute value of q, $\Sigma^*=\Sigma^{\rm lim}_{\rm min}$, $P_l=P_{\rm low}$, $P_h=P_{\rm high}$.

As a further example, the function *Fh* has been plotted in Fig. 2 for four different cases:

(*a*) $11\bar{2}4$ twin, $\Sigma=(4\nu+\mu)/\alpha$, $\Sigma^*=3$, $\mu^*/\nu^*=2/1$, $P_{\rm low}=2$, $P_{\rm high}=1$,
(*b*) $30\bar{3}2$ twin, $\Sigma=(3\nu+9\mu)/\alpha$, $\Sigma^*=4$, $\mu^*/\nu^*=1/1$, $P_{\rm low}=1$, $P_{\rm high}=3$,
(*c*) $9,3,\overline{12},1$ twin, $\Sigma=(7\nu+4\mu)/\alpha$, $\Sigma^*=8$, $\mu^*/\nu^*=1/4$, $P_{\rm low}=7$, $P_{\rm high}=1$,
(*d*) $41\bar{5}3$ twin, $\Sigma=(468\nu+84\mu)/\alpha$, $\Sigma^*=20$, $\mu^*/\nu^*=3/1$, $P_{\rm low}=13$, $P_{\rm high}=7$.

This last case is not a real twin as there is no 180° description; the largest angle description is a rotation of 167·2° for the [24 6 3] rotation axis and $m=1$.

Rhombohedral Bravais lattice

The function $Fr(\Sigma, c/a)$,

$$\Sigma=[(u^2+v^2+uv)2\rho+(3m^2+w^2)\mu]/\delta$$

for $(c/a)^2=3\mu/2\rho$ and g.c.d. $[\mu,(\mu-\rho)/3]=1$,

$(c/a)^2$ being a rational number, contains, in addition to the proper rhombohedral coincidence orientations, all the coincidences of the simple cubic ($\mu/\rho=1/1$),

Table 2. *Twin description of all the coincidence cases in an hP lattice with* $\Sigma^* \leq 7$

hkil and *uvw* are respectively the twin plane and the 180° rotation axis; $Fh = \Sigma^*\alpha$; μ^*/ν^* is the axial ratio corresponding to $\Sigma^* = \Sigma^{\rm lim}_{\rm min}$; $Pl\ (P_{\rm low}) + Ph(P_{\rm high}) = \Sigma^*$, Pl and Ph being the periodicities of $\Sigma^{\rm lim}$ for $(c/a)^2 < \mu^*/\nu^*$ (low) and $(c/a)^2 > \mu^*/\nu^*$ (high).

Σ^*	Twin plane *hkil*	*uvw*	*Fh*	μ^*/ν^*	$Pl+Ph$
2	$10\bar{1}1$	212	$3\nu+4\mu$	3/4	1+1
	$11\bar{2}1$	102	$\nu+4\mu$	1/4	1+1
	$10\bar{1}2$	211	$3\nu+\mu$	3/1	1+1
	$11\bar{2}2$	101	$\nu+\mu$	1/1	1+1
3	$20\bar{2}1$	214	$3\nu+16\mu$	3/8	1+2
	$22\bar{4}1$	104	$\nu+16\mu$	1/8	1+2
	$10\bar{1}4$	421	$12\nu+\mu$	6/1	2+1
	$11\bar{2}4$	201	$4\nu+\mu$	2/1	2+1
5	$40\bar{4}1$	218	$3\nu+64\mu$	3/16	1+4
	$44\bar{8}1$	108	$\nu+64\mu$	1/16	1+4
	$20\bar{2}3$	634	$27\nu+16\mu$	9/8	3+2
	$22\bar{4}3$	304	$9\nu+16\mu$	3/8	3+2
	$30\bar{3}4$	423	$12\nu+9\mu$	2/1	2+3
	$33\bar{6}4$	203	$4\nu+9\mu$	2/3	2+3
	$10\bar{1}8$	841	$48\nu+\mu$	12/1	4+1
	$11\bar{2}8$	401	$16\nu+\mu$	4/1	4+1
7	$40\bar{4}3$	638	$27\nu+64\mu$	9/16	3+4
	$20\bar{2}5$	10,5,4	$75\nu+16\mu$	15/8	5+2
	$30\bar{3}8$	843	$48\nu+9\mu$	4/1	4+3
	$60\bar{6}1$	2,1,12	$3\nu+144\mu$	1/8	1+6
	$1,0,\bar{1},12$	12,6,1	$108\nu+\mu$	18/1	6+1
4	$10\bar{1}3$	632	$27\nu+4\mu$	9/4	3+1
	$11\bar{2}3$	302	$9\nu+4\mu$	3/4	3+1
	$10\bar{1}6$	631	$27\nu+\mu$	9/1	3+1
	$11\bar{2}6$	301	$9\nu+1\mu$	3/1	3+1
	$30\bar{3}1$	216	$3\nu+36\mu$	1/4	1+3
	$33\bar{6}1$	106	$\nu+36\mu$	1/12	1+3
	$30\bar{3}2$	213	$3\nu+9\mu$	1/1	1+3
	$33\bar{6}2$	103	$\nu+9\mu$	1/3	1+3
6	$50\bar{5}1$	2,1,10	$3\nu+100\mu$	3/20	1+5
	$5,5,\overline{10},1$	1,0,10	$\nu+100\mu$	1/20	1+5
	$50\bar{5}2$	215	$3\nu+25\mu$	3/5	1+5
	$5,5,\overline{10},2$	105	$\nu+25\mu$	1/5	1+5
	$10\bar{1}5$	10,5,2	$75\nu+4\mu$	15/4	5+1
	$11\bar{2}5$	502	$25\nu+4\mu$	5/4	5+1
	$1,0,\bar{1},10$	10,5,1	$75\nu+\mu$	15/1	5+1
	$1,1,\bar{2},10$	501	$25\nu+\mu$	5/1	5+1
7	$44\bar{8}3$	308	$9\nu+64\mu$	3/16	3+4
	$22\bar{4}5$	504	$25\nu+16\mu$	5/8	5+2
	$33\bar{6}8$	403	$16\nu+9\mu$	4/3	4+3
	$6,6,\overline{12},1$	1,0,12	$\nu+144\mu$	1/24	1+6
	$1,1,\bar{2},12$	601	$36\nu+\mu$	6/1	6+1

body-centred cubic ($\mu/\rho = 1/4$) and face-centred cubic ($\mu/\rho = 4/1$). In particular, when the twin plane becomes a mirror plane for the corresponding c/a, the identity appears as $\Sigma = 1$. This complicates slightly the structure of the function *Fr* and leads in some rare cases to two $\Sigma^{\rm lim}_{\rm min}$ both equal and contiguous. The envelope of $\Sigma^{\rm lim}$ remains as before continuous and monotonic on its two parts with the appropriate periodicity.

The plot of *Fr* for the rhombohedral twin (01.2) and for $0 < c/a < 5$ and Σ up to 20 is represented in Fig. 3. The envelope of $\Sigma^{\rm lim}$ has a dual extremum for $\Sigma = 1^*$ ($\mu/\rho = 1/1$) and $\Sigma = 1°$ ($\mu/\rho = 4/1$), $P_{\rm low} = 1$ and $P_{\rm high} = 1$ but $\Sigma^{\rm lim}_{\rm min}$ is now different from $P_{\rm low} + P_{\rm high}$. However, if the particular cases $\Sigma = 1$ are excluded from the plot, there remain three independent sets of values with, for each of them,

$$\Sigma = 2 \text{ and } \mu/\rho = 2/5; \quad P_{\rm low} = 1 \text{ and } P_{\rm high} = 1;$$
$$\Sigma^{\rm lim}_{\rm min} = P_{\rm low} + P_{\rm high} = 2;$$
$$\Sigma = 2 \text{ and } \mu/\rho = 6/3; \quad P_{\rm low} = 1 \text{ and } P_{\rm high} = 1;$$
$$\Sigma^{\rm lim}_{\rm min} = P_{\rm low} + P_{\rm high} = 2;$$
$$\Sigma = 2 \text{ and } \mu/\rho = 10/1; \quad P_{\rm low} = 1 \text{ and } P_{\rm high} = 1;$$
$$\Sigma^{\rm lim}_{\rm min} = P_{\rm low} + P_{\rm high} = 2.$$

As an example, the coincidence case $\Sigma = 15$ and $\mu/\rho = 64/13$ or $c/a = 2{\cdot}717_5$ is found in Fig. 3 by the following linear combination:

$$6 \times (\Sigma = 1°, \mu/\nu = 4/1) + 1 \times (\Sigma = 2, \mu/\nu = 10/1)$$
$$+ 5 \times (\Sigma = 1°, \mu/\nu = 4/1) + 1 \times (\Sigma = 2, \mu/\nu = 10/1)$$

with the simple rule $\Sigma = \Sigma' + \Sigma''$, $\mu = \mu' + \mu''$, $\rho = \rho' + \rho''$, keeping the two neighbouring cases ′ and ″ as the two closest (with reference to c/a) of the final case.

The series of $\Sigma^{\rm lim}$ is detailed for some simple cases in Table 3 and the relevant information for all the coincidence cases with $\Sigma \leq 3$ is summarized in Table 4. It appears that for every $\Sigma^{\rm lim}$ the axial ratio is given by

$$\mu/[p(3\rho') + \rho] \quad \text{and} \quad [\mu + p(3\mu')]/\rho$$

on both sides of $\Sigma^* = \Sigma^{\rm lim}_{\rm min}$ defined by μ/ρ and μ', ρ' divisor of μ, ρ. $p = 0$ for Σ^*. This becomes $\mu^*/[p(3\rho°) + \rho^*]$ and $[\mu° + p(3\mu^*)]/\rho°$ for the two dual cases.

In most simple cases (*cf.* Table 4), $\mu = \mu'$ and $\rho = \rho'$; if not the 'odd rule' has to be applied on the corresponding side of Σ^*: low side for $\mu' \neq \mu$ and high side for $\rho' \neq \rho$. The odd rule implies that only the odd values of p are counted.

On both sides of Σ^* two singular values of Σ appear and are noted $\Sigma_{\rm low}$ and $\Sigma_{\rm high}$. These Σ values are related to the periodicities $P_{\rm low}$ and $P_{\rm high}$ by

$$3\Sigma^* = P_{\rm low} + P_{\rm high},$$
$$\Sigma_{\rm low} = \Sigma^* + P_{\rm low} \quad \text{and} \quad \Sigma_{\rm high} = \Sigma^* + P_{\rm high}$$

and in this case there is a continuity in the periodicity of $\Sigma^{\rm lim}$ on both sides of Σ^*.

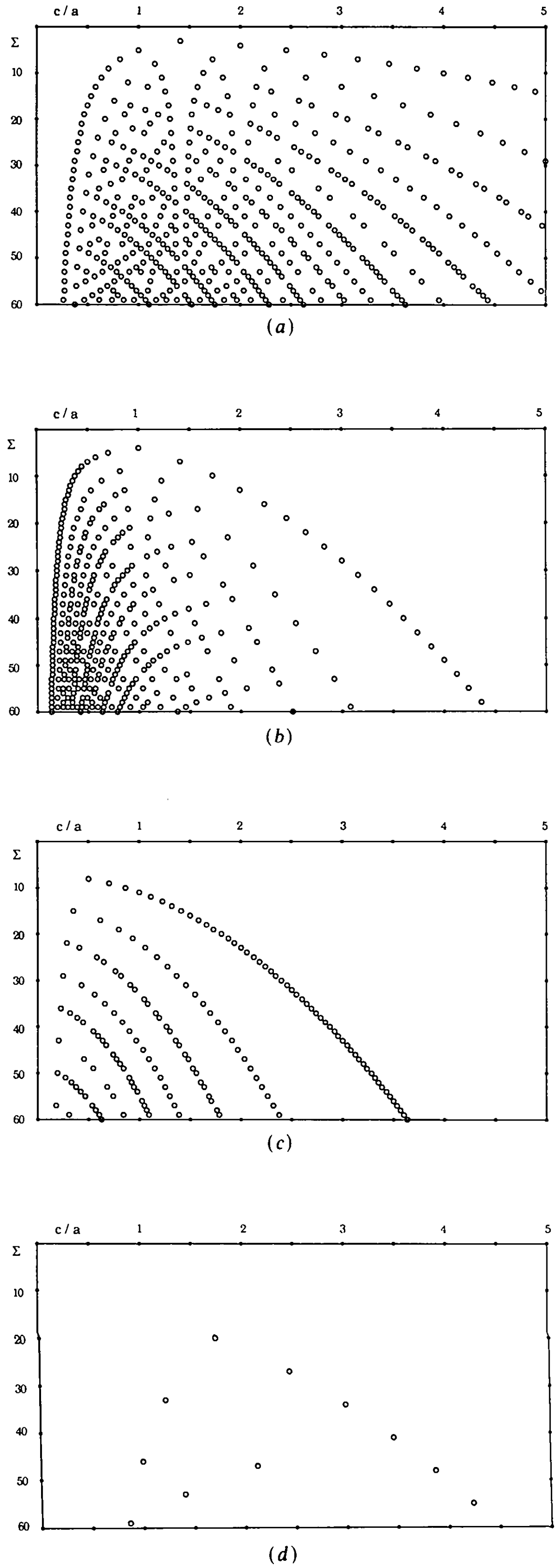

Fig. 2. Plot of *Fh* for the (*a*) $11\bar{2}4$ twin, $\Sigma^*=3$, $\mu^*/\nu^*=2/1$; (*b*) $30\bar{3}2$ twin, $\Sigma^*=4$, $\mu^*/\nu^*=1/1$; (*c*) $9,3,\overline{12},1$ twin, $\Sigma^*=8$, $\mu^*/\nu^*=1/4$; (*d*) $41\bar{5}3$ 'twin', $\Sigma^*=20$, $\mu^*/\nu^*=3/1$.

If the odd rule applies then the relation between Σ, P_{low} and P_{high} is changed to

$$3\Sigma^*=2P_{\text{low}}+P_{\text{high}} \quad \text{or} \quad 3\Sigma^*=P_{\text{low}}+2P_{\text{high}}$$

depending on which side the rule is effective (respectively high and low sides) and

$$\Sigma^*=p_{\text{low}}+p_{\text{high}}$$

$$\Sigma_{\text{low}}=\Sigma^*+p_{\text{low}} \quad \text{and} \quad \Sigma_{\text{high}}=\Sigma^*+p_{\text{high}}.$$

There is in this case an alteration of the periodicity at the level of Σ_{low}, Σ^* and Σ_{high}. As detailed in Table 3, for the (08.1) twin the odd rule does not apply:

$$\Sigma^*=3, \qquad 3\Sigma^*=9=P_{\text{low}}+P_{\text{high}}=1+8,$$

$$\Sigma_{\text{low}}=\Sigma^*+P_{\text{low}}=3+1=4,$$

$$\Sigma_{\text{high}}=\Sigma^*+P_{\text{high}}=3+8=11;$$

the sequence of Σ^{lim} becomes:

6	5	4	**3**	11	19	27
P_{low}		Σ_{low}	Σ^*	Σ_{high}		P_{high}.

For the (70.1) twin the odd rule applies on the high side:

$$\Sigma^*=3, \qquad 3\Sigma^*=9=2P_{\text{low}}+P_{\text{high}}=2\times1+7,$$

$$\Sigma^*=p_{\text{low}}+p_{\text{high}}=1+2$$

$$\Sigma_{\text{low}}=\Sigma^*+p_{\text{low}}=3+1=4,$$

$$\Sigma_{\text{high}}=\Sigma^*+p_{\text{high}}=3+2=5;$$

the sequence of Σ^{lim} becomes:

6	5	4	**3**	5	12	19
P_{low}		Σ_{low}	Σ^*	Σ_{high}		P_{high}
			p_{low}	p_{high}.		

A quasiperiodic description

Obviously, in real materials, $(c/a)^2$ has an irrational value and coincidences were understood as 'near

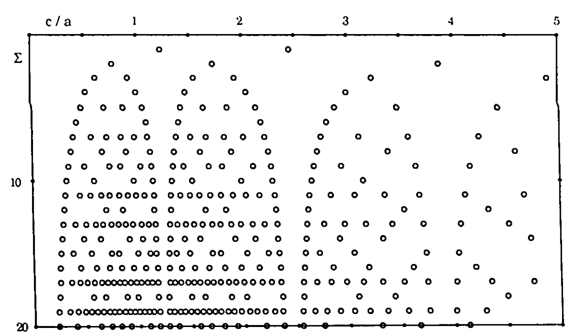

Fig. 3. Plot of *Fr* for the rhombohedral (01.2) twin; $0<(c/a)^2<5$ and Σ up to 20. $\Sigma^*=\Sigma^{\text{lim}}_{\text{min}}=1$ appears twice (1^* and 1°) for $\mu^*/\rho^*=1/1$ ($c/a=1{\cdot}224_7$), $\mu^\circ/\rho^\circ=4/1$ ($c/a=2{\cdot}449_5$).

Table 3. *Typical cases of twin orientations for an hR lattice and* $\Sigma^{lim}_{min}=1$*: (01.2) and (10.4) twin planes,* $\Sigma^{lim}_{min}=2$*: (05.1) and (40.1) twin planes,* $\Sigma^{lim}_{min}=3$*: (70.1) and (08.1) twin planes and the corresponding sets of* Σ_{lim}

(01.2) twin plane

Σ	4	3	2	1*	1°	2	3	4
μ/ρ	2/11	1/4	2/5	1/1	4/1	10/1	16/1	22/1
	$\frac{2}{9+2}$	$\frac{2}{6+2}$	$\frac{2}{3+2}$	$\frac{2}{2}$	$\frac{4}{1}$	$\frac{4+6}{1}$	$\frac{4+12}{1}$	$\frac{4+18}{1}$

(10.4) twin plane

				2+1			
Σ	7	5	3	1	2	3	4
μ/ρ	2/5	4/7	1/1	4/1	16/1	28/1	40/1
	$\frac{4}{9+1}$	$\frac{4}{6+1}$	$\frac{4}{3+1}$	$\frac{4}{1}$	$\frac{4+12}{1}$	$\frac{4+24}{1}$	$\frac{4+36}{1}$

(05.1) twin plane

				1+5			
Σ	5	4	3	2	7	12	17
μ/ρ	1/100	1/70	1/40	1/10	2/5	7/10	1/1
	$\frac{1}{90+10}$	$\frac{1}{60+10}$	$\frac{1}{30+10}$	$\frac{1}{10}$	$\frac{1+3}{10}$	$\frac{1+6}{10}$	$\frac{1+9}{10}$

(40.1) twin plane

			1	1+1	4		
Σ	5	4	3	2	3	7	11
μ/ρ	1/88	1/64	1/40	1/16	1/4	5/8	1/1
$\rho'=8$	$\frac{1}{72+16}$	$\frac{1}{48+16}$	$\frac{1}{24+16}$	$\frac{1}{16}$	$\frac{1+3}{16}$	$\frac{1+9}{16}$	$\frac{1+15}{16}$

(70.1) twin plane

			1	1+2	7		
Σ	6	5	4	3	5	12	19
μ/ρ	1/154	1/112	1/70	1/28	1/7	5/14	4/7
$\rho'=14$	$\frac{1}{126+28}$	$\frac{1}{84+28}$	$\frac{1}{42+28}$	$\frac{1}{28}$	$\frac{1+3}{2}$	$\frac{1+9}{28}$	$\frac{1+15}{28}$

(08.1) twin plane

			1	1+8	8		
Σ	6	5	4	3	11	19	27
μ/ρ	1/160	1/112	1/64	1/16	1/4	7/16	5/8
	$\frac{1}{144+16}$	$\frac{1}{96+16}$	$\frac{1}{48+16}$	$\frac{1}{16}$	$\frac{1+3}{16}$	$\frac{1+6}{16}$	$\frac{1+9}{16}$

coincidences': the experimental case being near to one or other exact coincidence case. However, the choice of this (these) exact case(s) remains the main problem. The best compromise was to keep simultaneously an acceptably low value of the index of coincidence Σ and a difference $\mu/\nu-(c/a)^2_{ex}$ as small as possible (Hagège & Nouet, 1989). Another approach was to identify the Burgers vector and/or the line direction of some intrinsic dislocations at the boundary and relate the corresponding displacement shift complete lattice (DSCL) to an exact coincidence orientation of a given Σ value (Chen & King, 1988). Technically, this method is difficult to use systematically and the discrimination between different cases remains hazardous.

As an irrational number can always be approximated by two rational numbers within a chosen precision, an irrational orientation can be approximated in the same way by two rational exact coincidence orientations. As demonstrated above, these two exact orientations are described by a periodic arrangement of elementary units; in the case of an irrational orientation the arrangement is no longer periodic but is defined by a deterministic rule and therefore ordered; the arrangement is quasiperiodic. The rule defining this quasiperiodicity is the same as that defining the coefficient of the linear combination of elementary units characteristic of the irrational orientation, and this linear combination is unique.

Table 4. *Twin description of all the coincidence cases for an hR lattice with* $\Sigma^*\le 3$.

hkil is the twin plane; μ/ρ corresponds to Σ^* (μ^*/ρ^* and μ°/ρ° for the two dual cases); the other parameters are defined in the text.

Σ^*	*hk.l*	μ^*/ρ^*	μ°/ρ°			*Pl + Ph*
	10.1	1/4	2/2			1+...+1
1		dual				(6*1)
	01.2	2/2	4/1			1+...+1
		dual				(6*1)
Σ^*	*hk.l*	μ/ρ	ρ', μ'	*Pl + Ph*		*q, p*
1	10.4	4/1	1, 4	2+1		all
	02.1	1/4	4, 1	1+2		all
Σ^*	*hk.l*	μ/ρ	ρ', μ'	*pl + ph*	*Pl + Ph*	*q, p*
	10.2	6/3	3, 6	3+3	3+3	all
	01.1	3/6	6, 3	3+3	3+3	all
	10.10	10/1	1, 10	5+1	5+1	all
	05.1	1/10	10,1	1+5	1+5	all
2	50.2	2/5	5, 2	1+5	1+5	all
	01.5	5/2	2, 5	5+1	5+1	all
	40.1	1/16	8, 1	1+1	2*1+4	odd+
	01.8	16/1	1, 10	1+1	4+2*1	odd−
	10.16	16/1	1, 16	8+1	8+1	all
	08.1	1/16	16, 1	1+8	1+8	all
	70.4	4/7	7, 4	2+7	2+7	all
	02.7	7/4	4, 7	7+2	7+2	all
	50.8	8/5	5, 8	4+5	4+5	all
	04.5	5/8	8, 5	5+4	5+4	all
	21.4	4/1	1, 4	2+7	2+7	all
3	12.2	2/2	1, 2	1+2	2*1+7	odd+
	21.1	1/4	2, 1	1+2	2*1+7	odd−
	70.1	1/28	14, 1	1+2	2*1+7	odd+
	01.14	28/1	1, 14	2+1	7+2*1	odd−
	10.7	14/2	2, 7	2+1	7+2*1	odd−
	07.2	2/14	7, 2	1+2	2*1+7	odd+
	20.5	10/4	4, 5	1+2	5+2*2	odd−
	05.4	4/10	5, 4	2+1	2*2+5	odd+

The orientation defined by this (m, u, v, w), all relatively prime integers, can be described, for any c/a, by a quasiperiodic arrangement of $\Sigma^{\rm lim}$.

Mechanical twins in h.c.p. metals

As shown above, $(10\bar{1}2)$ mechanical twins in h.c.p. metals are described by the quaternion (0, 2, 1, 1). By plotting for this quaternion $F(\Sigma, c/a)$, *i.e.* $\Sigma=(3\nu+\mu)/\alpha$ and $\alpha=1$ or 3, a set of $\Sigma^{\rm lim}$ (...7, 6, 5, 4, 3, 2, 3, 4, 5, 6, 7, ...) and a unique $\Sigma^{\rm lim}_{\rm min}=2$ appear in Fig. 1:

As an example $(10\bar{1}2)$ mechanical twins in zinc $[(c/a)_{\rm ex}=1{\cdot}856_{2\ldots}]$ will be described by the following algorithm:

Σ'	μ'/ν'	c/a	Σ''	μ''/ν''	c/a	then	Σ^+	μ^+/ν^+
2	3/1	$1\cdot732_1$	3	6/1	$2\cdot449_5$	then	5	9/2
2	3/1	$1\cdot732_1$	5	9/2	$2\cdot131_3$	then	7	12/3 (4/1)
2	3/1	$1\cdot732_1$	7	12/3	$2\cdot000_0$	then	9	15/4
2	3/1	$1\cdot732_1$	9	15/4	$1\cdot936_5$	then	11	18/5
2	3/1	$1\cdot732_1$	11	18/5	$1\cdot897_3$	then	13	21/6 (7/2)
2	3/1	$1\cdot732_1$	13	21/6	$1\cdot870_8$	then	15	24/7
15	24/7	$1\cdot851_6$	13	21/6	$1\cdot870_8$	then	28	45/13
15	24/7	$1\cdot851_6$	28	45/13	$1\cdot860_5$	then	43	69/20
15	24/7	$1\cdot851_6$	43	69/20	$1\cdot857_2$	then	58	93/27 (31/9)
58	93/27	$1\cdot855_9$	43	69/20	$1\cdot857_2$	then	101	162/47
58	93/27	$1\cdot855_9$	101	162/47	$1\cdot856_6$	then	159	255/74
58	93/27	$1\cdot855_9$	159	255/74	$1\cdot856_3$	then	217	348/101

$c/a = 1\cdot856_2$

with the simple rule $\Sigma^+ = \Sigma' + \Sigma''$, $\mu^+ = \mu' + \mu''$, $\nu^+ = \nu' + \nu''$ and up to a chosen precision.

With the following notation for the limiting boundaries:

Σ	μ/ν	c/a	
2	3/1	$1\cdot732_1$	as A
3	6/1	$2\cdot449_5$	as B,

the successive approximants are noted:

Σ	μ/ν	c/a	
5	9/2	$2\cdot121_3$	AB
7	12/3	$2\cdot000_0$	AAB or $2AB$
9	15/4	$1\cdot936_5$	$3AB$
11	18/5	$1\cdot897_4$	$4AB$
13	21/6	$1\cdot870_8$	$5AB$
15	24/7	$1\cdot851_6$	$6AB$
28	45/13	$1\cdot860_5$	$6AB5AB$
43	69/20	$1\cdot857_4$	$6AB6AB5AB$ or $2(6AB)5AB$
58	31/9	$1\cdot855_9$	$3(6AB)5AB$
101	162/47	$1\cdot856_6$	$3(6AB)5AB\ 2(6AB)5AB$
159	255/74	$1\cdot856_3$	$3(6AB)5AB\ 3(6AB)5AB\ 2(6AB)5AB$
217	348/101	$1\cdot856_2$	$3(6AB)5AB \ldots 3(6AB)5AB\ 2(6AB)5AB$

and finally for the real material zinc [$(c/a)_{ex} = 1\cdot856_{2\ldots}$], a quasiperiodic arrangement of

B units ($\Sigma = 3$) in a matrix A ($\Sigma = 2$),
or $5AB$ units ($\Sigma = 13$) in a matrix $6AB$ ($\Sigma 15$),
or $2(6AB)5AB$ units ($\Sigma = 43$) in a matrix $3(6AB)5AB$ ($\Sigma = 58$).

Generally, $(10\bar{1}2)$ mechanical twins in h.c.p. metals (Fig. 4) will be best described by a $\Sigma = 2$, $\mu/\nu = 3/1$ perturbed by a quasiperiodic arrangement of B, or B', units such as $\Sigma = 3$, $\mu/\nu = 6/1$ (B) for Zn and Cd and $\Sigma = 3$, $\mu/\nu = 3/2$ (B') for Mg, Zr, Ti, ... Each material, for each particular value of c/a, defines a particular quasiperiodicity of minor units.

Metal	$(c/a)_{ex}$	Best approximant ($\Sigma < 50$) Σ	μ/ν	quasiperiodicity
Ti	$1\cdot587_{9\ldots}$	46	63/25	$\ldots 3(B'4A)B'5A \ldots$
Mg	$1\cdot623_{6\ldots}$	47	66/15	$\ldots 2(B'6A)B'7A \ldots$
Zn	$1\cdot856_{2\ldots}$	43	69/20	$\ldots 2(6AB)5AB \ldots$

All the other usual mechanical twins $(10\bar{1}1)$, $(11\bar{2}2)$, $(11\bar{2}1)$ can be reconsidered in the same way following the values of $\Sigma^{\rm lim}_{\rm min}$ and $\Sigma^{\rm lim}$ in Table 3.

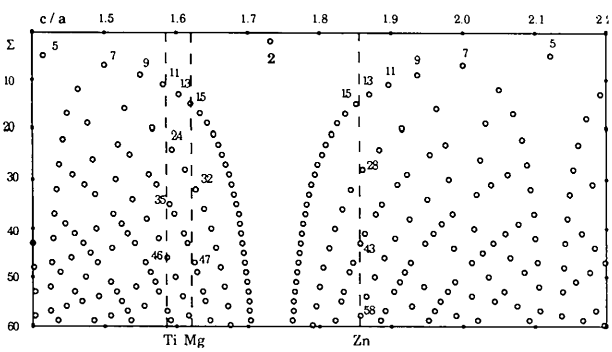

Fig. 4. Enlargement of the plot of *Fh* for the $(10\bar{1}2)$ mechanical twin: $1\cdot4 \leq c/a \leq 2\cdot2$ and Σ up to 60. The experimental values of c/a of Ti ($1.587_{9\ldots}$), Mg ($1.623_{6\ldots}$) and Zn ($1.856_{2\ldots}$) appear as dashed lines.

Interfaces in tungsten carbide

In tungsten carbide-cobalt (WC-Co) composites, interfaces in the hard phase [WC, $(c/a)_{ex} = 0\cdot976_{1\ldots}$], described in a hexagonal Bravais lattice, show often a low-energy configuration which has been described by $\Sigma = 2$, $\mu/\nu = 1$ and a quaternion $(0, 1, 1, 1)$ (Hagège, Nouet & Delavignette, 1980). This case belongs to the same subset as the $(11\bar{2}2)$ twins in h.c.p. metals (see Table 2). In that case $\Sigma = (\nu + \mu)$ ($\alpha = 1$ for any μ, ν) and $\Sigma^{\rm lim}$ and $\Sigma^{\rm lim}_{\rm min}$ are defined as follows:

$(c/a)^2$	1/6	1/5	1/4	1/3	1/2	**1/1**	2/1	3/1	4/1	5/1	6/1	...
Σ	7	6	5	4	3	**2**	3	4	5	6	7	...

$\Sigma^{\rm lim}_{\rm min}$.

This orientation will be described by the following algorithm:

Σ	μ/ν	c/a	Σ	μ/ν	c/a	then	Σ^+	μ^+/ν^+
3	1/2	$0\cdot707_1$	2	1/1	$1\cdot000_0$	then	5	2/3
5	2/3	$0\cdot816_5$	2	1/1	$1\cdot000_0$	then	7	3/4
⋮								
41	20/21	$0\cdot975_9$	2	1/1	$1\cdot000_0$	then	43	21/22
41	20/21	$0\cdot975_9$	43	21/22	$0\cdot977_0$	then	84	41/43

$c/a = 0\cdot976_5$.

With the following notation for the limiting boundaries:

Σ	μ/ν	c/a	
2	1/1	$1\cdot000_0$	as A
3	1/2	$0\cdot707_1$	as B,

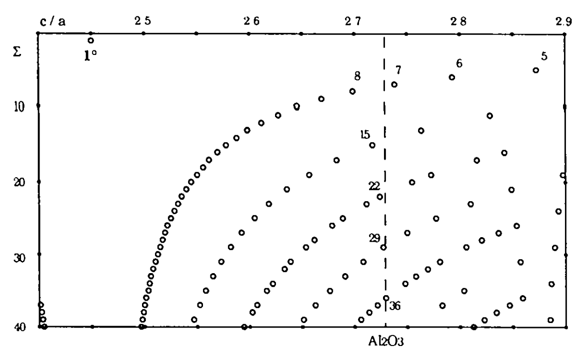

Fig. 5. Enlargement of the plot of *Fr* for the rhombohedral twin: $2\cdot4 \leq c/a \leq 3\cdot4$ and Σ up to 40. The experimental value of c/a of alumina appears as a dashed line.

the successive approximants are noted:

Σ	μ/ν	c/a	
5	2/3	$0{\cdot}816_5$	BA
7	3/4	$0{\cdot}866_0$	BAA or $B2A$
⋮			
41	20/21	$0{\cdot}975_9$	$B19A$
43	21/22	$0{\cdot}977_0$	$B20A$

and finally for the real material a quasiperiodic arrangement of B units ($\Sigma = 3$) in a matrix A ($\Sigma = 2$), with an average of minor unit every 19 to 20 A on a first approximation.

Rhombohedral twin in alumina

In the case of alumina (corundum or α-Al_2O_3: $c/a = 2{\cdot}729_4$), the lattice is hR and the rhombohedral twin is a common interface (Grimmer *et al.*, 1990) with a twin plane (01.2)

$$\Sigma = (\mu + 2\rho)/3\delta'.$$

$\Sigma^{\lim}$ and $\Sigma^{\lim}_{\min}$ are defined as follows (*cf.* also Table 3):

c/a	0·46	0·52	0·61	0·77	**1·22**	**2·45**	3·87	4·90	5·74	6·4
μ/ρ	1/7	2/11	1/4	2/5	**1/1**	**4/1**	10/1	16/1	22/1	28/1
Σ	5	4	3	2	1*	1°	2	3	4	5

$^*\Sigma^{\lim}_{\min}$.

This orientation for $(c/a)_{ex} = 2{\cdot}729_4$ will be described in Fig 5 by the following algorithm:

Σ	μ/ρ	c/a	Σ	μ/ρ	c/a	then	Σ	μ/ρ	c/a
1°	4/1	$2{\cdot}449_5$	2	10/1	$3{\cdot}873_0$	then	3	14/2	$3{\cdot}240_4$
1°	4/1	$2{\cdot}449_5$	3	14/2	$3{\cdot}240_4$	then	4	18/3	$3{\cdot}000_0$
1°	4/1	$2{\cdot}449_5$	4	18/3	$3{\cdot}000_0$	then	5	22/4	$2{\cdot}872_3$
1°	4/1	$2{\cdot}449_5$	5	22/4	$2{\cdot}872_3$	then	6	26/5	$2{\cdot}792_8$
1°	4/1	$2{\cdot}449_5$	6	26/5	$2{\cdot}792_8$	then	7	30/6	$2{\cdot}738_6$
1°	4/1	$2{\cdot}449_5$	7	30/6	$2{\cdot}738_6$	then	8	34/7	$2{\cdot}699_0$
8	34/7	$2{\cdot}699_0$	7	30/6	$2{\cdot}738_6$	then	15	64/13	$2{\cdot}717_5$
15	64/13	$2{\cdot}717_5$	7	30/6	$2{\cdot}738_6$	then	22	94/19	$2{\cdot}724_2$
22	94/19	$2{\cdot}724_2$	7	30/6	$2{\cdot}738_6$	then	29	124/25	$2{\cdot}727_6$
29	124/25	$2{\cdot}727_6$	7	30/6	$2{\cdot}738_6$	then	36	154/31	$2{\cdot}729_8$

If	1°	4/1	2·4495	is noted A
and	2	10/1	3·8730	is noted B

the successive approximants are noted:

Σ	μ/ρ	c/a	
3	7/1	$3{\cdot}240_4$	AB
4	6/1	3·0000	$A2B$
5	11/2	$2{\cdot}872_3$	$A3B$
6	26/5	$2{\cdot}792_8$	$A4B$
7	5/1	$2{\cdot}738_6$	$A5B$
8	34/7	$2{\cdot}699_0$	$A6B$
15	64/13	$2{\cdot}717_5$	$(A6B)(A5B)$
22	94/19	$2{\cdot}724_2$	$(A6B)2(A5B)$
29	124/25	$2{\cdot}727_6$	$(A6B)3(A5B)$
36	154/31	$2{\cdot}729_8$	$(A6B)4(A5B)$

and finally for the real material a quasiperiodic arrangement of B units ($\Sigma = 2$) in a matrix A ($\Sigma = 1°$), with an average of one minor unit B every 5 to 6 major units.

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