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The space groups of orthorhombic approximants to the icosahedral quasilattice

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Abstract. The space groups of the orthorhombic approximant lattices to the primitive icosahedral quasilattice are classified. There exist three Bravais classes: Pmmm, Cmmm and Immm. The basis vectors of the Bravais lattice of an approximant are parallel to two-, three- and/or fivefold axes of the quasilattice. It is found that there exist many non-symmorphic space groups with a common Bravais lattice in addition to symmorphic ones. This is because glides commonly appear.

1. Introduction

A quasicrystal has a regular atomic structure with a non-crystallographic point symmetry (see e.g. Janssen 1988); it is not periodic but quasiperiodic. It has been recognized that many phases of approximant crystals to a quasicrystal exist in the neighbourhood of the stoichiometry of the quasicrystal (Henley 1985, Knowles 1988, Ohashi 1989, Spaepen *et al* 1990, Audier and Guyot 1990, Zhang and Kuo 1991).

The structure of a quasicrystal is described by a quasilattice (QL), while that of its approximant crystal by a periodic approximant (PA) to the QL (Elser and Henley 1985, Knowles 1988). We have developed a theory of the space groups of the PA to a QL (Niizeki 1991a, b); a QL has PAs with different lattice constants and different space groups.

A QL is obtained by the cut-and-projection method from a mother lattice L which is a periodic lattice in higher dimensions than the physical dimensions (Katz and Duneau 1986, Janssen 1988); the mother lattice is cut with a strip before projected on to the physical space. Similarly, a PA to the QL is obtained by the same method from its mother lattice $\tilde{L}$, which is obtained by introducing a phason strain into L (Ishii 1989). The phason strain makes a lattice plane of $\tilde{L}$ overlap the physical space perfectly (Niizeki 1991a, b). Different PAs are obtained from a single mother lattice $\tilde{L}$ because there exists a degree of freedom known as the phase vector in the cut-and-projection method (Niizeki 1991a). The Bravais lattice of a PA is given by the restriction of $\tilde{L}$ onto the physical space, while the space group of the PA is determined by the point symmetry of the phase vector with respect to the shadow lattice, which is the projection of $\tilde{L}$ onto the internal space; a high symmetry PA is obtained when the phase vector is located on a special point of the shadow lattice.

The point group of the Bravais lattice of a PA is determined by the symmetry of the phason strain in $\tilde{L}$ (Ishii 1989). Dmitrienko (1987, 1990) discussed the space groups of the cubic PAs to icosahedral quasilattices (IQLs) by focusing on the reciprocal space properties, while Knowles (1988) discussed orthorhombic approximants. In this paper, we will present a complete classification of the space groups of orthorhombic PAs to the primitive IQL and also of cubic ones.

We shall introduce in section 2 the properties of the primitive IQL. The properties of the mother lattices of orthorhombic PAs to the IQL are extensively investigated in section 3. Several important examples of the non-primitive Bravais lattices appearing as the PAs are presented in section 4. PAs to the IQL are constructed in section 5 by the cut-and-projection method from the mother lattices. We shall introduce in section 6 special points, lines and planes of the shadow lattice. The space groups of the orthorhombic PAs to the IQL are completely classified in section 7. Section 8 is devoted to discussion.

2. The primitive icosahedral quasilattice

The mother lattice L of the primitive IQL (Pm$\bar{3}\bar{5}$) in three dimensions (3D) is a simple hypercubic lattice in 6D. The 6D Euclidean space into which L is embedded is decomposed into the physical space and the internal space as $E_6 = E_3 \oplus E_3'$. The basis vectors $\boldsymbol{\varepsilon}_i = (\boldsymbol{e}_i, \boldsymbol{e}_i')$ of L are given as

$$\begin{pmatrix} \boldsymbol{e}_1 & \boldsymbol{e}_2 & \boldsymbol{e}_3 & \boldsymbol{e}_4 & \boldsymbol{e}_5 & \boldsymbol{e}_6 \\ \boldsymbol{e}_1' & \boldsymbol{e}_2' & \boldsymbol{e}_3' & \boldsymbol{e}_4' & \boldsymbol{e}_5' & \boldsymbol{e}_6' \end{pmatrix} = \begin{pmatrix} \tau & 0 & 1 & -1 & \tau & 0 \\ 1 & \tau & 0 & 0 & -1 & \tau \\ 0 & 1 & \tau & \tau & 0 & -1 \\ 1 & 0 & -\tau & \tau & 1 & 0 \\ -\tau & 1 & 0 & 0 & \tau & 1 \\ 0 & -\tau & 1 & 1 & 0 & \tau \end{pmatrix} \tag{1}$$

where the first (or the last) three components represent $\boldsymbol{e}_i$ (or $\boldsymbol{e}_i'$) and $\tau = (1+\sqrt{5})/2$ is the golden ratio. Note that $\boldsymbol{\varepsilon}_i \cdot \boldsymbol{\varepsilon}_j = 2(a_{\mathrm{R}})^2 \delta_{i,j}$ with $a_{\mathrm{R}} = \sqrt{\tau+2}$.

Twleve vectors $\pm\boldsymbol{e}_i$ (or $\pm\boldsymbol{e}_i'$) are vertex vectors of an icosahedron Y (or Y') in E_3 (or E_3'). We show in figure 1 the projection of Y onto plane perpendicular to the threefold axis $\boldsymbol{e}_1 + \boldsymbol{e}_2 + \boldsymbol{e}_3$; the threefold rotation C_3 around this axis permutes cyclically

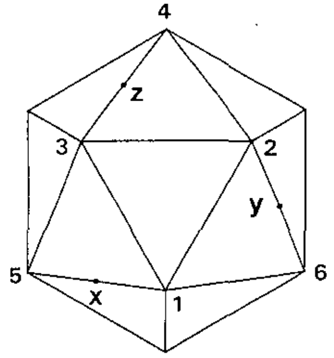

Figure 1. The projection of the icosahedron Y onto the plane perpendicular to a threefold axis. The centre of Y is located on the origin of E_3 and the six numbered vertices of Y show $\boldsymbol{e}_i$. x, y and z axes of the Cartesian coordinate system of E_3 are parallel to twofold axes which pass the middle points of the three edges indicated. Two fivefold axes and two threefold ones are included in the xy-plane.

the members of the triplets $\{e_1, e_2, e_3\}$ and $\{e_4, e_5, e_6\}$. Three twofold axes which are orthogonal to each other are chosen as the three axes of the Cartesian coordinate system of E_3 (or E_3'). The point group of Y is equal to $\mathrm{m}\bar{3}\bar{5}(Y_h)$.

The projection of L onto E_3 is a dense set, $L_\mathrm{p}=\{\Sigma_i n_i e_i \mid n_i \in Z\}$, because e_i are linearly independent over Z. L_p is called a pre-quasilattice. L_p is mathematically a Z-module. An IQL is a discrete subset of L_p. A lattice vector $\Sigma_i n_i e_i$ of L_p is indexed as $[n_1 n_2 n_3 n_4 n_5 n_6]$. The projection L_p' of L onto E_3' is a also pre-quasilattice. L_p is invariant against the quasi-space group $g_\mathrm{p}=Y_h * L_\mathrm{p}$ $(=\{\{\sigma|l\}|\sigma \in Y_h,\ l \in L\})$, a semi-direct product. Y_h is lifted to a 6D point group, which is usually identified with Y_h. The 6D point group Y_h leaves E_3 and E_3' invariant and g_p is the restriction of the 6D space group $Y_h * L$ of L onto E_3.

Only three of six e_i (or e_i') are linearly independent over the algebraic field $Q[\tau]$. The linear relationship among e_i along a two-, three- or fivefold axis of Y is given by

$$(e_1+e_5)/\tau-(e_3-e_4)=0$$

$$(e_1+e_2+e_3)/\rho-(e_4+e_5+e_6)=0$$

or

$$\sqrt{5}e_1-(e_2+e_3-e_4+e_5+e_6)=0,$$

where $\rho=2+\sqrt{5}$ $(=\tau^3)$. e_i' satisfy similar linear relationships but τ, ρ and $\sqrt{5}$ are replaced by their algebraic conjugates, $-1/\tau$, $-1/\rho$ and $-\sqrt{5}$.

An IQL

$$Q(\phi, W)=\left\{\sum_i n_i e_i \,\middle|\, n_i \in Z, \sum_i n_i e_i' + \phi \in W\right\} \tag{2}$$

is characterized by ϕ $(\in E_3')$, the phase vector, and W $(\subset E_3')$, the window. $Q(\phi, W)$ has Y_h as its macroscopic point symmetry group provided that W is invariant against Y_h. Two IQLs with a common window but different phase vectors are locally isomorphic.

If W is a rhombic triacontahedron whose edge length is a_R, then $Q(\phi, W)$ is a 3D-Penrose tiling (Katz and Duneau 1986) with prolate rhombohedra and oblate ones; a_R is equal to the edge length of the rhombohedra. The volumes of the two types of rhombohedra are given by $\Omega_\mathrm{P}=2\tau^2$ and $\Omega_\mathrm{O}=2\tau$.

3. The mother lattices of orthorhombic approximants to the IQL

3.1. An orthorhombic distortion of L

We shall introduce an orthorhombic distortion into L so that the resulting lattice $\tilde{L}$ becomes commensurate with E_3. This is implemented by approximating the incommensurate ratio τ in the fourth, fifth or sixth row of (1) by its rational approximant τ_1, τ_2 or τ_3, respectively, where $\tau_i=p_i/q_i$ (Henley 1985, Knowles 1988, Ohashi 1989). A best approximant is obtained if q_i and p_i are consecutive Fibonacci numbers. Fibonacci numbers F_k satisfy the recursion relation $F_{k+1}=F_k+F_{k-1}$ with the initial conditions $F_0=0$ and $F_1=1$. F_k are determined, alternatively, as integers satisfying the equation $F_k+\tau F_{k+1}=\tau^{k+1}$. The basis vectors of $\tilde{L}$ are given by $\tilde{e}_i=(e_i, \tilde{e}_i')$ with

$$(\tilde{e}_1' \quad \tilde{e}_2' \quad \tilde{e}_3' \quad \tilde{e}_4' \quad \tilde{e}_5' \quad \tilde{e}_6')=(b_1 \quad b_2 \quad b_3)J \tag{3}$$

where $\boldsymbol{b}_1=(b_1, 0, 0)$, $\boldsymbol{b}_2=(0, b_2, 0)$ and $\boldsymbol{b}_3=(0, 0, b_3)$ and

$$J=\begin{pmatrix} q_1 & 0 & -p_1 & p_1 & q_1 & 0 \\ -p_2 & q_2 & 0 & 0 & p_2 & q_2 \\ 0 & -p_3 & q_3 & q_3 & 0 & p_3 \end{pmatrix}. \tag{4}$$

Note that $b_i=1/q_i$ but the exact values of b_i are indifferent to the properties of the PA obtained from $\tilde{L}$ because the internal space is ultimately crushed by the projection. In fact, we obtain $b_i=\sqrt{5}\tau/(p_i\tau+q_i)$ if $\tilde{L}$ is derived by introducing a linear phason strain into L (Niizeki 1991b). This choice is superior to that because it works even if $p_i/q_i=1/0$.

$\tilde{L}$ is characterized by the triplet $\langle\tau_1, \tau_2, \tau_3\rangle$. We shall abbreviate the triplet as $\langle\tau_1\rangle$ in the case of $\tau_1=\tau_2=\tau_3$. C_3 permutes τ_1, τ_2 and τ_3 cyclically, so that $\langle\tau_1, \tau_2, \tau_3\rangle$ is congruent with $\langle\tau_2, \tau_3, \tau_1\rangle$ and $\langle\tau_3, \tau_1, \tau_2\rangle$ (but not congruent with $\langle\tau_1, \tau_3, \tau_2\rangle$ and its cyclic permutations).

3.2. The Bravais lattice of a PA

The Bravais lattice which represents the translational symmetry of a PA derived from $\tilde{L}$ is given by $L_B=\tilde{L}\cap E_3$, i.e. the restriction of $\tilde{L}$ onto E_3 (Niizeki 1991a). The point group G of L_B is mmm(D_{2h}), i.e. orthorhombic, in the general case, but m$\bar{3}$(T_h), i.e. tetrahedral, in the special case $\langle\tau_1\rangle$ (Elser and Henley 1985). The space group of L_B is given by $g_B=G * L_B$.

Let $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ or $\boldsymbol{a}_3$ be the shortest lattice vector of L_B among those which are parallel to the first, second or third axis of E_3, respectively. Then we obtain

$$(\boldsymbol{a}_1 \quad \boldsymbol{a}_2 \quad \boldsymbol{a}_3)=(\boldsymbol{e}_1 \quad \boldsymbol{e}_2 \quad \boldsymbol{e}_3 \quad \boldsymbol{e}_4 \quad \boldsymbol{e}_5 \quad \boldsymbol{e}_6)K \tag{5}$$

with K being a 6×3 integer matrix whose transpose is given by

$${}^tK=\begin{pmatrix} p_1 & 0 & q_1 & -q_1 & p_1 & 0 \\ q_2 & p_2 & 0 & 0 & -q_2 & p_2 \\ 0 & q_3 & p_3 & p_3 & 0 & -q_3 \end{pmatrix}. \tag{6}$$

The three columns of K are the indices of $\boldsymbol{a}_i$. Since $J\,{}^tK=0$, we obtain $(\tilde{\boldsymbol{e}}'_1\tilde{\boldsymbol{e}}'_2\tilde{\boldsymbol{e}}'_3\tilde{\boldsymbol{e}}'_4\tilde{\boldsymbol{e}}'_5\tilde{\boldsymbol{e}}'_6)\,{}^tK=0$. The lattice constants of the rectangular unit cell of L_B are given by $a_i=|\boldsymbol{a}_i|=2(p_i\tau+q_i)$. Note that $p_i\tau+q_i$ are powers of τ.

E_3 is a hyper-lattice plane of $\tilde{L}$ and is indexed by K or by the dual index J (Niizeki 1991b). If K is 'unimodular',† $\boldsymbol{a}_i$ are basis vectors of L_B and L_B belongs to Pmmm. This is the case as will be shown shortly if and only if $p_1p_2p_3+q_1q_2q_3$ is odd or, equivalently, if the following condition is satisfied:

Condition 1. p_i or q_i are all odd but one of p_i or q_i is even.

If this is not the case, L_B belongs to Cmmm, Immm or Fmmm according to:
(i) $(\boldsymbol{a}_1+\boldsymbol{a}_2)/2\in L_B$ and $(\boldsymbol{a}_2+\boldsymbol{a}_3)/2\notin L_B$,
(ii) $(\boldsymbol{a}_1+\boldsymbol{a}_2+\boldsymbol{a}_3)/2\in L_B$ or
(iii) $(\boldsymbol{a}_1+\boldsymbol{a}_2)/2\in L_B$, $(\boldsymbol{a}_2+\boldsymbol{a}_3)/2\in L_B$ and $(\boldsymbol{a}_3+\boldsymbol{a}_1)/2\in L_B$,

respectively.

† A rectangular integer matrix is called 'unimodular' if it is embedded into the conventional unimodular matrix (Niizeki 1991b).

Since

$$\boldsymbol{a}_1+\boldsymbol{a}_2=(p_1+q_2)\boldsymbol{e}_1+p_2(\boldsymbol{e}_2+\boldsymbol{e}_6)+q_1(\boldsymbol{e}_3-\boldsymbol{e}_4)+(p_1-q_2)\boldsymbol{e}_5,$$

we can conclude that the condition $(\boldsymbol{a}_1+\boldsymbol{a}_2)/2\in L_B$ is satisfied if p_1+q_2, p_2 and q_1 are all even; p_1-q_2 is even if p_1+q_2 is. It follows that p_1 and q_2 must both be odd because p_1/q_1 and p_2/q_2 are simple fractions. Thus, whether or not the condition $(\boldsymbol{a}_1+\boldsymbol{a}_2)/2\in L_B$ is satisfied is determined by the parities of p_i and q_i. The same is true for the other conditions above because a division by 2 is included in every condition. The ratio p_i/q_i can assume the three cases, $+/-$, $-/+$ and $-/-$. The Bravais class of L_B is determined as in table 1(a). Condition 1 above is nothing but that L_B belongs to neither of Cmmm and Immm. Im$\bar{3}$ and Pm$\bar{3}$ are cubic Bravais classes. Note that Fmmm and Fm$\bar{3}$ never appear as the Bravais lattices of PAs to the IQL.

Table 1. Bravais classes of (a) L_B ($=\tilde{L}\cap E_3$) and (b) the shadow lattice L_s. The symbol $*$ means that the relevant parity is arbitrary, while ● means that the parity is common between the relevant integers. Condition 1 is given in the text. Note that L_B (or L_s) belongs to Immm (or Fmmm) if $\langle\tau_1,\tau_2,\tau_3\rangle$ is transformed into the form in the third row of (a) (or (b)) by a cyclic permutation of τ_i. L_B or L_s belongs to Ammm (or Bmmm) if $C_3\langle\tau_1,\tau_2,\tau_3\rangle$ (or $(C_3)^2\langle\tau_1,\tau_2,\tau_3\rangle$) takes the form in the second row of (a) (or (b)).

(a)

Bravais class	Parity	Example
Pmmm or Pm$\bar{3}$	Condition 1	$\langle 2/1,\ 1/1,\ 1/1\rangle$, $\langle 2/1\rangle$, $\langle 3/2\rangle$
Cmmm	$\langle -/+,\ +/-,\ */*\rangle$	$\langle 3/2, 2/1, 2/1\rangle$, $\langle 3/2,\ 8/5,\ 1/1\rangle$
Immm or Im$\bar{3}$	$\langle \pm/-,\ -/\pm,\ -/-\rangle$	$\langle 2/1,\ 3/2,\ 1/1\rangle$, $\langle 1/1\rangle$, $\langle 5/3\rangle$

(b)

Bravais class	Parity	Example
Pmmm or Pm$\bar{3}$	Condition 1	$\langle 2/1,\ 1/1,\ 1/1\rangle$, $\langle 2/1\rangle$, $\langle 3/2\rangle$
Cmmm	$\langle +/-,\ -/+,\ */*\rangle$	$\langle 2/1,\ 3/2,\ 1/1\rangle$, $\langle 8/5,\ 3/2,\ 1/1\rangle$
Fmmm or Fm$\bar{3}$	$\langle -/\pm,\ \pm/-,\ -/-\rangle$	$\langle 3/2,\ 2/1,\ 1/1\rangle$, $\langle 1/1\rangle$, $\langle 5/3\rangle$

In the case where L_B does not belong to the primitive Bravais class (Pmmm), its basis vectors, $\boldsymbol{a}'_i$, are related to $\boldsymbol{a}_i$ as $(\boldsymbol{a}_1\boldsymbol{a}_2\boldsymbol{a}_3)=(\boldsymbol{a}'_1\boldsymbol{a}'_2\boldsymbol{a}'_3)H$, where H is given by

$$\text{(I)}\begin{pmatrix}1&1&0\\-1&1&0\\0&0&1\end{pmatrix}\qquad\text{or}\qquad\text{(II)}\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix}$$

according to whether L_B belongs to Cmmm or Immm, respectively. We shall denote these matrices as H_{I} or H_{II}, respectively. If follows that K is decomposed as $K=K'H$, where K' is a 6×3 'unimodular' matrix. $\boldsymbol{a}'_i$ are related to $\boldsymbol{e}_i$ by a similar equation to (5) but with K' in place of K. K' is called a reduced form of K.

The volume of the rectangular unit cell of L_B is given by $\Omega=a_1a_2a_3=8\tau^n$ with n being an integer. $\Omega/\Omega_O=4\tau^{n-1}=4(F_{n-1}\tau+F_{n-2})$, so that $\Omega=4(F_{n-1}\Omega_P+F_{n-2}\Omega_O)$. It follows that the number of prolate (or oblate) rhombohedra of a PA in the rectangular unit cell is given by $4F_{n-1}$ (or $4F_{n-2}$) and the total number by $4F_n$. By an elementary topological argument, we can show that the total number ($4F_n$) is also equal to the number of the lattice points of the PA in the orthorhombic unit cell.

3.3. *The shadow lattice*

The projection of $\tilde{L}$ onto E_3' is a discrete set in contrast to L_p'. It is, in fact, a Bravais lattice called the shadow lattice (Niizeki 1991a), which is denoted as L_s. A lattice vector of L_s is written as $m_1\boldsymbol{b}_1+m_2\boldsymbol{b}_2+m_3\boldsymbol{b}_3$, where $\boldsymbol{m}\equiv(m_1, m_2, m_3)=J\boldsymbol{n}$ with $\boldsymbol{n}\in\boldsymbol{Z}^6$. That is

$$L_s=\{m_1\boldsymbol{b}_1+m_2\boldsymbol{b}_2+m_3\boldsymbol{b}_3 \mid m\in J\boldsymbol{Z}^6\} \tag{7}$$

where $J\boldsymbol{Z}^6\equiv\{J\boldsymbol{n}\mid \boldsymbol{n}\in\boldsymbol{Z}^6\}$ is a submodule of $\boldsymbol{Z}^3$ (the simple cubic lattice). L_s as well as L_B has G as its point group with $G=\mathrm{mmm}$ or $\mathrm{m}\bar{3}$. The space group of L_s is given by $g_s=G*L_s$.

The Bravais class to which L_s belongs is determined by the parities of p_i and q_i and the rules are given in table 1(b), which are proved in appendix 1. Note that the case Immm never appears and also that L_s and L_B belong together to Pmmm. $\boldsymbol{b}_i$ are the basis vectors of L_s only in the case of Pmmm. The basis vectors $\boldsymbol{b}_i'$ in other cases are given by $(\boldsymbol{b}_1'\boldsymbol{b}_2'\boldsymbol{b}_3')=(\boldsymbol{b}_1\boldsymbol{b}_2\boldsymbol{b}_3)H$.

There exists a natural surjection φ from L_p onto L_s; $\Sigma_i n_i\boldsymbol{e}_i\in L_p\to\Sigma_i n_i\boldsymbol{e}_i'\in L_s$. φ is a homomorphism between the two $\boldsymbol{Z}$-modules and L_B is its kernel. It is naturally extended to a homomorphism from $\tilde{g}_p\equiv G*L_p$ $(\subset g_p)$ to g_s (Niizeki 1991a); φ acts on G as an identity operation.

4. Several important cases of the non-primitive Bravais lattices

4.1. *The Fibonacci numbers and their analogues*

We begin by investigating the parity sequence of the Fibonacci series $\{F_k\}=\{0, 1, 1, 2, 3, 5, 8, 13, \ldots\}$. From the equality $\tau^3=2\tau+1$, we obtain another recursion relation, $F_{k+3}=2F_{k+1}+F_k$. It follows that F_k and F_{k+3} have a common parity. More precisely, we can conclude from $F_0=0$ and $F_1=1$ that F_k is even if $k\equiv 0 \bmod 3$ but is odd otherwise. $G_k\equiv F_{3k}/2$ are generated by $G_{k+1}=4G_k+G_{k-1}$ with $G_0=0$ and $G_1=1$; $\{G_k\}=\{0, 1, 4, 17, 72, 305, \ldots\}$. The parity alternates in the series G_k. G_{k+1}/G_k is a best approximant to ρ $(=2+\sqrt{5})$, which satisfies $\rho^2=4\rho+1$. Moreover we have $G_k+G_{k+1}\rho=\rho^{k+1}$. Two series of odd Fibonacci numbers F_{3k+1} and F_{3k+2} satisfy the same recursion relation as that of G_k and we can conclude from the initial conditions that $F_{3k+1}=G_{k+1}-G_k$ and $F_{3k+2}=G_{k+1}+G_k$.

$H_k\equiv G_{k+1}-2G_k$ $(=2G_k+G_{k-1})$ satisfy the same recursion relation as that of G_k but with different initial conditions, $H_0=1$ and $H_1=2$; $\{H_k\}=\{1, 2, 9, 38, 161, \ldots\}$. $H_k+\sqrt{5}G_k=\rho^k$ and H_k/G_k $(=G_{k+1}/G_k-2)$ is a best approximant to $\sqrt{5}$ $(=\rho-2)$ (Kat and Duneau 1986).

4.2. *Im$\bar{3}$*

We shall consider the case $\langle F_{3k+2}/F_{3k+1}\rangle$ in more detail. L_B belongs to Im$\bar{3}$ and $\boldsymbol{a}_0'\equiv(\boldsymbol{a}_1+\boldsymbol{a}_2+\boldsymbol{a}_3)/2$ belongs to L_B; $\boldsymbol{a}_0'=r(\boldsymbol{e}_1+\boldsymbol{e}_2+\boldsymbol{e}_3)+s(\boldsymbol{e}_4+\boldsymbol{e}_5+\boldsymbol{e}_6)$ with $r=G_{k+1}$ and $s=G_k$. We may write $\boldsymbol{a}_0'=\tau^{3k+2}$ (1, 1, 1) and L_B is generated by $\boldsymbol{a}_i'=\boldsymbol{a}_0'-\boldsymbol{a}_i$, $i=1$-3. $\pm\boldsymbol{a}_i'$ are parallel to threefold axes of Y. $\boldsymbol{a}_i'$ are indexed by K', the reduced form of K; K' is written as $K'=[\bar{s}rsr\bar{r}s/s\bar{s}rsr\bar{r}/rs\bar{s}\bar{r}sr]$, where the three groups of six integers partitioned by '/' denote the three columns of K' and a bar is put on a minus index.

The appearance of G_{k+1} and G_k in K' is due to the fact that G_{k+1}/G_k is a best approximant to the incommensurate ratio ρ associated with the threefold axes.

4.3. *Immm*

In the case of $\langle F_k/F_{k-1}, F_{k+1}/F_k, F_{k+2}/F_{k+1}\rangle$, L_B belongs to Immm because it is written as $\langle q/(p-q), p/q, (p+q)/p\rangle$ with $p=F_{k+1}$ and $q=F_k$. Then $(\pm\boldsymbol{a}_1\pm\boldsymbol{a}_2\pm\boldsymbol{a}_3)/2$ belong to L_B and are parallel to twofold axes, $\pm(\boldsymbol{e}_2+\boldsymbol{e}_3)$, $\pm(\boldsymbol{e}_2+\boldsymbol{e}_4)$, $\pm(\boldsymbol{e}_3-\boldsymbol{e}_6)$ and $\pm(\boldsymbol{e}_4-\boldsymbol{e}_6)$. Note that $a_1:a_2:a_3=1:\tau:\tau^2$. K' is written as $K'=[0pqp\bar{q}0/00pqq\bar{p}/q0\bar{q}\bar{p}0p]$; p/q is a best approximant to the irrational τ associated with the twofold axes.

4.4. *Cmmm*

In the case where L_B belongs to Cmmm, the centring occurs in the plane perpendicular to the third axis. The 2D lattice cmm on the plane is characterized by two approximants τ_1 $(=-/+)$ and τ_2 $(=+/-)$; Cmmm is a vertical stacking of cmm. The basis vectors of cmm are $\boldsymbol{a}_1'=(\boldsymbol{a}_1+\boldsymbol{a}_2)/2$ and $\boldsymbol{a}_2'=(-\boldsymbol{a}_1+\boldsymbol{a}_2)/2$ with $|\boldsymbol{a}_1'|=|\boldsymbol{a}_2'|$. Case 1: $\tau_1=F_{3k+1}/F_{3k}$ $(=(G_{k+1}-G_k)/(2G_k))$ and $\tau_2=F_{3k}/F_{3k-1}$ $(=2G_k/(G_k+G_{k-1}))$ and case 2: $\tau_1=F_{3k+1}/F_{3k}$ and $\tau_2=F_{3k+3}/F_{3k+2}$ $(=2G_{k+1}/(G_{k+1}+G_k))$ are of particular interest. $\boldsymbol{a}_1'$ and $\boldsymbol{a}_2'$ are indexed in case 1 by $[tsss\bar{s}s]$ and $[\bar{s}s\bar{s}s\bar{t}s]$ with $t=H_k$, so that $\boldsymbol{a}_1'=\rho^k\boldsymbol{e}_1$ and $\boldsymbol{a}_2'=\rho^k\boldsymbol{e}_5$, which are parallel to fivefold axes of Y. Similarly, we obtain in case 2 that $\boldsymbol{a}_1'=[rrs\bar{s}\bar{s}r]=\rho^k(\boldsymbol{e}_1+\boldsymbol{e}_2+\boldsymbol{e}_6)$ with $r=G_{k+1}$ and $s=G_k$ and $\boldsymbol{a}_2'=[sr\bar{s}s\bar{r}r]=\rho^k(-\boldsymbol{e}_2+\boldsymbol{e}_5-\boldsymbol{e}_6)$, which are parallel to threefold axes. t/s (or r/s) is a best approximant to the incommensurate ratio $\sqrt{5}$ (or ρ) associated with the five- (or three-) fold axis.

The fact that L_B has centring of type 1 (or 2) is due to the presence of two five- (or three-) fold axes which are perpendicular to a twofold axis of Y (see figure 1). The angle between the two five- (or three-) fold axes is given by $\cos^{-1}(1/\sqrt{5})=63.43°$ (or $\cos^{-1}(\sqrt{5}/3)=41.81°$), which represents the acute inner angle of the rhombic unit cell of the 2D lattice cmm.

5. Periodic approximants

We begin with the following expression for a PA to $Q(\boldsymbol{\phi}, W)$:

$$\tilde{Q}(\boldsymbol{\phi})=\{\boldsymbol{u}\,|\,\boldsymbol{u}\in L_p, \varphi(\boldsymbol{u})\in\boldsymbol{\phi}+\tilde{W}\} \tag{8}$$

where $\tilde{W}$ is an appropriate distortion of W. The point group of $\tilde{W}$ is equal to G. $\tilde{Q}(\boldsymbol{\phi})$ is a periodic set of points and its Bravais lattice is given by L_B. If $\boldsymbol{\phi}'=\boldsymbol{\phi}+\boldsymbol{v}$ with $\boldsymbol{v}\in L_s$, we obtain $\tilde{Q}(\boldsymbol{\phi}')=\boldsymbol{u}+\tilde{Q}(\boldsymbol{\phi})$ with $\boldsymbol{u}\in\varphi^{-1}(\boldsymbol{v})$. That is, $\tilde{Q}(\boldsymbol{\phi}')$ is congruent with $\tilde{Q}(\boldsymbol{\phi})$ if $\boldsymbol{\phi}'\equiv\boldsymbol{\phi}$ mod L_s (Niizeki 1991a). The number of the lattice points of $\tilde{Q}(\boldsymbol{\phi})$ in a unit cell is equal to that of L_s in the domain $\boldsymbol{\phi}+\tilde{W}$ (Niizeki 1991a).

Two PAs with different phase vectors are usually different from each other in contrast to the case of the QL. The space group of $\tilde{Q}(\boldsymbol{\phi})$ is given by $g(\boldsymbol{\phi})=\varphi^{-1}(g_s(\boldsymbol{\phi}))$ (Niizeki 1991a), where

$$g_s(\boldsymbol{\phi})=\{\{\sigma|\boldsymbol{v}\}\,|\,\{\sigma|\boldsymbol{v}\}\in g_s, \{\sigma|\boldsymbol{v}\}\boldsymbol{\phi}=\boldsymbol{\phi}\} \tag{9}$$

is the point group of $\boldsymbol{\phi}$ with respect to L_s. It follows that

$$g(\boldsymbol{\phi})=\{\{\sigma|\boldsymbol{u}\}\,|\,\{\sigma|\boldsymbol{v}\}\in g_s(\boldsymbol{\phi}), \boldsymbol{u}\in\varphi^{-1}(\boldsymbol{v})\}. \tag{10}$$

The point group of $\tilde{Q}(\boldsymbol{\phi})$ is given by $G(\boldsymbol{\phi})=\{\sigma|\{\sigma|v\}\in g_s(\boldsymbol{\phi})\}$, which is isomorphic to $g_s(\boldsymbol{\phi})$. $G(\boldsymbol{\phi})$ is a subgroup of G.

6. Special points, lines and planes of L_s

We can define special manifolds (points, lines and planes) in E_3' with respect to L_s; a special manifold is the centre, the axis or the plane of a centring subgroup of g_s, a polar one or the mirror one, respectively. Equivalent special manifolds with respect to g_s form a class, which has a conventional symbol in solid state physics (Bradley and Cracknell 1972). In particular, the lattice points of L_s are special points (SPs) of full symmetry and form the class Γ.

If a unit cell of L_s is fixed, a representative of each class of SPs is included in the cell. We shall sometimes identify the represntative with the class. A vector $\boldsymbol{x}$ in E_3' is indexed with $\boldsymbol{b}_i$ as $\boldsymbol{x}=[x_1x_2x_3]\equiv x_1\boldsymbol{b}_1+x_2\boldsymbol{b}_2+x_3\boldsymbol{b}_3$.

Pmmm has eight classes of SPs, Γ, X, Y, Z, S, T, U and R, whose point groups are mmm. Their representatives are [000], $[h00]$, $[0h0]$, $[00h]$, $[0hh]$, $[h0h]$, $[hh0]$ and $[hhh]$, respectively, where we mean $h=1/2$ throughout this paper. Cmmm has four classes of SPs with point group mmm, i.e. Γ, Y, Z and T, while Fmmm has two, Γ and Y. The representatives of the six are [000], [100], $[00h]$, $[10h]$, [000] and [100], respectively. Pmmm and Cmmm have no classes of SPs with point group 222, while Fmmm has one class, W, whose representative is $[hhh]$.

Every special line (or plane) includes SPs. Special planes are classified into type I or II according to whether or not they pass lattice points of L_s.

Pmmm has three classes of type II special planes, which are parallel to the three mirrors of the point group mmm. If an SP of Pmmm has a half-integer index, it is located on a type II special plane which is perpendicular to the axis relevant to the index. Cmmm has only one class of type II special planes, which are perpendicular to the third axis. SPs Z and T of Cmmm are located on them. Fmmm has no classes of type II special planes.

7. The space groups of the regular approximants

$\tilde{Q}(\boldsymbol{\phi})$ is called a regular approximant if it belongs to the same Bravais class as that of L_B. The point group of a regular approximant must be mmm, mm2(C_{2V}) or 222(D_2) if $G=$ mmm, i.e. the case of the orthorhombic approxiant but m$\bar{3}$ or 23(T) if $G=$ m$\bar{3}$. mm2 is a polar group but the other four are centring groups. We confine our considerations to regular approximants, which are obtained with phase vectors located on special points or lines of L_s.

The space group $g(\boldsymbol{\phi})$ of a regular approximant is determined by the class of the special manifold on which $\boldsymbol{\phi}$ is located. If $G(\boldsymbol{\phi})=$ mm2, $\boldsymbol{\phi}$ is located on a special line of L_s. The special line passes an SP, whose point group is mmm. Let $\boldsymbol{\phi}'$ be the position vector of the SP. Then, $g_s(\boldsymbol{\phi})$ is a subgroup of $g_s(\boldsymbol{\phi}')$ and $g(\boldsymbol{\phi})$ is a subgroup of $g(\boldsymbol{\phi}')$. In fact, $g(\boldsymbol{\phi})$ is determined as $g(\boldsymbol{\phi})=\{\{\sigma|\boldsymbol{u}\}|\{\sigma|\boldsymbol{u}\}\in g(\boldsymbol{\phi}'),\ \sigma\in G(\boldsymbol{\phi})\}$. Therefore, we can restrict our considerations to the PAs associated with SPs of L_s. If $\boldsymbol{\phi}$ is located on the SP X of L_s, we may write $g(\boldsymbol{\phi})$ as $g(X)$.

It can easily be shown that $g(\boldsymbol{\phi})$ has a mirror if $\boldsymbol{\phi}$ is located on a type I special plane of L_s; the mirror plane is parallel to the special plane (Niizeki 1991a). On the other hand, if ϕ is located on a type II special plane of L_s, $g(\phi)$ has no such mirrors but has glides which are parallel to the special plane, which will be proved shortly. A glide is denoted as a, b or c according to whether the translation accompanying it is $\boldsymbol{a}_1/2$, $\boldsymbol{a}_2/2$ or $\boldsymbol{a}_3/2$, respectively, while it is denoted as n if the translation is $(\boldsymbol{a}_2+\boldsymbol{a}_3)/2$, $(\boldsymbol{a}_3+\boldsymbol{a}_1)/2$ or $(\boldsymbol{a}_1+\boldsymbol{a}_2)/2$.

We consider at the moment $\tilde{Q}(\phi)$, the case where $G(\phi)=\mathrm{mmm}$. We begin with the case where L_s has a class of type II special planes perpendicular to the third axis. We can prove as implemented in appendix 2 that, if ϕ is located on one of the special planes, $g(\phi)$ has glides of type a or b according to whether the parities of p_i and q_i in $\langle p_1/q_1, p_2/q_2, p_3/q_3\rangle$ conform to $\langle +/-, */*, */-\rangle$ or $\langle */*, -/+, -/*\rangle$, respectively, while it has glides of type n in the cases $\langle -/-, \pi_1/-, \pi_2/-\rangle$ and $\langle -/\pi_1, -/-, -/\pi_2\rangle$, where π_1 and π_2 are not together equal to $-$. Using the equality $C_3\langle \tau_1, \tau_2, \tau_3\rangle = \langle \tau_3, \tau_1, \tau_2\rangle$, we can derive similar results for the case of type II special planes perpendicular to other axes. In the case of $\langle */-, +/-, */*\rangle$, for example, the glides perpendicular to the first axis are of type b. These results are sufficient for us to determine $g(\phi)$ in the case of $G(\phi)=\mathrm{mmm}$.

Each term in $\langle p_1/q_1, p_2/q_2, p_3/q_3\rangle$ can assume three cases, $+/-$, $-/+$ and $-/-$, and there exist 27 ($=3^3$) parity combinations. They are classified into 11 (Nos 1–7 and 1′–4′) as listed in the second column of table 2 because a cyclic permutation of τ_i in $\langle \tau_1, \tau_2, \tau_3\rangle$ yields the same lattice. The types of the glides associated with type II special

Table 2. The space groups of the regular orthorhombic approximants associated with SPs of L_s and cubic ones. There exist 11 cases depending on the parity combinations of p_i and q_i in $\langle p_1/q_1, p_2/q_2, p_3/q_3\rangle$. In the division of 'Bravais class', the first (or second) column shows those of L_B (or L_s). The symbols P, I or F refer to the primitive orthorhombic, the body-centred one or the face-centred one, respectively, while A, B or C to A-, B- or C-centred one. The three columns under the heading 'glide' show the glides perpendicular to the first, second and third axes in this order; an asterisk shows that no glides exist at that place. The column of 'space group' is composed of two subdivisions referring to orthorhombic approximants and the cubic ones. In the case of a primitive orthorhombic approximant, the space group in parentheses shows the prototype and space groups obtained from it by replacing any number of the glides by mirrors are also allowed. Parity combinations are inverted between n and n', $n=1$–4, in the sense that the parities of numerators and those of the denominators are interchanged. The space groups are isomorphic between such a pair, e.g. Pbca of No. 1 and Pcab of No. 1′. The space group associated with a special line of L_s is obtained as a subgroup of the one listed in the table.

No	Parity combination	Bravais class		Glide			Space group	
1	$\langle +/-, +/-, +/-\rangle$	P	P	b	c	a	(Pbca)	$\mathrm{Pm\bar{3}}$, $\mathrm{Pa\bar{3}}$
1′	$\langle -/+, -/+, -/+\rangle$	P	P	c	a	b	(Pcab)	$\mathrm{Pm\bar{3}}$, $\mathrm{Pb\bar{3}}$
2	$\langle +/-, +/-, -/-\rangle$	P	P	b	n	a	(Pbna)	
2′	$\langle -/+, -/+, -/-\rangle$	P	P	c	n	b	(Pcnb)	
3	$\langle -/-, -/-, +/-\rangle$	P	P	n	c	n	(Pncn)	
3′	$\langle -/-, -/-, -/+\rangle$	P	P	n	n	b	(Pnnb)	
4	$\langle -/+, +/-, +/-\rangle$	C	B	*	c	*	Cmmm, Cmcm	
4′	$\langle -/+, +/-, -/+\rangle$	C	A	c	*	*	Cmmm, Ccmm	
5	$\langle -/+, +/-, -/-\rangle$	C	F	*	*	*	Cmmm, $\mathrm{C222_1}$	
6	$\langle +/-, -/+, -/-\rangle$	I	C	*	*	a	Immm, Imma	
7	$\langle -/-, -/-, -/-\rangle$	I	F	*	*	*	Immm, I222	$\mathrm{Im\bar{3}}$, I23

planes are listed in the fifth column of the table. Using the results, we can easily classify the space groups whose point groups are mmm. Consider, for example, the case of No. 1 in the table, i.e. $\langle +/-, +/-, +/- \rangle$. Then L_B and L_s belong to Pmmm and the space groups associated with SPs Γ, X, Y, Z, S, T, U and R of L_s are Pmmm, Pbmm, Pmcm, Pmma, Pmca, Pbma, Pbcm and Pbca, respectively; the last space group, Pbca, is a prototype of them and others are obtained from the prototype by replacing one or more glides by the mirror(s).

Note that both $g(\Gamma)$ and $g(Y)$ are equal to Cmmm (or Immm) for Nos 4, 4′ and 5 (or 6 and 7) in table 2, while $g(Z)$ and $g(T)$ to Cmcm, Ccmm or Imma for Nos 4, 4′ or 6, respectively. Note, however, that each pair of PAs with the same space group have different structures.

The case where L_s belongs to Fmmm needs an additional consideration because its SP W has the point group 222. It is shown in appendix 3 that the space group of the PA associated with W is C222$_1$ or I222 according to whether L_B belongs to Cmmm (No. 5) or Immm (No. 7), respectively.

8. Discussion

There exist two alternatives for introducing the Cartesian coordinate system into Y (the icosahedron) so that the three axes are parallel to the twofold axes of Y; we have adopted one of them. The other is obtained from ours by rotating it through $\pi/2$ around the first axis (cf. figure 1). This is the coordinate system adopted by Dmitrienko (1990). In this system, the results in table 2 are interchanged between Nos n and n' with $n = 1$–4. Therefore, two space groups of such a pair (e.g. Pbca of No. 1 and Pcab of No. 1′) are isomorphic. Note, however, that the two space groups can be distinguished by their orientations with respect to the pseudo-icosahedral symmetry of the PAs.

The cubic approximants are treated as special cases of the orthorhombic ones. Since the point symmetry is higher, regular cubic approximants are greatly restricted. Consider, for example, case No. 1 in table 2. Then, Pmmm and Pbca are associated with Γ and R and they are lifted in the cubic case to Pm$\bar{3}$ and Pa$\bar{3}$, respectively, because the point groups of Γ and R become m$\bar{3}$. Other space groups remain unchanged and are not regular cubic approximants. By similar arguments, we obtain other cubic approximants as listed in table 2. The present results agree with those of Dmitrienko (1987, 1990) except one point; he obtained I2$_1$3 instead of I23 for the case $\langle -/- \rangle$.

Since the primitive IQL has a self-similarity whose scale is ρ $(=\tau^3)$, we can generate from a given PA to the IQL another one by deflation and rescaling (Niizeki 1991b). The unit cell of the new PA is ρ-times that of the original one and the space group is common between the two. This is the reason why the parities of p_i and q_i are of vital importance in table 2.

Spaepen *et al* (1990) have found in the Ga–Mg–Zn system an orthorhombic approximant $\langle 3/2, 2/1, 2/1 \rangle$, which belongs to No. 4 in table 2; L_B = Cmmm and L_s = Bmmm. They reported that the Bravais lattice of this approximant is the base-centred orthorhombic in agreement with the present theory. The two basis vectors in the basal plane are parallel to fivefold axes. $g(Z) = g(T)$ = Cmcm with $Z = [0h0]$ and $T = [1h0]$ are SPs of Bmmm. Cmc2$_1$ is a subgroup of Cmcm and is the space group of $\tilde{Q}(\boldsymbol{\phi})$ with $\boldsymbol{\phi} = [0h\zeta]$, $0 < \zeta < 1$, which is located on the special line A; the special line passes not only Z but also T because $[1h0] \equiv [0h1]$ mod L_s. This space group is identical to the space group of the model structure constructed by Ohashi (1989) for this approximant crystal; the model is derived on the basis of the canonical cell packing model by Henley (1991).

Spaepen *et al* have reported the three cubic approximants $\langle 1/1\rangle$, $\langle 2/1\rangle$ and $\langle 3/2\rangle$ for the same system; the first one belongs to the body-centred cubic Bravais class but the latter two to the primitive one in agreement with the present theory. Henley (1991) constructed structural models for the latter two approximants. Their space groups are reported to be $\mathrm{Pa}\bar{3}\langle 2/1\rangle$ and $\mathrm{Pa}\bar{3}\langle 3/2\rangle$ but the latter should be assigned to $\mathrm{Pb}\bar{3}\langle 3/2\rangle$ in our coordinate system (see also Dmitrienko 1990). Note that two cubic crystals $Mg_2Cu_2Al_5$ and Mg_2Zn_{11} reported by Samson (1949a, b) are considered to be approximant crystals of type $\langle 1/0\rangle$ (Ohashi 1989); their sace groups are $\mathrm{Pm}\bar{3}$.

Audier and Guyot (1990), Spaepen *et al* (1990) reported rhombohedral approximant crystals to the icosahedral quasicrystals. The icosahedral QL has a variety of rhombohedral approximants, which will be discussed elsewhere.

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Appendix 1

We consider a different deformation of L from that in the text. That is, we shall replace τ in each of the first three rows of (1) by $\tau_i = p_i/q_i$ with i being the row number. Then, the resulting lattice $\hat{L}$ is commensurate with E_3'. The physical space components $\hat{e}_i$ of the basis vectors $\hat{\varepsilon}_i$ of $\hat{L}$ are represented by a similar equation to (3) but J is replaced by $\hat{J} \equiv {}^t K$ (cf. (6)). $\hat{L}_{\mathrm{B}} \equiv \hat{L} \cap E_3'$ is a 3D Bravais lattice whose basis vectors $\hat{a}_i$ are represented by a similar equation to (5) but K is replaced by $\hat{K} \equiv {}^t J$ (cf. (4)). The point group of $\hat{L}_{\mathrm{B}}$ is the same as that of L_{B}.

Since $\hat{K}$ $(= {}^t J)$ is obtained from K by the replacements: $p_i \to q_i$ and $q_i \to -p_i$, we can conclude that $\hat{L}_{\mathrm{B}}$ belongs to Pmmm, Cmmm or Immm according to whether parities of p_i and q_i satisfy the first, second or third condition in the second column of table 1(b); the parities of the denominators and numerators are inverted in these columns between tables 1(a) and (b). It follows that J $(= {}^t(\hat{K}))$ is 'unimodular' in the case of Pmmm. Since a 'unimodular' 3×6 matrix represents a surjection from $\boldsymbol{Z}^6$ onto $\boldsymbol{Z}^3$, we can conclude that $J\boldsymbol{Z}^6 = \boldsymbol{Z}^3$ for this case, so that L_{s} belongs to Pmmm. On the other hand, if $\hat{L}$ belongs to Cmmm or Immm, J is decomposed as HJ' with $H = H_{\mathrm{I}}$ or H_{II} and J' being 'unimodular'. Then we obtain $J\boldsymbol{Z}^6 = H\boldsymbol{Z}^3$, which is equal to $\{\boldsymbol{m} \mid \boldsymbol{m} \in \boldsymbol{Z}^3, m_1 + m_2 = \text{even}\}$ or $\{\boldsymbol{m} \mid \boldsymbol{m} \in \boldsymbol{Z}^3, m_1 + m_2 + m_3 = \text{even}\}$ for the case Cmmm or Immm, so that L_{s} belongs to Cmmm or Fmmm, respectively.

Appendix 2

We begin with a lemma: let $\boldsymbol{u} \in L_p$ and assume that (i) $\boldsymbol{t} \equiv \boldsymbol{u} + \sigma_3 \boldsymbol{u} \in L_{\mathrm{B}}$ with $\sigma_3 \in \mathrm{mmm}$ being the mirror perpendicular to the third axis, (ii) $\boldsymbol{t} \neq 0$ and (iii) $\boldsymbol{t}/2 \notin L_{\mathrm{B}}$. Then, $\alpha \equiv \{\sigma_3 \mid \boldsymbol{u}\} \in g_{\mathrm{p}}$ is a glide and the translation accompanying α is $\boldsymbol{t}/2$ because $\alpha^2 = \{E \mid \boldsymbol{t}\}$. Assume furthermore that (iv) $\boldsymbol{v} \equiv \varphi(\boldsymbol{u})$ takes the form $\boldsymbol{v} = k_3 \boldsymbol{b}_3$ with k_3 being an odd integer. Then, $\{\sigma_3|\boldsymbol{v}\}$ $(=\varphi(\alpha))$ is a type II mirror of L_s because the mirror cuts the third axis at $k_3\boldsymbol{b}_3/2$. It follows that α is a glide of $\tilde{Q}(\boldsymbol{\phi})$ provided that $\boldsymbol{\phi}$ is located on that mirror plane.

We shall apply the above lemma to each of the four cases in the text. In the case of $\langle +/-, */*, */-\rangle$, p_1 is even but q_1 and q_3 are odd and $\boldsymbol{u}=(p_1/2)$ $(\boldsymbol{e}_1+\boldsymbol{e}_5)+q_1\boldsymbol{e}_3$ satisfies the conditions of the lemma; we obtain that $k_3=q_1q_3$ and $\boldsymbol{t}=\boldsymbol{a}_1$. It follows that α is the a glide. The case $\langle */*, -/+, -/*\rangle$ is treated similarly; $\boldsymbol{u}=(q_2/2)$ $(\boldsymbol{e}_1-\boldsymbol{e}_5)+p_2\boldsymbol{e}_2$, $k_3=-p_2p_3$ and $\boldsymbol{t}=\boldsymbol{a}_2$, so that α is the b glide.

Finally we consider the case where p_1 and q_2 are both odd. Let $\boldsymbol{u}\equiv n_1\boldsymbol{e}_1+p_2\boldsymbol{e}_2+q_1\boldsymbol{e}_3+n_5\boldsymbol{e}_5$ with $n_1=(p_1+q_2)/2$ and $n_5=(p_1-q_2)/2$. Then we obtain that $k_3=-p_2p_3+q_1q_3$ and $\boldsymbol{t}=\boldsymbol{a}_1+\boldsymbol{a}_2$. It follows that α is the n glide provided that k_3 is odd. This applies to the last two cases in the text.

Appendix 3

We consider the case $\langle -/\pi, \pi/-, -/-\rangle$ with $\pi=+$ or $-$. Then, L_s belongs to Immm and $\boldsymbol{\phi}\equiv(-p_1p_3\boldsymbol{b}_1+q_2q_3\boldsymbol{b}_2-q_3p_3\boldsymbol{b}_3)/2$ belongs to class W of SPs of L_s because $\boldsymbol{\phi}\equiv(\boldsymbol{b}_1+\boldsymbol{b}_2+\boldsymbol{b}_3)/2$ mod L_s. Let R_i, $i=1$-3, be the rotations through π around the three axes of the point group 222 of W. Then $g_s(\boldsymbol{\phi})$ $(\simeq 222)$ is generated by $\{R_i|\boldsymbol{v}^{(i)}\}$, $i=1$-3, with $\boldsymbol{v}^{(i)}\equiv\boldsymbol{\phi}-R_i\boldsymbol{\phi}\in L_s$; we can easily check that $\boldsymbol{v}^{(i)}=\varphi(\boldsymbol{u}^{(i)})$ with $\boldsymbol{u}^{(1)}=q_3\boldsymbol{e}_2$, $\boldsymbol{u}^{(2)}=-p_3\boldsymbol{e}_4$ and $\boldsymbol{u}^{(3)}=q_3\boldsymbol{e}_2+p_3\boldsymbol{e}_3$. Therefore $g(\boldsymbol{\phi})=L_B+\alpha_1L_B+\alpha_2L_B+\alpha_3L_B$ with $\alpha_i=\{R_i|\boldsymbol{u}^{(i)}\}$, where L_B is identified with $\{\{E|\boldsymbol{u}\}|\boldsymbol{u}\in L_B\}$. α_1 and α_2 are rotations because $\boldsymbol{u}^{(1)}+R_1\boldsymbol{u}^{(1)}=0$ and $\boldsymbol{u}^{(2)}+R_2\boldsymbol{u}^{(2)}=0$, while α_3 is a screw because $\boldsymbol{u}^{(3)}+R_3\boldsymbol{u}^{(3)}=\boldsymbol{a}_3$. Then, we can concude that $g(W)=\mathrm{C}222_1$ for the case $\pi=+$. On the other hand, $\boldsymbol{t}\equiv(\boldsymbol{a}_1+\boldsymbol{a}_2+\boldsymbol{a}_3)/2\in L_B$ for the case $\pi=-$ and $\boldsymbol{t}+R_3\boldsymbol{t}=\boldsymbol{a}_3$, so that $\alpha_3'\equiv\{E|-\boldsymbol{t}\}\alpha_3$ is a rotation and we obtain $g(W)=\mathrm{I}222$ for this case.

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