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A New Description of Pentagonal Frank–Kasper Phases and a Possible Structure Model of the Icosahedral Quasicrystal

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Abstract

The structure of pentagonal Frank-Kasper phases can be recovered from the projection of a common $MgCu_2$ cube described in a six-dimensional space. From the close structural relationship between the newly discovered icosahedral quasicrystal and the Frank-Kasper phases, a structure model has been proposed for the former.

1. Introduction

Penrose (1974) first pointed out that a two-dimensional (2D) plane can be tiled by two rhombi, 72-108 and 36-144° respectively, with a fivefold symmetry. Later, this was developed to the three-dimensional (3D) case by Mackay (1982*a*, *b*), who used two rhombohedra, 63·43 and 116·57° respectively, displaying the icosahedral $2/m\bar{3}\bar{5}$ symmetry. This has attracted much attention lately on account of the discovery of an icosahedral quasicrystal (Shechtman, Blech, Gratias & Cahn, 1984).

An icosahedron has 12 vertices and six fivefold axes passing through its centre and vertices. The 3D Penrose lattice has been described by using a six-axes system and it was therefore called a quasilattice by Mackay (1982*a*, *b*). Consequently, this can also be described in terms of the projection of a 6D simple cubic lattice onto a 3D hyperplane [see, for example, Kramer & Neri (1984) and Elser (1986)]. If the projection is carried out onto an incommensurate hyperplane, a 3D quasilattice is recovered.

The structure of pentagonal Frank-Kasper (FK) phases was known to consist mainly of icosahedra (Frank & Kasper, 1958, 1959) and this close relationship between FK phases and the icosahedral phase has guided some investigators to obtain new icosahedral phases in Ti_2Ni (Zhang, Ye & Kuo, 1985), $Mg_{32}(Al, Zn)_{49}$ (Ramachandrarao & Sastry, 1985) and V-Ni-Si (Kuo, Zhou & Li, 1987). Moreover, structure models of 2D and 3D quasicrystals have already been derived from their close relationship to the FK phases (Yang & Kuo, 1986).

According to Anderson (1978), the structure of the pentagonal FK phases can be recovered by applying various symmetry operations, such as twinning, reflection, rotation, inversion *etc.*, to the rhombohedral unit (60°) of the f.c.c. $MgCu_2$ structure and the Zr_4Al_3 unit. Since this 60° rhombohedral unit is quite like the acute rhombohedron (63·43°) of the icosahedral phase, it is natural to inquire into the possibility, by projection of the 6D $MgCu_2$ onto a 3D hyperplane, of obtaining the structure of both the pentagonal FK phases and the icosahedral phase. The present investigation is devoted mainly to a new description of the FK phases, and in the meantime a possible structure model for the quasicrystal is proposed. A preliminary report has already been published (Yang & Kuo, 1986) and a similar study on the structure of the $Mg_{32}(Al, Zn)_{49}$ icosahedral phase has also appeared (Henley & Elser, 1986).

2. Projection method

In the case of the projection of a 2D lattice onto a 1D space (Fig. 1), Elser (1986) pointed out that when $\tan\alpha$ is an irrational number an incommensurate structure will result. This applies only to the case where the direction of projection is normal to the

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projection plane. As a matter of fact, both the projection direction and projection plane can vary independently. In such a case, whether the projected structure is commensurate or incommensurate depends on whether the subspace selected for projection is rational or irrational, irrespective of the projection direction. This point can be clearly seen in Fig. 1. When a straight line AB passes only through a lattice point C but no other point, then $\tan\alpha$ is an irrational number. Draw a line $A'B'$ parallel to AB and project all lattice points lying between these two lines perpendicularly onto AB at $\ldots m_1, m_2, \ldots, m_{14}, \ldots$. Obviously, only two projected lengths, $r_1 = m_1m_2 = a\cos\alpha$ and $r_2 = m_2m_3 = a\sin\alpha$, result and they form an aperiodic Fibonacci series. Now draw another pair of parallel lines DF and $D'F'$ making an angle α' with the X axis, where $\tan\alpha'$ is a rational number, say $\frac{1}{2}$. When all lattice points between this pair of lines are projected also perpendicularly onto AB at $\ldots n_1, n_2, \ldots, n_{12}, \ldots$, the projected lengths are still $r_1 = n_2n_3$ and $r_2 = n_1n_2$ with an irrational ratio r_2/r_1, but they now form $r_2r_1r_1r_2r_1r_1\ldots$, a periodic series which is determined by the periodic arrangement of lattice points on DF and $D'F'$. By separating the projected plane (or hyperplane) from the projected direction and choosing either an irrational or a rational plane, it is possible to obtain either an incommensurate structure such as the icosahedral phase or a commensurate structure of a FK phase by a projection from 6D to 3D.

Let E^6 be a 6D vector space, Z and δ be the set of integers and real numbers respectively, $\mathbf{b}_1$, $\mathbf{b}_2, \ldots, \mathbf{b}_6$ the set of basis vectors of a 6D lattice, $\mathbf{q}_j$ $(j = 1, 2, \ldots, 6)$ the projection of $\mathbf{b}_j$ in 3D space and $\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_6$ the set of vectors which span E^6.

Let L be the set of 6D lattice vectors $\mathbf{f}$; then

$$L = \left\{ \mathbf{f} \in E^6 \middle| \mathbf{f} = \sum_{i=1}^{6} u_i \mathbf{b}_i,\ u_i \in Z \right\}.$$

We define a subspace G in E^6 by

$$G = \left\{ \mathbf{t} \in E^6 \middle| \mathbf{t} = \sum_{j=1}^{6} \alpha_j \mathbf{c}_j,\ \alpha_1, \alpha_2, \alpha_3 \in [-\infty, +\infty],\ \alpha_i \in [\beta_{i1}, \beta_{i2}]\ (i = 4, 5, 6),\quad \beta_{ij} \in \delta \right\}. \tag{1}$$

The value of $(\beta_{i2} - \beta_{i1})$ $(i = 4, 5, 6)$ can be chosen for a known crystal. Generally $|\beta_{i2} - \beta_{i1}| \simeq 0 \to 1$.

Let L' be a subset of L, and

$$L' = \left\{ \mathbf{r} \in E^6 \middle| \mathbf{r} = \sum_{i=1}^{6} m_i \mathbf{b}_i,\ m_i \in Z,\ \mathbf{r} \in L \cap G \right\}.$$

Let $\mathbf{r}_p$ be the projection of r in 3D space; then

$$\mathbf{r}_p = \sum_{i=1}^{6} m_i \mathbf{q}_i. \tag{2}$$

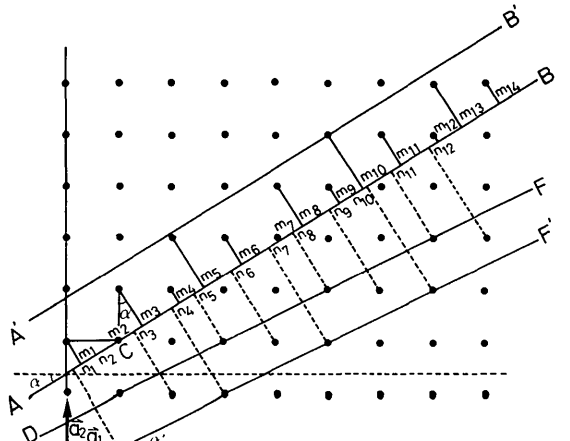


Fig. 1. Projection of a 2D lattice onto a 1D space illustrating the importance of the selection of projecting subspace (AB, $A'B'$ or DF, $D'F'$). AB is an irrational line passing through only one lattice point C and the lattice points between AB and $A'B'$, projected perpendicularly on AB, give an aperiodic incommensurate series of points $(m_1, m_2, m_3, \ldots)$. DF is a rational line lattice and the lattice points between DF and $D'F'$, projected also perpendicularly on AB, form a periodic commensurate series of points $(n_1, n_2, n_3, \ldots)$.

3. Method of calculation

3.1. *Projection matrix P and transformation matrix Ω*

In order to calculate the projection vector $\mathbf{r}_p$, we have to use matrix algebra. In this paper, we use a capital English or Greek letter to denote a matrix and a corresponding small one with subscripts *i, j, k etc.* to denote an element of the matrix. For example, c_{ij} is an element of the matrix C and $\tilde{C}$ is the transpose of the matrix C.

With this matrix notation, (2) becomes

$$\mathbf{r}_p = \tilde{M}Q \tag{3}$$

where

$$\tilde{M} = [m_1 m_2 \ldots m_6], \qquad \tilde{Q} = [\mathbf{q}_1 \mathbf{q}_2 \ldots \mathbf{q}_6].$$

For an icosahedral phase, $\mathbf{q}_i$ $(i = 1, 2, \ldots 6)$ are directed to six of the vertices of an icosahedron from its centre. As shown in Fig. 2, the centre of an icosahedron is positioned at the origin of the 3D Cartesian system with $\mathbf{i}_2$ and $\mathbf{i}_3$ parallel to one of the 2 and $\bar{5}$ axes of the icosahedron, respectively.

We impose the condition

$$Q = \Omega I^{(1)} \tag{4}$$

where

$$\tilde{I}^{(1)} = [\mathbf{i}_1 \mathbf{i}_2 \mathbf{i}_3];$$

then

$$\Omega = \begin{bmatrix} \sin\theta & 0 & \cos\theta \\ \sin\theta\cos\varphi & \sin\theta\sin\varphi & \cos\theta \\ \sin\theta\cos 2\varphi & \sin\theta\sin 2\varphi & \cos\theta \\ \sin\theta\cos 3\varphi & \sin\theta\sin 3\varphi & \cos\theta \\ \sin\theta\cos 4\varphi & \sin\theta\sin 4\varphi & \cos\theta \\ 0 & 0 & 1 \end{bmatrix} \quad (4a)$$

For a 3D icosahedral quasicrystal, $\theta = \tan^{-1} 2 = 63{\cdot}43°$ and $\varphi = 72°$; for a pentagonal FK phase, θ and φ can be slightly different from these values.

Substituting (4) into (3), we obtain

$$\mathbf{r}_p = \tilde{M}\Omega I^{(1)}. \quad (5)$$

If we set

$$Q = PB, \quad (6)$$

then

$$\mathbf{r}_p = \tilde{M}PB, \quad (7)$$

where P is the projection matrix, with the property that

$$P^2 = P.$$

One can use both (5) and (7) to calculate quasilattice vectors $\mathbf{r}_p$, but (7) is much more complicated than (5). This is discussed in Appendix 1.

The problem is how to choose the m_i ($i = 1$ to 6) so that $\mathbf{r} = \sum_{i=1}^{6} m_i \mathbf{b}_i$ is located in L', the subset of L. This will be shown in the following section.

3.2. *Formulae for calculating lattice constants and atomic coordinates*

Let

$$C = SB, \quad (8)$$

where $\tilde{C} = [\mathbf{c}_1\mathbf{c}_2 \ldots \mathbf{c}_6]$ and S is the 6×6 transformation matrix.

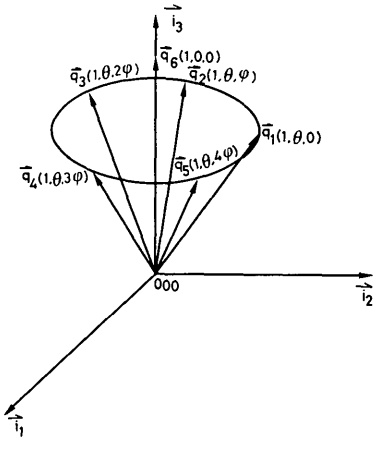


Fig. 2. $\mathbf{q}_j$ are vectors directed from the centre of an icosahedron towards its six vertices with $\mathbf{q}_6$ parallel to $\mathbf{i}_3$ and $\mathbf{q}_1$ on the plane defined by $\mathbf{i}_2$ and $\mathbf{i}_3$. $\mathbf{i}_j$ are the basis vectors of a Cartesian system. The values in parentheses are polar coordinates.

From (8)

$$B = S^{-1}C = UC;$$

then

$$U = S^{-1}.$$

A lattice vector $\mathbf{r}$ can be expressed as

$$\mathbf{r} = \tilde{M}B = \tilde{M}UC \quad (9)$$

or

$$\mathbf{r} = \sum \alpha_i \mathbf{c}_i. \quad (10)$$

From (9) and (10),

$$\alpha_i = \sum_{j=1}^{6} m_j u_{ij}. \quad (11)$$

We have to choose m_i ($i = 1$ to 6) such that the α_i ($i = 4, 5, 6$) satisfy (1). If the elements of the first one, two or three rows in the matrix S are irrational numbers, *i.e.* one, two or three of the vectors $\mathbf{c}_1$, $\mathbf{c}_2$ and $\mathbf{c}_3$ are irrational directions, the projected structure will be a 1D, 2D or 3D quasicrystal.

Let $\mathbf{c}_1$, $\mathbf{c}_2$ and $\mathbf{c}_3$ all be rational directions; $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$, the projection of $\mathbf{c}_1$, $\mathbf{c}_2$ and $\mathbf{c}_3$ respectively, will be the basis of a 3D crystalline phase, analogous to (2),

$$A = S^{(3)}Q = S^{(3)}\Omega I \quad (12a)$$

and

$$I = (S^{(3)}\Omega)^{-1}A \quad (12b)^*$$

where $\tilde{A} = [\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3]$; $S^{(3)}$ denotes the first three rows of the matrix S. Formula (12a) gives the lattice constants of the primitive cell of the projected structure.

From (5) and (12b)

$$\mathbf{r}_p = \tilde{M}\Omega(S^{(3)}\Omega)^{-1}A.$$

Sometimes the origin of the 3D unit cell is displaced from that of the 6D one by $\mathbf{r}_0 = \tilde{A}B$; then

$$\mathbf{r}_p = (\tilde{M} - \hat{\Lambda})\Omega(S^{(3)}\Omega)^{-1}A = [xyz]A \quad (13)$$

where $\Lambda = (\lambda_1\lambda_2 \ldots \lambda_6)$, $\lambda_j \in \delta$. Formula (13) gives the atomic coordinates $[xyz]$ in the projected structure.

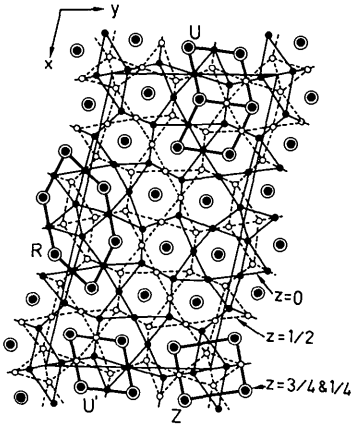
4. Frank–Kasper phases

First, the basic structure of $MgCu_2$ will be analysed; this will form the basis for further discussion. This structure has a f.c.c. lattice with 24 atoms, its primitive cell being a 60° rhombohedron with an edge length equal to $a/\sqrt{2}$. Each rhombohedron has six atoms at 000, $\frac{1}{2}00$ⵔ, $\frac{x}{8}\frac{x}{8}\frac{x}{8}$ ($x = 3$ and 5). In the 6D space, the corresponding $MgCu_2$ rhombohedron will have 27 atoms (see Appendix 2) located at: 000000 (one),

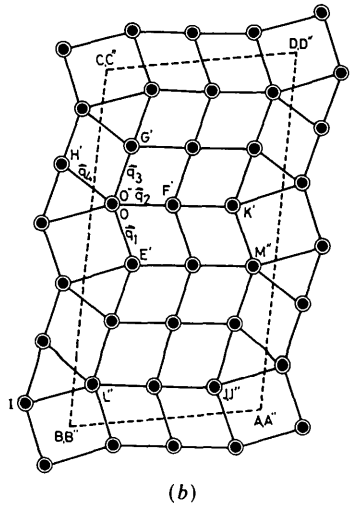
* Ω has no inverse matrix but $(S^{(3)}\Omega)$ is a 3×3 matrix and of course has an inverse matrix.

$\frac{1}{2}00000\circlearrowright$ (six), $\pm(\frac{3}{8}\frac{3}{8}000\frac{3}{8})$, $\pm(0\frac{3}{8}\frac{3}{8}00\frac{3}{8})$, $\pm(00\frac{3}{8}\frac{3}{8}0\frac{3}{8})$, $\pm(000\frac{3}{8}\frac{3}{8}\frac{3}{8})$, $\pm(\frac{3}{8}000\frac{3}{8}\frac{3}{8})$, $\pm(\frac{3}{8}\frac{3}{8}0\frac{3}{8}00)$, $\pm(0\frac{3}{8}\frac{3}{8}0\frac{3}{8}0)$, $\pm(\frac{3}{8}0\frac{3}{8}\frac{3}{8}00)$, $\pm(0\frac{3}{8}0\frac{3}{8}\frac{3}{8}0)$, $\pm(\frac{3}{8}0\frac{3}{8}0\frac{3}{8}0)$.

Once θ and φ are selected, the matrix Ω is known from (4*a*). The important step in obtaining a projected crystal structure is to define the S matrix or the six vectors $\mathbf{c}_j$. In the following the complex structure of the monoclinic Mg_4Zn_7 ($Z = 110$ atoms, $a = 2{\cdot}596$, $b = 1{\cdot}428$, $c = 0{\cdot}524$ nm, $\gamma = 102{\cdot}5°$) (Yarmolyuk, Kripyakevich & Mel'nik, 1975) will be used as an illustrative example. Along the unique axis, namely the [001] direction, Mg_4Zn_7 has a layer structure (Fig. 3*a*) consisting of four layers: the primary layers have pentagon-triangle networks at $z = 0$ and $\frac{1}{2}$, the latter being rotated 36° from the former, forming pentagonal antiprisms; the secondary layers are at $z = \pm\frac{1}{4}$ with nodes located at the centres of these pentagonal antiprisms forming interlocked icosahedra. Therefore, the layer structure of Mg_4Zn_7 can be represented by the secondary layer as shown in Fig. 3(*b*), in which filled circles and letters without a prime represent the nodes at $z = \frac{1}{4}$, open circles and letters with a prime those at $z = \frac{3}{4}$ and letters with a double prime those at $z = \frac{5}{4}$. *ABCDA"B"C"D"* represents a unit cell in Mg_4Zn_7 with $\mathbf{a}_1 = AD$, $\mathbf{a}_2 = AB$, $\mathbf{a}_3 = AA''$. Let *OE'*, *OF'*, *OG'*, *OH'* and *OO"* denote the projected vectors $\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3, \mathbf{q}_4$ and $\mathbf{q}_6$, respectively, in the 3D hyperplane projected from the vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$, $\mathbf{b}_4$, and $\mathbf{b}_6$, respectively, of a 6D cubic crystal. Then $JK' = 2\mathbf{q}_3 - \mathbf{q}_1$, $JI = -2\mathbf{q}_2 - \mathbf{q}_3 + \mathbf{q}_4 + \mathbf{q}_6$, $JJ'' = \mathbf{q}_6$, $JM'' = 2\mathbf{q}_3$ and $JL'' = -2\mathbf{q}_2$ are the projected vectors onto the 3D hyperplane of vectors $\mathbf{c}_1$, $\mathbf{c}_2$, $\mathbf{c}_3$, $\mathbf{c}_4$ and $\mathbf{c}_5$ in the 6D space. If $\mathbf{q}_5$ is the projection of $\mathbf{c}_6$, then



(*a*)



(*b*)

Fig. 3. (*a*) Mg_4Zn_7 structure projected on (001) (Yarmolyuk *et al.*, 1975). (*b*) The secondary layer of Mg_4Zn_7, $Z = \frac{1}{4}, \frac{3}{4}$ (letters with a prime) and $\frac{5}{4}$ (letters with a double prime) illustrating its unit cell *ABCDA"B"C"D"*, vectors $\mathbf{q}_j$ representing an icosahedron and the projected vectors *JK'*, *JI*, *JJ"*, *JM"*, *JL"* of the selected 6D subspace.

$$S = \begin{bmatrix} \bar{1} & 0 & 2 & 0 & 0 & 0 \\ 0 & \bar{2} & \bar{1} & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & \bar{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

with the limiting conditions:

$$0 < \alpha_4 < 1$$
$$-1 < \alpha_5 < 0$$
$$\alpha_6 = 0.$$

Then all the lattice points in the secondary layer and therefore the lattice parameter of the primitive cell of Mg_4Zn_7 can be calculated. If one converts these lattice parameters to those of the Bravais monoclinic cell, the calculated lattice parameters become $b/a = 0{\cdot}5470$, $c/a = 0{\cdot}2012$, $\alpha = 90$, $\beta = 90$ and $\gamma = 102{\cdot}8°$, and they are in good agreement with the experimental data (see Table 1): $b/a = 0{\cdot}5501$, $c/a = 0{\cdot}2019$, $\alpha = 90$, $\beta = 90$, $\gamma = 102{\cdot}5°$. The S, θ and φ, β_{ij}, and the calculated and experimental data of lattice parameters for the other nine FK phases are also given in Table 1. Obviously, most of the deviations of b/a and c/a are below 1% (maximum deviation 2·6%) and the deviations of α, β and γ are within 0·56°.

If the limiting conditions are relaxed to

$$0 < \alpha_4 < 1{\cdot}2$$
$$-1{\cdot}2 < \alpha_5 < 0$$

and one uses the atom positions in the 6D $MgCu_2$ rhombohedron, the atom positions in the Mg_4Zn_7 structure can be calculated as shown in Table 2. For the atom positions of the 110 atoms in Mg_4Zn_7, the average deviation compared with the shortest atom distances is 3·69%. A similar calculation was carried out for another FK phase with a rather complex structure, X phase ($Mn_{45}Co_{40}Si_{45}$), and the results are shown in Table 3. The average deviation of 74

Table 1. *Calculated lattice parameters of FK phases by cut and projection method from a 6D $MgCu_2$ cube compared with experimental data*

FK phases	Matrix S	β_{ij} β_{11}	β_{12}	β_{21}	β_{22}	β_{31}	β_{32}	Projection angles θ(°)	φ(°)	Calculated / Experimental b/a	c/a	lattice constants α(°)	β(°)	γ(°)	References
$MgCu_2$	$S^{(1)}$	0	0	0	0	0	0	60	70·53	1	1	90	90	90	Friauf (1927)
										1	1	90	90	90	
$MgZn_2$	$S^{(2)}$	0	1	0	0	0	0	60	70·53	1	1·633	90	90	120	Friauf (1927)
										1	1·647	90	90	120	
$MgNi_2$	$S^{(3)}$	0	1	0	0	0	0	60	70·53	1	3·266	90	90	120	Laves & Witte (1935)
										1	3·282	90	90	120	
Zr_4Al_3	$S^{(4)}$	0	0	0	0	0	0	60	72	1	1·108	90	90	120	Wilson, Thomas &
										1	0·992	90	90	120	Spooner (1960)
Fe_7W_6	$S^{(5)}$	0	1	0	0	0	0	60	72	1	5·526	89·43	89·43	120	Westgren (1936)
										1	5·432	90	90	120	
W_2FeSi	$S^{(6)}$	0	1	0	1	0	0	60	72	0·8506	0·5164	90	90	90	Kripyakevich &
										0·8421	0·5122	90	90	90	Yarmolyuk (1974)
M	$S^{(7)}$	0	1	0	1	0	0	60	72	0·5878	0·3036	90	90	90	Shoemaker & Shoemaker
										0·5721	0·3033	90	90	90	(1967)
$(Co_{0·57}Si_{0·43})_3V_2$	$S^{(8)}$	0	1	0	1	0	0	60	72	0·4425	0·2688	90	90	98·40	Kripyakevich & Yamolyuk
										0·4397	0·2714	90	90	99·2	(1970)
X phase	$S^{(9)}$	−0·25	1	−0·25	0·75	0	0	60	72	0·7987	0·2996	90	90	90	Manor, Shoemaker &
										0·8032	0·3074	90	90	90	Shoemaker (1972)
Mg_4Zn_7	$S^{(10)}$	0	1·20	−1·20	0	0	0	60	72	0·5470	0·2012	90	90	102·8	Yarmolyuk, Kripyakevich
										0·5501	0·2019	90	90	102·5	& Mel'nik (1975)

$$S^{(1)}=\begin{bmatrix}1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&1&0&0&0\\0&0&0&1&0&0\\0&0&0&0&1&0\\0&0&0&0&0&1\end{bmatrix}\quad S^{(2)}=\begin{bmatrix}0&\bar1&0&0&0&0\\0&1&0&0&0&\bar1\\1&0&\bar1&0&0&0\\1&0&0&0&0&-\frac12\\0&0&0&1&0&0\\0&0&0&0&1&0\end{bmatrix}\quad S^{(3)}=\begin{bmatrix}0&\bar1&0&0&0&0\\0&1&0&0&0&\bar1\\2&0&\bar2&0&0&0\\2&0&0&0&0&\bar1\\0&0&0&1&0&0\\0&0&0&0&1&0\end{bmatrix}\quad S^{(4)}=\begin{bmatrix}\bar1&0&0&0&0&0\\1&0&0&0&0&\bar1\\0&0&1&\bar1&0&0\\0&1&0&0&0&0\\0&0&0&1&0&0\\0&0&0&0&1&0\end{bmatrix}$$

$$S^{(5)}=\begin{bmatrix}\bar1&0&0&0&0&0\\1&0&0&0&0&\bar1\\0&1&1&\bar1&0&0\\0&1&0&0&0&-\frac12\\0&0&0&0&1&0\\0&0&0&1&0&0\end{bmatrix}\quad S^{(6)}=\begin{bmatrix}\bar1&0&\bar1&1&1&0\\\bar1&0&1&0&0&0\\0&0&0&0&0&1\\\bar1&0&0&0&0&\frac12\\\bar1&0&0&0&1&0\\0&1&0&0&0&0\end{bmatrix}\quad S^{(7)}=\begin{bmatrix}2&0&0&\bar2&0&0\\\bar1&1&1&\bar1&0&0\\0&0&0&0&0&1\\2&0&0&0&0&\bar1\\0&0&\bar1&1&0&0\\0&0&0&0&1&0\end{bmatrix}\quad S^{(8)}=\begin{bmatrix}\bar1&1&1&0&0&-\frac12\\0&0&\bar1&1&0&0\\0&0&0&0&0&1\\0&\bar1&0&0&0&\frac12\\0&0&\bar1&0&0&\frac12\\0&0&0&0&1&0\end{bmatrix}$$

$$S^{(9)}=\begin{bmatrix}1&\bar2&\bar2&1&0&1\\1&1&\bar1&\bar1&0&0\\0&0&0&0&0&1\\0&\bar2&0&0&0&1\\0&0&2&0&0&\bar1\\0&0&0&0&1&0\end{bmatrix}\quad S^{(10)}=\begin{bmatrix}\bar1&0&2&0&0&0\\0&\bar2&\bar1&1&0&1\\0&0&0&0&0&1\\0&2&0&0&0&1\\0&0&\bar2&0&0&1\\0&0&0&0&1&0\end{bmatrix}$$

atom positions is 3·85%. Such good agreement may serve to show the possibility of using this projection method to obtain crystal structures of a number of pentagonal FK phases from a common 6D $MgCu_2$ cube.

5. A possible structure model of the icosahedral phase

As mentioned above, the 3D Penrose lattice consists of acute and obtuse rhombohedra; a 2D projection of it is shown in Fig. 4. Its resemblance to a FK phase is quite obvious, in such respects as the different orientations (U and U') and twining (U) of the acute rhombohedra; the rectangular unit Z and the compound unit R in the second layer of Mg_4Zn_7 as shown in Fig. 3(a) can all be found in Fig. 4. This has led the present authors to propose a structure model for the 2D quasicrystals (Yang & Kuo, 1986).

In the 3D quasicrystal the acute rhombohedra, by adopting different orientations and twinning, form the main skeleton and the obtuse rhombohedra fill the empty space left by the former. Since the acute rhombohedra can be considered as slightly distorted $MgCu_2$ rhombohedral units, now 63·43° instead of 60°, the structure model of the icosahedral quasicrystals can therefore be derived from the $MgCu_2$ structures as shown in Fig. 5. The atom positions in the acute rhombohedron shown in Fig. 5(b) and those in the obtuse rhombohedron can easily be fixed as shown in Fig. 5(a), if the fact that the obtuse and actue rhombohedra have a face in common is taken into consideration. However, this obtuse rhombohedron is too thin to allow any atom to be located inside it.

Since the $MgCu_2$-type structure is known to consist of the $Z16$ Kasper polyhedron, also known as the Friauf–Laves polyhedron, there must be a somewhat distorted one in this structure model. If one assumes the rhombohedral cell edge to be 0·476 nm, the distances from the central atom of this polyhedron to

Table 2. *Calculated coordinates of* Mg_4Zn_7 *by cut and projection from a 6D* $MgCu_2$ *cube compared with experimental ones: space group B2/m,* $a = 25{\cdot}96$, $b = 14{\cdot}28$, $c = 5{\cdot}24$ Å

Atom	Position	Experimental coordinates x	y	z	Calculated coordinates x	y	z	Atomic deviation Δd(Å)	Coordinates in 6D crystal	α_4	α_5
4Mg(1)	4(*i*)	0·307	0·351	0	0·303	0·353	0	0·11	$(0\bar{1}010\bar{1})+(0\frac{3}{8}\frac{3}{8}00\frac{3}{8})$	0·6875	−0·6875
4Mg(2)	4(*i*)	0·177	0·321	0	0·176	0·322	0	0·03	$(01\bar{1}10\bar{1})+(0\frac{2}{8}\frac{2}{8}00\frac{2}{8})$	0·3125	−0·8125
4Mg(3)	4(*i*)	0·166	0·747	0	0·161	0·745	0	0·13	$(02\bar{1}100)+(0\frac{2}{8}\frac{2}{8}00\frac{2}{8})$	0·1875	−0·1875
4Mg(4)	4(*i*)	0·361	0·570	0	0·359	0·580	0	0·16	$(02\bar{0}10\bar{1})+(0\frac{3}{8}\frac{3}{8}00\frac{3}{8})$	0·8125	−0·3125
4Mg(5)	4(*i*)	0·129	0·108	0	0·120	0·095	0	0·27	$(00\bar{1}10\bar{1})+(0\frac{3}{8}\frac{3}{8}00\frac{3}{8})$	0·1875	−1·1875
4Mg(6)	4(*i*)	0·213	0·977	0	0·215	0·973	0	0·09	$(02\bar{1}100)+(00\frac{3}{8}\frac{3}{8}0\frac{3}{8})$	0·3750	−0·3750
4Mg(7)	4(*i*)	0·033	0·726	0	0·035	0·720	0	0·11	$(02\bar{1}100)+(\frac{3}{8}\frac{3}{8}000\frac{3}{8})$	0·3750	−0·1875
4Mg(8)	4(*i*)	0·479	0·602	0	0·486	0·605	0	0·18	$(\bar{1}21\bar{1}0\bar{1})+(\frac{3}{8}\frac{3}{8}000\frac{3}{8})$	0·6250	−0·3125
4Mg(9)	4(*i*)	0·445	0·957	0	0·448	0·960	0	0·08	$(02\bar{0}10\bar{1})+(00\frac{5}{8}\frac{5}{8}0\frac{5}{8})$	1·1250	−0·6250
4Mg(10)	4(*i*)	0·008	0·903	0	0·010	0·912	0	0·13	$\frac{1}{2}[(\bar{1}0\frac{3}{2}000)+(002\frac{1}{2}0\bar{1})]$	0·5000	−0·2500
8Zn(1)	8(*j*)	0·070	0·248	0·25	0·067	0·242	0·25	0·10	$(00\bar{1}100)$	0·0000	−1·0000
8Zn(2)	8(*j*)	0·232	0·173	0·25	0·229	0·175	0·25	0·09	$(00010\bar{1})+(00000\frac{1}{2})$	0·5000	−1·0000
8Zn(3)	8(*j*)	0·108	0·898	0·25	0·108	0·892	0·25	0·09	$(02\bar{1}101)$	0·0000	0·0000
8Zn(4)	8(*j*)	0·086	0·569	0·25	0·088	0·567	0·25	0·06	$(01\bar{1}100)+(00000\frac{1}{2})$	0·0000	−0·5000
4Zn(5)	4(*i*)	0·079	0·409	0	0·077	0·405	0	0·07	$(01\bar{1}100)+(0\frac{1}{2}0000)$	0·0000	−0·7500
4Zn(6)	4(*i*)	0·168	0·533	0	0·169	0·533	0	0·03	$(01\bar{1}100)+(00\frac{1}{2}000)$	0·2500	−1·0000
4Zn(7)	4(*i*)	0·256	0·657	0	0·260	0·662	0	0·11	$(02\bar{0}100)+(0\frac{1}{2}0000)$	0·5000	−0·2500
4Zn(8)	4(*i*)	0·313	0·138	0	0·311	0·142	0	0·09	$(00010\bar{1})+(00\frac{1}{2}000)$	0·7500	−1·0000
4Zn(9)	4(*i*)	0·402	0·266	0	0·402	0·271	0	0·07	$(0\bar{1}110\bar{1})+(0\frac{1}{2}0000)$	1·0000	−0·7500
4Zn(10)	4(*i*)	0·346	0·787	0	0·352	0·791	0	0·15	$(02\bar{0}100)+(00\frac{1}{2}000)$	0·7500	0·0000
4Zn(11)	4(*i*)	0·330	0·966	0	0·331	0·967	0	0·03	$(02\bar{0}100)+(000\frac{1}{2}00)$	0·7500	−0·5000
4Zn(12)	4(*i*)	0·479	0·178	0	0·479	0·175	0	0·04	$(\bar{1}0110\bar{1})+(\frac{1}{2}00000)$	0·5000	−1·0000
4Zn(13)	4(*f*)	0·25	0·5	0·25	0·25	0·5	0·25	0·00	$(0\bar{1}010\bar{1})+(00000\frac{1}{2})$	0·5000	−0·5000
2Zn(14)	2(*c*)	0	0·5	0	0	0·5	0	0·00	$(01\bar{1}100)+(\frac{1}{2}00000)$	0·5000	−0·5000

The average of $\Delta d/d$ is 3·69%. The origin is at $(10\bar{1}10\bar{1})$.

Table 3. *Calculated coordinates of X phase* ($Mn_{45}Co_{40}Si_{15}$) *by cut and projection method from a 6D* $MgCu_2$ *cube compared with experimental ones: space group Pnnm,* $a = 15{\cdot}43$, $b = 12{\cdot}39$, $c = 4{\cdot}74$ Å

No.	Atom	Position	Experimental coordinates x	y	z	Calculated coordinates x	y	z	Atomic deviation Δd(Å)	Coordinates in 6D crystal	α_4	α_5
1	CoMn	8(*h*)	0·1106	0·0858	0·2428	0·1050	0·0955	0·2500	0·15	$(0\bar{1}0000)+(00000\frac{1}{2})$	0·0000	0·5000
2	CoMn	8(*h*)	0·1759	0·3980	0·2354	0·1851	0·4045	0·2500	0·18	$(1\bar{1}0000)+(00000\frac{1}{2})$	0·7500	0·2500
3	CoMnSi	8(*h*)	0·3981	0·2104	0·2536	0·3950	0·2135	0·2500	0·06	$(1\bar{2}0000)+(00000\frac{1}{2})$	0·7500	0·7500
4	Si	4(*g*)	0·2156	0·9917	0	0·2099	0·1000	0	0·14	$(1\bar{1}\bar{1}\bar{1}01)+(0\frac{1}{2}0000)$	0·7500	0·7500
5	CoMn	4(*g*)	0·3607	0·0573	0	0·3550	0·0590	0	0·09	$(02\bar{0}001)+(\frac{1}{2}00000)$	0·3750	0·7500
6	CoMn	4(*g*)	0·4986	0·3107	0	0·5000	0·3090	0	0·03	$(12\bar{1}001)+(00\frac{1}{2}000)$	0·5000	0·7500
7	Si	2(*b*)	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	0	0·00	$(12\bar{1}001)+(0\frac{1}{2}0000)$	0·2500	0·5000
8	Si	4(*g*)	0·3546	0·7424	0	0·3550	0·7500	0	0·09	$(1\bar{1}\bar{1}\bar{1}01)+(000\frac{1}{2}00)$	0·1250	0·6250
9	CoMn	4(*g*)	0·2092	0·8023	0	0·2099	0·8090	0	0·08	$(1\bar{1}\bar{1}\bar{1}01)+(00\frac{1}{2}000)$	0·2500	1·0000
10	Mn	4(*g*)	0·0701	0·5292	0	0·0725	0·5295	0	0·04	$\frac{1}{2}[(\frac{1}{2}\bar{1}0\bar{1}01)+(1\frac{1}{2}0000)]$	0·6875	0·4375
11	Mn	4(*g*)	0·4728	0·8993	0	0·4761	0·9080	0	0·12	$(1\bar{1}2\bar{1}01)+(00\frac{3}{8}\frac{3}{8}0\frac{3}{8})$	−0·2188	0·7187
12	Mn	4(*g*)	0·0551	0·2779	0	0·0563	0·2830	0	0·07	$(0\bar{1}0000)+(\frac{3}{8}\frac{3}{8}000\frac{3}{8})$	0·2813	0·2188
13	Mn	4(*g*)	0·2360	0·2130	0	0·2338	0·2170	0	0·06	$(02\bar{0}000)+(\frac{2}{8}\frac{2}{8}000\frac{2}{8})$	0·4688	0·5313
14	Mn	4(*g*)	0·3394	0·3990	0	0·3426	0·4045	0	0·08	$(12\bar{1}000)+(0\frac{2}{8}\frac{2}{8}00\frac{2}{8})$	0·5563	0·4375
15	Mn	4(*g*)	0·2351	0·5865	0	0·2338	0·5920	0	0·07	$(1\bar{1}\bar{1}\bar{1}00)+(00\frac{5}{8}\frac{5}{8}0\frac{5}{8})$	0·4688	0·5313
16	Mn	4(*g*)	0·0506	0·9026	0	0·0525	0·9045	0	0·04	$(1\bar{1}\bar{1}\bar{1}00)+(0\frac{5}{8}\frac{5}{8}00\frac{5}{8})$	0·3125	0·6875

The average of $\Delta d/d$ is 3·85%. The origin is at $(0\bar{2}1000)$.

its 12 closest atoms at 1 to 12 (Fig. 5*b*) are 0·277 (1 to 3), 0·288 (4 to 6) and 0·293 nm (7 to 12), respectively. These are comparable to the interatomic distances of 0·291 and 0·279 nm, respectively, for Ta–Ta and Ta–Co pairs in the equilibrium $TaCo_2$ phase ($a = 0{\cdot}673$ nm). Moreover, the atomic volumes of the acute and obtuse rhombohedra are 0·0136 and 0·0126 nm^3 respectively, while the average atomic volume in $TaCo_2$ is 0·0127 nm^3. It is of interest to note that the edge length of the rhombohedron is $a/\sqrt{2} = 0{\cdot}476$ nm, in good agreement with the 0·46 nm obtained by Elser (1986).

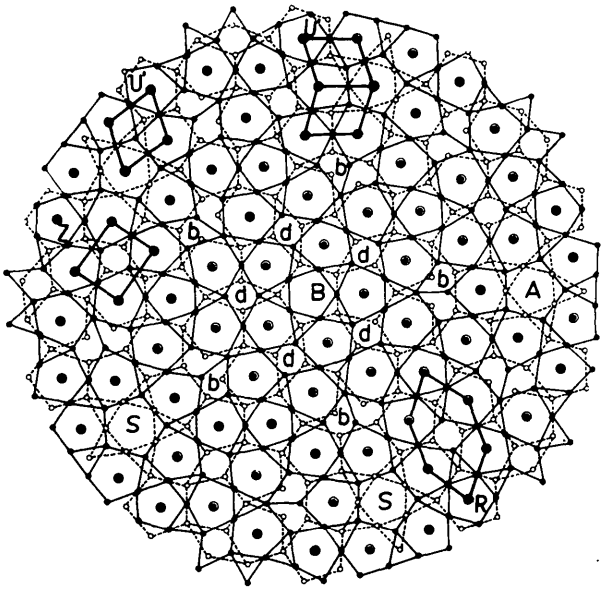


Fig. 4. 2D fivefold quasicrystal structure.

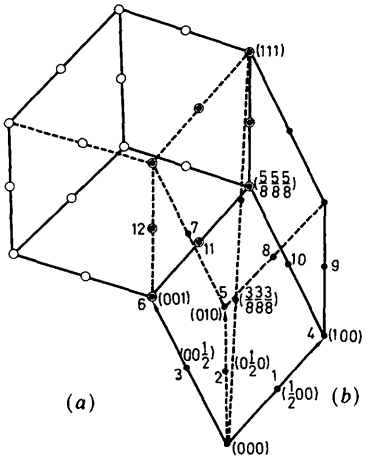


Fig. 5. Structure model of the icosahedral quasicrystal consisting of obtuse (*a*) and acute (*b*) rhombohedra having a common interface. The acute rhombohedron ($\alpha = 63{\cdot}43°$) is a slightly distorted rhombohedral unit cell of the f.c.c. $MgCu_2$ structure ($\alpha = 60°$).

6. Concluding remarks

In the past Frank & Kasper (1958, 1959) have discussed the fundamentals of the geometrical nature of the FK phases. Andersson (1978) applied symmetry operations to the $MgCu_2$ rhombohedral and Zr_4Al_3 rectangular units to recover a large number of the pentagonal FK phases. Recently in this laboratory we have used the juxtaposition of pentagonal antiprisms to explain the domain structures of FK phases (Ye, Li & Kuo 1985; Ye, Wang & Kuo 1985*a*, *b*; Li & Kuo, 1985) as well as the structure of new FK phases (Wang, Ye & Kuo, 1985). In this paper a new description of the structure of FK phases has been described which has the following merits: (1) the structures of FK phases are described analytically by well defined mathematical equations; (2) all known structures of pentagonal FK phases can be recovered from a common 6D $MgCu_2$ cube by a projection method; (3) the structure relationship between the icosahedral phase and the pentagonal FK phases is made more clear; and (4) the transition structure between the icosahedral phase and the equilibrium FK phase can be speculated upon.

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APPENDIX 1

Projection matrix *P*

From (5) and (7) we have

$$\Omega I^{(1)} = PB.$$

Assuming

$$I = \begin{bmatrix} I^{(1)} \\ I^{(2)} \end{bmatrix}$$

and

$$I^{(2)} = \begin{bmatrix} \mathbf{i}_4 \\ \mathbf{i}_5 \\ \mathbf{i}_6 \end{bmatrix}$$

in which $\mathbf{i}_1, \mathbf{i}_2, \ldots, \mathbf{i}_6$ are the basis vectors in the 6D Cartesian system, let

$$B = RI;$$

then

$$\Omega I = PRI,$$

or

$$P = \Omega R^{-1}.$$

For P to be a projection matrix, it is necessary that

$$PP = \Omega R^{-1}\Omega R^{-1} = \Omega(R^{-1}\Omega)R^{-1} = \Omega R^{-1} = P, \qquad (A1)$$

or

$$R^{-1}\Omega = E, \qquad (A1')$$

where E is the unit matrix.

If R can be decomposed into two 6×3 matrices Ω and Γ,

$$R = [\Omega\Gamma],$$

and R^{-1} to two 3×6 matrices Ω' and Γ'

$$R^{-1} = \begin{bmatrix}\Omega'\\ \Gamma'\end{bmatrix}$$

then

$$\Omega R^{-1} = \Omega\Omega' + \Omega\Gamma'$$

and

$$B = RR^{-1}B = [\Omega\Gamma]\begin{bmatrix}\Omega'\\ \Gamma'\end{bmatrix}B = (\Omega\Omega' + \Gamma\Gamma')B.$$

Let

$$\Omega\Omega' = P, \qquad (A2)$$

$$\Gamma\Gamma' = P'; \qquad (A3)$$

then

$$B = (P + P')B$$

where P and P' are projection matrices along the parallel and perpendicular directions respectively. Since

$$R^{-1}R = E$$

then

$$\begin{bmatrix}\Omega'\\ \Gamma'\end{bmatrix}[\Omega\Gamma] = \begin{bmatrix}\Omega'\Omega & \Omega'\Gamma\\ \Gamma'\Omega & \Gamma'\Gamma\end{bmatrix} = \begin{bmatrix}E^{(3)} & 0\\ 0 & E^{(3)}\end{bmatrix}$$

where $E^{(3)}$ is the unit matrix of order 3. Then

$$\Omega'\Omega = \Gamma'\Gamma = E^{(3)} \qquad (A4)$$

$$\Omega'\Gamma = \Gamma'\Omega = 0. \qquad (A5)$$

Then

$$R^{-1}\Omega = \begin{bmatrix}\Omega'\\ \Gamma'\end{bmatrix}\Omega = \begin{bmatrix}\Omega'\Omega\\ \Gamma'\Omega\end{bmatrix} = \begin{bmatrix}E^{(3)}\\ 0\end{bmatrix} = E^{(3)};$$

thus $(A1')$ and $(A1)$ are proved.

Similarly, it can be proved that

$$P'P' = P'.$$

Once the 6×3 matrix of order 3 is arbitrarily given, then R^{-1}, Ω' and P can be obtained. It is most convenient to choose Γ so that the number of basis vectors of a unit cell that are perpendicular and of equal modulus is a maximum. This is especially so when

$$\tilde{\Omega}\Gamma = 0.$$

Let

$$\Omega' = X\tilde{\Omega};$$

then

$$\Omega'\Gamma = X\tilde{\Omega}\Gamma = 0,$$

where X is a 3×3 matrix. From $(A4)$,

$$\Omega'\Omega = X\tilde{\Omega}\Omega = E^{(3)},$$

one obtains

$$X = (\tilde{\Omega}\Omega)^{-1}$$

and

$$\Omega' = (\tilde{\Omega}\Omega)^{-1}\tilde{\Omega}.$$

From $(A2)$

$$P = \Omega(\tilde{\Omega}\Omega)^{-1}\tilde{\Omega}. \qquad (A6)$$

From the Ω given in $(4a)$,

$$p_{ij} = \alpha\cos[(i-1)\varphi]\cos[(j-1)\varphi] + \beta\sin[(i-1)\varphi]\sin[(j-1)\varphi] + \gamma\cos^2\theta \qquad i = 1,2,\ldots,5,\quad j = 1,2,\ldots,5;$$

$$p_{6j} = p_{j6} = \gamma\cos^2\theta \qquad j = 1,2,\ldots,6;$$

$$p_{66} = \gamma;$$

where

$$\alpha = \left[\sum_{j=0}^{4}\cos^2(j\varphi)\right]^{-1}$$

$$\beta = \left[\sum_{j=0}^{4}\sin^2(j\varphi)\right]^{-1}$$

$$\gamma = (5\cos^2\theta + 1)^{-1}.$$

For $\theta = \tan^{-1}2 = 63{\cdot}43°$, $\varphi = 72°$,

$$P = \frac{\sqrt{5}}{10}\begin{bmatrix}\sqrt{5} & 1 & \bar{1} & \bar{1} & 1 & 1\\ 1 & \sqrt{5} & 1 & \bar{1} & \bar{1} & 1\\ \bar{1} & 1 & \sqrt{5} & 1 & \bar{1} & 1\\ \bar{1} & \bar{1} & 1 & \sqrt{5} & 1 & 1\\ 1 & \bar{1} & \bar{1} & 1 & \sqrt{5} & 1\\ 1 & 1 & 1 & 1 & 1 & \sqrt{5}\end{bmatrix}.$$

For $\theta = 60°$, $\varphi = 72°$,

$$P = \frac{5}{10}\begin{bmatrix}\sqrt{5} & 1 & \bar{1} & \bar{1} & 1 & 2/\sqrt{5}\\ 1 & \sqrt{5} & 1 & \bar{1} & \bar{1} & 2/\sqrt{5}\\ \bar{1} & 1 & \sqrt{5} & 1 & \bar{1} & 2/\sqrt{5}\\ \bar{1} & \bar{1} & 1 & \sqrt{5} & 1 & 2/\sqrt{5}\\ 1 & \bar{1} & \bar{1} & 1 & \sqrt{5} & 2/\sqrt{5}\\ 2/\sqrt{5} & 2/\sqrt{5} & 2/\sqrt{5} & 2/\sqrt{5} & 2/\sqrt{5} & \sqrt{5}\end{bmatrix}.$$

For $\theta = 60°$, $\psi = \cos^{-1}\frac{1}{3} = 70{\cdot}53°$,

$$\alpha = 2{\cdot}4857,\quad \beta = 2{\cdot}5142,\quad \gamma = 2{\cdot}25.$$

From the three different P matrices, it is clear that it is easier to use (5) than (7) to obtain $\mathbf{r}_p$.

APPENDIX 2

Atoms in the 6D $MgCu_2$ rhombohedron

Let us assume that the acute rhombohedron ($\alpha = 63{\cdot}43°$) of the 3D Penrose tiling has a similar structure to the 3D $MgCu_2$ rhombohedron ($\alpha = 60°$) which has two atoms at $\pm(\frac{3}{8}\frac{3}{8}\frac{3}{8})$ in addition to those at the vertices and the centres of edges. This acute rhombohedron can have 20 different orientations. But one half of them are in the opposite direction to the other half, so that only ten independent orientations exist. Let the basis vectors be $\mathbf{q}_i$, $\mathbf{q}_j$ and $\mathbf{q}_k$, where the set i, j, k may have the values

$$(126),\quad (236),\quad (346),\quad (456),\quad (156),$$

$$(12\bar{4}),\quad (23\bar{4}),\quad (\bar{1}34),\quad (\bar{2}54),\quad (1\bar{3}5).$$

The coordinates of these 20 atoms inside the rhombohedron are

$$\pm(\tfrac{3}{8}\tfrac{3}{8}00\tfrac{3}{8}),\quad \pm(0\tfrac{3}{8}\tfrac{3}{8}0\tfrac{3}{8}),\quad \pm(00\tfrac{3}{8}\tfrac{3}{8}0\tfrac{3}{8}),$$

$$\pm(000\tfrac{3}{8}\tfrac{3}{8}\tfrac{3}{8}),\quad \pm(\tfrac{3}{8}00\tfrac{3}{8}\tfrac{3}{8}),\quad \pm(\tfrac{3}{8}\tfrac{3}{8}0\bar{\tfrac{3}{8}}0),$$

$$\pm(0\tfrac{3}{8}\tfrac{3}{8}0\bar{\tfrac{3}{8}}),\quad \pm(\bar{\tfrac{3}{8}}0\tfrac{3}{8}\tfrac{3}{8}0),\quad \pm(0\bar{\tfrac{3}{8}}0\tfrac{3}{8}\tfrac{3}{8}),$$

$$\pm(\tfrac{3}{8}0\bar{\tfrac{3}{8}}0\tfrac{3}{8}).$$

Together with the atom at the origin and six more atoms on the centres of the edges with coordinates $(\frac{1}{2}00000)_{\mathrm{O}}$, there are altogether 27 atoms. Since the $\mathbf{q}_i$ are the projection of $\mathbf{b}_i$, these 27 atoms can be considered as projected from a 6D unit cell. By projecting such a 6D unit cell onto a 3D hyperplane, the atomic positions in the icosahedral quasicrystal can be obtained.

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Debye–Waller Coefficient of Nb by the Elastic Neutron Diffraction Method

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Abstract

The Debye–Waller exponent B and the Debye temperature Θ for niobium have been determined at room temperature by the elastic neutron diffraction method using a triple-axis neutron spectrometer. The contribution of TDS to the diffraction peaks was found to be negligible. The value of B thus found was 0·55 (5) Å^2. The Debye temperature Θ was 262 (12) K. The results are compared with values obtained by other techniques.

Introduction

From a diffraction experiment one could, in principle, obtain information about lattice-dynamical properties such as the mean square displacement of an atom and the Debye temperature of the material.

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