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A symmetrical indexing scheme for decagonal quasicrystals analogous to Miller–Bravais indexing of hexagonal crystals

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The problems of redundancy and superfluous indices in indexing the planes and axes in a decagonal quasicrystal are considered, using a scheme of five coplanar vectors in the quasiperiodic plane and one perpendicular vector. Of all the indexing schemes in use, this scheme offers the maximum advantage. An analogy is drawn to the hexagonal system using Miller–Bravais indices. Based on this, a symmetry-based indexing system for decagonal phases is devised that follows a simplified approximate zone law analogous to the exact zone law for the hexagonal case. The indices based on this scheme will be designated as 'Frank indices'. High-symmetry electron diffraction zone-axis patterns as well as powder X-ray diffraction patterns are indexed using Frank indices and compared with those of other indexing schemes.

1. Introduction

It is understood that a decagonal phase exhibiting two-dimensional quasiperiodicity as well as one-dimensional periodicity (Bendersky, 1985; Chattopadhyay *et al.*, 1985) requires a minimum of five basis vectors for indexing the quasilattices. Five-index schemes in which four of the base vectors are coplanar with a fifth perpendicular to them, along the tenfold symmetry axis, have been used extensively. Steurer and his co-workers (Steurer, 1989; Steurer & Mayer, 1989; Steurer & Kuo, 1990) and Cervellino *et al.* (1998) identified the unit cell at a minimum higher dimensional lattice through Patterson analysis and used it for indexing. Similarly, Yamamoto & Ishihara (1988) used five-integer indices for the planes and proposed a corresponding scheme for directions in decagonal structures. These indexing schemes avoid redundancy of indices by exploiting the fact that only four planar vectors are required to index two-dimensional quasiperiodic patterns in a plane (Janssen, 1988). However, the symmetry of the structure is not elegantly represented by this kind of indexing – the relation between index sets of symmetrically related spots is far from obvious. Moreover, in these schemes the relation between reciprocal space and direct space is derived by projection from a five-dimensional non-orthogonal lattice onto a three-dimensional subspace. As a consequence, it is not at all straightforward, using these schemes, to understand the symmetry-related planes and directions and to interpret the experimental electron and X-ray diffraction patterns.

A six-index scheme for decagonal quasicrystals has been used by Fitz Gerald and co-workers (Fitz Gerald, 1988; Choy *et al.*, 1988). Five base vectors are coplanar, corresponding to the five vertices of a regular pentagon; the sixth, perpendicular to them, is along the axis of tenfold symmetry. In this kind of scheme, the indices for diffraction spots related by the tenfold symmetry differ only by permutations and sign changes, so the symmetry of the structure is clearly and simply represented. However, because of the redundancy in the set of base vectors, the problem of non-uniqueness arises. The six-index scheme we introduce here, which we designate as 'Frank indexing', solves the non-uniqueness problem and adopts a straightforward relationship between reciprocal space and direct space that leads to a simple zone law. The situation for decagonal quasicrystals is very closely analogous to the indexing of hexagonal crystals, for which either a three-index scheme or a four-index scheme can be employed, but the four-index Frank–Weber scheme has a greater elegance and logic because it reflects the symmetry of the structure.

The problem of non-uniqueness in the Fitz Gerald-type six-index schemes was addressed by Mukhopadhyay *et al.* (1989), who suggested a 'least path criterion' (LPC) in order to assign unique indices. A mathematical proof of the uniqueness was provided by Mukhopadhyay & Lord (2002).

Other more complex indexing schemes exist for decagonal quasicrystals. Koopmans *et al.* (1987) provided an indexing scheme for the diffraction pattern of decagonal phases by extending the structural model advocated by Ho (1986), where a pentagonal bipyramid of base vectors is derived from a distorted icosahedral basis. This kind of approach may be regarded as analogous to the use of a rhombohedral basis for indexing hexagonal and trigonal crystals. Mandal & Lele (1991), Prasad *et al.* (1997) and Mandal *et al.* (2003) employed a similar distorted icosahedral basis, projected from a six-dimensional orthogonal unit cell, where the magnitude of one base vector is different from the others. Aragon *et al.* (1990) also used the same six base vectors but with a different scaling constant for indexing. A curious indexing method was introduced by Dalton *et al.* (1992), who advocated a scheme based on two appropriately distorted icosahedra rotated 36° about a common axis (*i.e.* periodic axis), giving an index set of 11 integers.

The redundant four-index scheme for indexing hexagonal crystals (Weber, 1922; Frank, 1965) is now accepted as standard and its superiority over the non-redundant three-index scheme is now taken for granted. In spite of the close analogy between the hexagonal and the decagonal cases, this does not appear to have happened in the case of decagonal quasicrystals: the five-index scheme is very commonly employed. In a sense, it is analogous to the three-index scheme earlier used for indexing hexagonal crystals. The main aim of the present work is to draw attention to this analogy between the hexagonal and decagonal cases and, in the process of doing so, to clarify some of the problems arising from the use of redundant axes and superfluous indices.

2. Indexing using a redundant axis

The indexing of directions and planes when there are redundant axes is an important challenge. The two-dimensional hexagonal lattice provides the simplest example of the use of a redundant axis. Two axes suffice but a third can be introduced to bring out the symmetry. This leads to multiple indexing possibilities. To retain uniqueness, one way is to impose a restriction that $u + v + w = 0$. This condition can be understood in terms of projection from a three-dimensional cube. It is the zone law applied to the zone axis [111], the axis of projection. Frank (1965) showed that a three-dimensional hexagonal lattice can similarly be obtained by projection from four dimensions. His observations can be briefly summarized as follows: let $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$, $\mathbf{e}_4$ be the axes of a Cartesian coordinate system in four-dimensional space and consider the four-dimensional lattice given by the points with position vectors

$$\mathbf{e}_1u^1 + \mathbf{e}_2u^2 + \mathbf{e}_3u^3 + (\lambda\mathbf{e}_4)u^4 \quad (1)$$

and its reciprocal lattice, given by

$$h_1\mathbf{e}_1 + h_2\mathbf{e}_2 + h_3\mathbf{e}_3 + h_4(\mathbf{e}_4/\lambda). \quad (2)$$

(u^i and h_i are integers.) The zone law takes the simple form

$$h_1u^1 + h_2u^2 + h_3u^3 + h_4u^4 = 0. \quad (3)$$

Projection along the [1110] axis onto the three-dimensional space $u^1 + u^2 + u^3 = 0$ gives a three-dimensional hexagonal lattice with $c/a = \lambda\surd(3/2)$. The indices $[u^1u^2u^3u^4]$ and $(h_1h_2h_3h_4)$ and the zone law (3) for the hexagonal lattice are inherited from the four-dimensional lattice. For the particular case $\lambda = 1$, the four-dimensional lattice is (hyper)cubic and the hexagonal lattice is "Frank's cubic hexagonal lattice" (Ranganathan *et al.*, 2002).

2.1. Algebraic geometry

If $\mathbf{e}_i$ ($i = 1, \ldots, N$) is a set of vectors in Euclidean n space E_n, an N-tuple of real numbers $[u^1, u^2, \ldots, u^N]$ determines a position vector

$$\mathbf{u} = \mathbf{e}_iu^i. \quad (4)$$

(We adopt the Einstein summation convention: where a label appears twice in an expression, once as a subscript and once as a superscript, a summation is implied. Thus, for example, $\mathbf{e}_iu^i = \mathbf{e}_1u^1 + \mathbf{e}_2u^2 + \ldots + \mathbf{e}_Nu^N$.) A vector $\mathbf{h}$ determines an N-tuple $(h_1, h_2, \ldots, h_N)$,

$$h_i = \mathbf{h}\cdot\mathbf{e}_i. \quad (5)$$

A hyperplane with unit normal $\mathbf{n}$, at a distance d from the origin, is given by the equation

$$\mathbf{n}\cdot\mathbf{x} = d. \quad (6)$$

Writing $\mathbf{h} = \mathbf{n}/d$, the condition $\mathbf{u}\cdot\mathbf{n} = 0$ for a vector $\mathbf{u}$ to be parallel to this plane then implies

$$h_iu^i = h_1u^1 + h_2u^2 + \ldots + h_Nu^N = 0. \quad (7)$$

The axis along $\mathbf{e}_i$, given parametrically by $\mathbf{x} = \lambda\mathbf{e}_i$, cuts the hyperplane (6) at $\lambda = 1/h_i$, *i.e.* the numbers h_i are equal to the reciprocals of the intercepts of the plane, with the N axes:

$$(h_1, h_2, \ldots, h_N) = (1/\lambda_1, 1/\lambda_2, \ldots, 1/\lambda_N). \quad (8)$$

The above simple concepts are the foundations for the indexing methods employed in crystallography. Observe the considerable generality of the above statements. There is no assumption that the vectors $\mathbf{e}_i$ be linearly independent, nor do we need to assume $n = N$. The above statements remain valid whether $N > n$ [as in the use of a superfluous axis for the indexing of hexagonal crystals, first introduced by Weber (1922), or in the indexing of quasicrystals] or $N < n$ (as when three-dimensional space is regarded as a subspace of a space of higher dimensions). In crystallographic applications, the u^i are *integers* and the points with position vectors $\mathbf{u}$ given by (1) constitute a lattice. The ratios $u^1 : u^2 : \ldots : u^N$ determine a *zone axis*. The lattice planes intersect the axes at rational values of λ_i, so that the h_i given by (5) are *rational*. Families of parallel crystal planes are determined by the ratios $h_1 : h_2 : \ldots : h_N$, so that families of parallel planes may be indexed by sets of *integers* h_i, the *Miller indices*. Equation (4) is of course the familiar *zone law*. When $N = n$ and the vectors $\mathbf{e}_i$ are linearly independent, the *reciprocal lattice* can be defined simply as the lattice generated by the vectors $\mathbf{e}^i$ that satisfy

$$\mathbf{e}^i\cdot\mathbf{e}_j = \delta^i_j \quad (9)$$

(where the δ^i_j are the components of the unit $N \times N$ matrix). The families of crystal planes of the original lattice are then conveniently related to the points of the reciprocal lattice through

$$\mathbf{h} = h_i \mathbf{e}^i. \tag{10}$$

So far, all is simple and straightforward and well known. Indeed, it is 'standard text book material'. Our aim has been to present it in the clearest and briefest possible way, to establish our notational conventions and to set the scene for what we intend as a definitive treatment of the subtleties that arise when $N > n$. We shall emphasize two important particular cases – the Weber four-index scheme for hexagonal crystals and the indexing problem raised by decagonal quasicrystals – and highlight their similarities and their differences. *The problems that arise in cases of linearly dependent base vectors all have one source: the failure of equation (9).*

2.2. The hexagonal lattice

A plane hexagonal lattice can be generated by two vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ of equal length subtending an angle of 120°. The reciprocal vectors $\mathbf{e}^1$ and $\mathbf{e}^2$ given by (9) are equal in length and subtend an angle of 60°. The indexing method that is now standard for trigonal and hexagonal systems employs a superfluous base vector $\mathbf{e}_3$, defined by

$$\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3 = 0. \tag{11}$$

A fourth vector $\mathbf{e}_4$ perpendicular to the plane, along the sixfold axis, completes the set of generating vectors for a three-dimensional hexagonal lattice. The point symmetry of the structure is then properly represented in the system of zone-axis indices $[u^1, u^2, u^3, u^4]$.

Frank (1965) considered, and solved, the problem of dealing similarly with the reciprocal vectors. The reciprocal lattice generated by $\mathbf{e}^1$ and $\mathbf{e}^2$ [obtained from (9) with $N = n = 2$] is of course also a hexagonal lattice, so it can be generated by three redundant vectors in the proper 120° configuration, such as $\mathbf{e}^1$, $\mathbf{e}^2 - \mathbf{e}^1$ and $-\mathbf{e}^2$, but the usefulness of the reciprocal-lattice concept for indexing planes is then lost. The solution presented by Frank was to regard the plane hexagonal lattice as a projection from a three-dimensional primitive cubic lattice along the [111] direction onto the plane $x + y + z = 0$.

The columns of the matrix

$$a\begin{pmatrix} \mathrm{c}_0 & \mathrm{c}_1 & \mathrm{c}_2 \\ \mathrm{s}_0 & \mathrm{s}_1 & \mathrm{s}_2 \\ 1/\sqrt{2} & 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} = \frac{a}{2}\begin{pmatrix} 2 & -1 & -1 \\ 0 & \sqrt{3} & -\sqrt{3} \\ \sqrt{2} & \sqrt{2} & \sqrt{2} \end{pmatrix}, \tag{12}$$

where $\mathrm{c}_r = \cos(2r\pi/3)$ and $\mathrm{s}_r = \sin(2r\pi/3)$ can be interpreted as the Cartesian components of a *cube* of edge length $a\surd(3/2)$. Projection onto the plane $z = 0$ (perpendicular to the [111] axis of the cube) then gives the three base vectors

$$(\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3) = a\begin{pmatrix} \mathrm{c}_0 & \mathrm{c}_1 & \mathrm{c}_2 \\ \mathrm{s}_0 & \mathrm{s}_1 & \mathrm{s}_2 \\ 0 & 0 & 0 \end{pmatrix} = \frac{a}{2}\begin{pmatrix} 2 & -1 & -1 \\ 0 & \sqrt{3} & -\sqrt{3} \\ 0 & 0 & 0 \end{pmatrix}, \tag{13}$$

for a plane hexagonal lattice of edge length a. For the three-dimensional hexagonal lattice, one can simply introduce a fourth vector perpendicular to these three:

$$\mathbf{e}_4 = c\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{14}$$

The four vectors ($\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$, $\mathbf{e}_4$) are readily obtained by projection from a four-dimensional lattice. When $c/a = \surd(3/2)$ (Frank's 'cubic hexagonal' lattice), the four-dimensional lattice is (hyper)cubic.

The reciprocal hexagonal lattice proposed by Frank is obtained by projection from the reciprocal of the lattice in the higher dimension. This gives

$$(\mathbf{e}^1\mathbf{e}^2\mathbf{e}^3) = \frac{2}{3a}\begin{pmatrix} \mathrm{c}_0 & \mathrm{c}_1 & \mathrm{c}_2 \\ \mathrm{s}_0 & \mathrm{s}_1 & \mathrm{s}_2 \\ 0 & 0 & 0 \end{pmatrix} = \frac{1}{3a}\begin{pmatrix} 2 & -1 & -1 \\ 0 & \sqrt{3} & -\sqrt{3} \\ 0 & 0 & 0 \end{pmatrix},$$
$$\mathbf{e}^4 = \frac{1}{c}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{15}$$

An alternative approach to the problem of reciprocal vectors, when linearly dependent base vectors are involved, makes use of the concept of the *generalized inverse* of a matrix (Ben-Israel & Greville, 1977). The method was explored by Mackay (1977), who showed that, in the case of the Weber indexing for a hexagonal lattice, it leads to the same reciprocal lattice as the one given by Frank, defined by equation (10). The indexing problem for quasicrystals has been discussed in terms of generalized inverses by Lord (2003).

The definition (9) of the reciprocal vectors in the case of linearly independent base vectors simply amounts to finding the inverse of a matrix. If the components of the vectors $\mathbf{e}_i$ (referred to a Cartesian coordinate system) are written as the columns of a matrix E, then the components of the reciprocal vectors $\mathbf{e}^i$ are given by the rows of the inverse matrix E^{-1}. The corresponding matrix E for a set of redundant axes has no inverse – it is in general not even a square matrix. However, *every* matrix E possesses a unique *Moore–Penrose inverse* (M–P inverse) E^* satisfying

$$E^{**} = E, \quad EE^* = (EE^*)^T, \quad E^*E = (E^*E)^T,$$
$$EE^*E = E, \quad E^*EE^* = E^* \tag{16}$$

(superscript T denotes matrix transpose). The M–P inverse of the matrix given in (13) is in fact the matrix given in (15) (Lord, 2003); the projection method and the generalized inverse method are equivalent. The M–P inverse is a valuable concept for dealing with problems that arise from redundancy of axes (Mackay, 1977; Mandal, 1994; Lord, 2003).

Recall that the indices defined by (4) and (5) satisfy the zone law (7) *independently of whether or not the base vectors are linearly dependent*, and that these indices h_i are the reciprocals of the intercepts of a lattice plane with the axes. However, when the reciprocal base vectors for a hexagonal lattice are defined by equation (13), as in Frank's scheme, these indices h_i are *not* the same as the indices appearing in (10). Let us therefore write (k_1, k_2, k_3) for the components of reciprocal vectors,

$$\mathbf{h} = k_i \mathbf{e}^i. \tag{17}$$

The h_i and k_i are related through

$$h_i = k_j P_i^j, \tag{18}$$

where

$$P_i^j = \mathbf{e}^j \cdot \mathbf{e}_i = \frac{1}{3}\begin{pmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix}. \tag{19}$$

In terms of the indices k_i, the zone law takes the form

$$k_j P_i^j u^i = 0 \tag{20}$$

($k_4 = h_4$). Written out in full,

$$\begin{aligned} 2(k_1u^1 + k_2u^2 + k_3u^3) - (k_2u^1 + k_3u^1 + k_3u^2 \\ + k_1u^2 + k_1u^3 + k_2u^3) + 3k_4u^4 = 0. \end{aligned} \tag{21}$$

Note that, because of (5) and (11) [and as can be seen from (18) and the fact that the first three column sums of P are zero],

$$h_1 + h_2 + h_3 = 0 \tag{22}$$

is satisfied *identically*, but that [also because of (11) and as can be seen from (18) and the fact that the first three row sums of P are zero] there is a freedom of choice for the index sets k_i: ($k_1 + m$, $k_2 + m$, $k_3 + m$) and (k_1, k_2, k_3), for any rational m, represent the same family of planes. Choosing $m = -(k_1 + k_2 + k_3)/3$ gives indices k_i that satisfy

$$k_1 + k_2 + k_3 = 0. \tag{23}$$

Then the k_i are *identical* to the Miller–Bravais indices h_i and the complicated zone law (20) reduces to the usual

$$h_1u^1 + h_2u^2 + h_3u^3 + h_4u^4 = 0. \tag{24}$$

From the form of (4) and (11), there is a corresponding freedom of choice for the indices u^i: $[u^1 + m', u^2 + m', u^3 + m']$ and $[u^1, u^2, u^3]$ represent the same zone axis $\mathbf{u}$. Choosing $m' = -(u^1 + u^2 + u^3)/3$, we get the Weber zone-axis symbols, satisfying

$$u^1 + u^2 + u^3 = 0. \tag{25}$$

If we choose to satisfy either (23) or (25) (or both), the simple zone law applies. If neither are satisfied, then the appropriate zone law is the more complicated equation (21).

2.3. The decagonal quasilattice

The indexing of directions and planes in quasilattices is an important challenge. Whereas, for the hexagonal system discussed above, the employment of an indexing scheme with $N > n$ is optional, in quasicrystals this condition is an essential feature of the structure. A large number of indexing schemes have been proposed for the indexing of decagonal quasicrystals. The scheme used by Choy *et al.* (1988) and Fitz Gerald *et al.* (1988) has five coplanar vectors $\mathbf{e}_1, \ldots, \mathbf{e}_5$ corresponding to position vectors of a regular pentagon and therefore satisfying

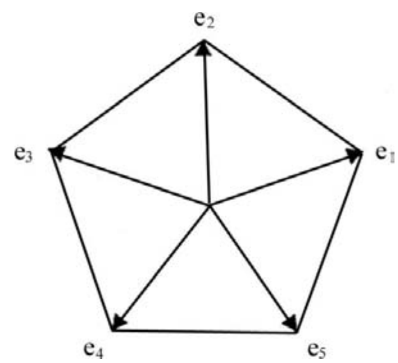

Figure 1
Pentagonal basis vector used for indexing in the decagonal plane.

$$\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3 + \mathbf{e}_4 + \mathbf{e}_5 = 0 \tag{26}$$

(Fig. 1). Their components with respect to a Cartesian coordinate system in the plane can be taken to be the columns of the matrix

$$\begin{aligned} E &= a\begin{pmatrix} c_0 & c_1 & c_2 & c_3 & c_4 \\ s_0 & s_1 & s_2 & s_3 & s_4 \end{pmatrix} \\ &= \frac{a}{2}\begin{pmatrix} 2 & -\sigma & -\tau & -\tau & -\sigma \\ 0 & \beta\tau & \beta & -\beta & -\beta\tau \end{pmatrix}, \end{aligned} \tag{27}$$

where $c_r = \cos(2r\pi/5)$, $s_r = \sin(2r\pi/5)$, $\tau = (1 + \surd 5)/2$, $\sigma = 1 - \tau$, $\beta = \surd(3 - \tau)$.

These vectors are obtained by projection onto a plane of the vectors in five dimensions whose Cartesian components are given by the columns of

$$\begin{aligned} &a\begin{pmatrix} c_0 & c_1 & c_2 & c_3 & c_4 \\ s_0 & s_1 & s_2 & s_3 & s_4 \\ c_0 & c_3 & c_1 & c_4 & c_2 \\ s_0 & s_3 & s_1 & s_4 & s_2 \\ 1/\surd 2 & 1/\surd 2 & 1/\surd 2 & 1/\surd 2 & 1/\surd 2 \end{pmatrix} \\ &= \frac{a}{2}\begin{pmatrix} 2 & -\sigma & -\tau & -\tau & -\sigma \\ 0 & \beta\tau & \beta & -\beta & -\beta\tau \\ 2 & -\tau & -\sigma & -\sigma & -\tau \\ 0 & -\beta & \beta\tau & -\beta\tau & \beta \\ 1/\surd 2 & 1/\surd 2 & 1/\surd 2 & 1/\surd 2 & 1/\surd 2 \end{pmatrix}. \end{aligned} \tag{28}$$

These five vectors in five dimensions are the edges of a hypercube of edge length $a\surd(5/2)$.

The M–P inverse of E is

$$E^* = \frac{2}{5a^2}E^T \tag{29}$$

(Lord, 2003). The reciprocal vectors, given by the rows of E^*, are then

$$\mathbf{e}^i = \frac{2}{5a^2}\mathbf{e}_i. \tag{30}$$

Equation (9) is replaced by

$$\mathbf{e}^j \cdot \mathbf{e}_i = P_i^j, \tag{31}$$

where

$$P = E^* E = \frac{1}{5}\begin{pmatrix} 2 & -\sigma & -\tau & -\tau & -\sigma \\ -\sigma & 2 & -\sigma & -\tau & -\tau \\ -\tau & -\sigma & 2 & -\sigma & -\tau \\ -\tau & -\tau & -\sigma & 2 & -\sigma \\ -\sigma & -\tau & -\tau & -\sigma & 2 \end{pmatrix}. \qquad (32)$$

The treatment of the decagonal case is now clearly analogous to Frank's treatment of the hexagonal case. Adding a sixth vector $\mathbf{e}_6$ perpendicular to the plane (*i.e.* along the axis of tenfold symmetry – the periodic direction) seems to be the most natural and relevant reference system for the underlying structure of these decagonal quasicrystals.

The complicated zone law analogous to (20) is now

$$k_i P^i_j u^j + k_6 u^6 = 0 \qquad (33)$$

with P given by (32). Written out in full, this is

$$\begin{aligned} &2(k_1u^1 + k_2u^2 + k_3u^3 + k_4u^4 + k_5u^5) \\ &\quad + (\tau - 1)(k_2u^1 + k_3u^2 + k_4u^3 + k_5u^4 + k_1u^5 + k_1u^2 + k_2u^3 \\ &\quad + k_3u^4 + k_4u^5 + k_5u^1) - \tau(k_3u^1 + k_4u^2 + k_5u^3 + k_1u^4 \\ &\quad + k_2u^5 + k_1u^3 + k_2u^4 + k_3u^5 + k_4u^1 + k_5u^2) + 5k_6u^6 \qquad (34) \end{aligned}$$

(Singh & Ranganathan, 1996).

2.4. The indexing scheme of Fitz Gerald

In spite of the close analogy with the hexagonal case, the problem of finding a satisfactory indexing scheme for decagonal quasicrystals raises problems that are absent from the hexagonal analogy. In the hexagonal case, the projection from four dimensions to three requires a splitting of the four-dimensional space into two orthogonal spaces, the three-space and a *one*-dimensional space perpendicular to it. Thus only *one* condition ($k_1 + k_2 + k_3 = 0$) is required to guarantee that the orthogonality condition for vectors in three dimensions is manifested in the three-dimensional subspace as the simple zone law, and to bring about the identity of the two kinds of index, the h_i of (10) and the k_i of (17).

For projection from six dimensions to three, the six-dimensional space is split into two orthogonal three-spaces, and *three* conditions are required. They are contained in the identity

$$\mathbf{h}Q = 0, \qquad (35)$$

where Q is the rank-3 matrix $I - P$. The indices h_i that satisfy the simple zone law

$$h_1u^1 + h_2u^2 + h_3u^3 + h_4u^4 + h_5u^5 + h_6u^6 = 0 \qquad (36)$$

are necessarily *irrational*, whereas the *integer* indices k_i satisfy the very complicated zone law (34).

Fitz Gerald *et al.* (1988) and Choy *et al.* (1988) devised a practical approach that avoids these difficulties. They were able to label the diffraction peaks in patterns associated with important zone axes of decagonal quasicrystals with sets of six *integer* indices k_i satisfying

$$k_1u^1 + k_2u^2 + k_3u^3 + k_4u^4 + k_5u^5 + k_6u^6 = 0. \qquad (37)$$

As is clear from our discussion, this is not a zone law; as pointed out by Fitz Gerald *et al.*, it 'looks superficially like' the simple zone law. The reciprocal vectors obtained from the indices k_i do not actually belong to the zone axis labelled by u^i. But they are surprisingly close – the vectors $\mathbf{k} = k_i\mathbf{e}^i$ and $\mathbf{u} = \mathbf{e}_iu^i$ tend to be nearly perpendicular.

We shall refer to the indexing scheme based on the *approximate zone law* (37) as the Fitz Gerald (FG) scheme.

Some insight into the possible reason for the effectiveness of the FG scheme has been provided by Singh & Ranganathan (1996), who showed that the complicated zone law (34) approaches condition (37), in a certain limit. A simple way of establishing this is to observe that

$$\tau\mathbf{e}_i = \mathbf{e}_j T^j_i,\ T = \begin{pmatrix} 0 & 0 & -1 & -1 & 0 \\ 0 & 0 & 0 & -1 & -1 \\ -1 & 0 & 0 & 0 & -1 \\ -1 & -1 & 0 & 0 & 0 \\ 0 & -1 & -1 & 0 & 0 \end{pmatrix}. \qquad (38)$$

Applying T repeatedly to $\mathbf{u} = \mathbf{e}_iu^i$ produces the inflationary sequence $\mathbf{u}$, $\tau\mathbf{u}$, $\tau^2\mathbf{u}, \ldots$. The corresponding sequence of indices, starting from [$1\,\bar{1}\,0\,0\,0$], is

$$\begin{array}{c} 1\,\bar{1}\,0\,0\,0 \\ 0\,0\,\bar{1}\,0\,1 \\ 1\,\bar{1}\,\bar{1}\,0\,1 \\ 1\,\bar{1}\,\bar{2}\,0\,2 \\ 2\,\bar{2}\,\bar{3}\,0\,3 \\ 3\,\bar{3}\,\bar{5}\,0\,5 \\ 5\,\bar{5}\,\bar{8}\,0\,8 \\ \ldots \end{array}$$

Each row is the sum of the two previous rows – hence the appearance of Fibonacci numbers. Since the ratio of two successive terms in the Fibonacci series 1, 1, 2, 3, 5, 8, 13, ... tends, in the limit, to τ, we deduce that the ratios $u^1 : u^2 : u^3 : u^4 : u^5$ of the indices in the above sequence tend, in the limit, to $1 : \bar{1} : \bar{\tau} : 0 : \tau$.

Now observe that $[u^1, u^2, u^3, u^4, u^5] = [1, \bar{1}, \bar{\tau}, 0, \tau]$ satisfies

$$P^j_iu^i = u^j. \qquad (39)$$

Thus, in the limit, the zone law (34) tends to the simpler law (37). This is for the inflationary sequence starting from [$1\,\bar{1}\,0\,0\,0$]. But, since P is a cyclic matrix, the same result will obviously hold starting from any cyclic permutations of [$1\,\bar{1}\,0\,0\,0$]. But then, *any* index set satisfying

$$u^1 + u^2 + u^3 + u^4 + u^5 = 0 \qquad (40)$$

is a linear combination of the cyclic permutations of [$1\,\bar{1}\,0\,0\,0$]. Hence the convergence of the complicated zone law to the simpler form is established for any inflationary sequence.

2.5. Redundancy of index sets

Fitz Gerald *et al.* and Choy *et al.* did not address the problem of non-uniqueness of indices in the FG scheme. The redundancy in the index sets $[u^1, u^2, u^3, u^4, u^5]$ and $(k_1, k_2, k_3, k_4, k_5)$ would appear at first sight to be a more serious problem than the corresponding problem for the hexagonal lattice. Changes in the index sets of the form

$$u^i \to u^i + Q^i_j m'^j, \quad k_i \to k_i + m_j Q^j_i, \tag{41}$$

where $Q = I - P$ have no effect on the indices

$$h_i = k_j P^j_i \tag{42}$$

and no effect on the zone law (33) (because $PQ = QP = 0$). However, for *rational* indices u^i or k_i the transformations (41) are to be restricted to the addition of a quintuple of rational numbers that are a linear combination of the rows (or columns) of Q. The only possibility is then

$$[u^1, u^2, u^3, u^4, u^5] \to [u^1 + m', u^2 + m', u^3 + m', u^4 + m', u^5 + m'], \tag{43}$$

$$(k_1, k_2, k_3, k_4, k_5) \to (k_1 + m, k_2 + m, k_3 + m, k_4 + m, k_5 + m) \tag{44}$$

with rational m, m'. So the analogy with the hexagonal case is preserved.

There are essentially just three reasonable ways of obtaining unique indexing from the FG scheme, corresponding to different choices of m (and/or m') in (43).

(I) *Five-index schemes*. The redundancy can be removed by employing only four of the five coplanar base vectors. This was suggested by Janssen (1988) and has been applied extensively (Yamamoto & Ishihara, 1988; Steurer, 1989; Steurer & Kuo, 1990; Steurer *et al.*, 1993). These authors employ a projection method to obtain the base vectors and the reciprocal base vectors, projecting from five dimensions to three dimensions. To simplify the presentation, we consider the projection from four dimensions to two dimensions, starting from the four dimensions whose unit cell is given by the four vectors whose Cartesian coordinates are the columns of

$$\frac{2}{5a}\begin{pmatrix} c_1 & c_2 & c_3 & c_4 \\ s_1 & s_2 & s_3 & s_4 \\ c_3 & c_1 & c_4 & c_2 \\ s_3 & s_1 & s_4 & s_2 \end{pmatrix} \tag{45}$$

[$c_r = \cos(2\pi r/5)$, $s_r = \sin(2\pi r/5)$]. Projection onto the two-dimensional subspace given by the first two rows gives the four reciprocal vectors ($\mathbf{e}^2$, $\mathbf{e}^3$, $\mathbf{e}^4$, $\mathbf{e}^5$), identical to those of the FG scheme. In the scheme adopted by Yamamoto and Steurer, the four base vectors for direct space (*i.e.* for zone-axis symbols) are obtained by projection of the lattice reciprocal to the lattice given by (45). This leads to a complication because the lattice is not a hypercubic lattice. The transposed inverse of (45) is

$$a\begin{pmatrix} c_1 - 1 & c_2 - 1 & c_3 - 1 & c_4 - 1 \\ s_1 & s_2 & s_3 & s_4 \\ c_3 - 1 & c_1 - 1 & c_4 - 1 & c_2 - 1 \\ s_3 & s_1 & s_4 & s_2 \end{pmatrix}, \tag{46}$$

so that the four planar base vectors in direct space are ($\mathbf{e}_2 - \mathbf{e}_1$, $\mathbf{e}_3 - \mathbf{e}_1$, $\mathbf{e}_4 - \mathbf{e}_1$, $\mathbf{e}_5 - \mathbf{e}_1$). The five-index schemes eliminate the non-uniqueness of the redundant six-axis scheme, but at the expense of obscuring the underlying decagonal structure. In a five-index scheme, symmetry-related vectors acquire indices that look totally different. From the above description, it is apparent that there are essentially five different five-index schemes (related to each other by the fivefold rotational symmetry) depending on which of the five planar pentagonal base vectors is discarded. The zone law is lost in these schemes.

(II) *The least path criterion (LPC)*. The LPC scheme proposed by Mukhopadhyay *et al.* (1989) is an alternative way of dealing with the problem of redundancy inherent in indexing schemes when the base vectors are linearly dependent. It solves the problem by setting one of the indices to zero, thus removing a redundant axis, but it is not always the same axis that is eliminated. LPC indexing minimizes $|k_1| + |k_2| + |k_3| + |k_4| + |k_5|$. As shown by Mukhopadhyay & Lord (2002), this is achieved by applying the transformation (44) with $-m$ equal to the integer that takes the middle position (*i.e.* the third position) when the k_i ($i = 1, \ldots, 5$) are arranged in numerical order. The LPC scheme has the advantage of providing unique indices while preserving the attractive feature of the FG system: that the symmetries of the decagonal structure are manifested in the indexing system simply by sign changes and permutations. The least path criterion can, of course, also be applied to the zone-axis symbols u^i. A disadvantage of the system is that, if both zone-axis indices and reciprocal indices are LPC, the simple zone law (37) is lost.

(III) *Frank indexing*. The unique indexing scheme proposed here is precisely analogous to the Miller–Bravais indexing of hexagonal lattices. Frank indices satisfy

$$k_1 + k_2 + k_3 + k_4 + k_5 = 0$$

[analogous to (23)]. This is achieved by a transformation (44) with $m = -(k_1 + k_2 + k_3 + k_4 + k_5)/5$ to the FG indices. To ensure that Frank indices are integers, this amounts to a multiplication of the six-integer sets by the matrix

$$M = \begin{pmatrix} 4 & -1 & -1 & -1 & -1 & 0 \\ -1 & 4 & -1 & -1 & -1 & 0 \\ -1 & -1 & 4 & -1 & -1 & 0 \\ -1 & -1 & -1 & 4 & -1 & 0 \\ -1 & -1 & -1 & -1 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 5 \end{pmatrix}. \tag{47}$$

This scheme has several advantages over the other two schemes: it respects the decagonal symmetry of the structure it is describing; the decagonal symmetries correspond simply to sign changes and permutations in the index sets; the validity of the simple approximate zone law (37) is assured because the identities $k_1 + k_2 + k_3 + k_4 + k_5 = 0$ and $u^1 + u^2 + u^3 + u^4 + u^5 = 0$ are the defining features of the Frank scheme.

3. Translation between indexing schemes

The five-index schemes used by Yamamoto & Ishihara (1988) and by Steurer and his co-workers (Steurer, 1989; Steurer & Kuo, 1990; Steurer *et al.*, 1993) originated from the formalism

Table 1
Important reflections observed in the powder X-ray diffraction pattern obtained from Al–Cu–Co decagonal quasicrystalline phases (Fig. 2).

The LPC, Steurer and Frank indices are displayed. The fundamental reciprocal constants for the Frank scheme are chosen to be the same as in the LPC scheme.

Label	d (nm)	Intensity (I/I_{max})	LPC indices	Frank indices	Steurer indices	Yamamoto indices
1	0.388	35	1, 0, −1, −1, 0, 0	−2, 3, −2, −2, 3, 0	1, 0, 0, 0, 0	0, 0, −1−1, 0
2	0.330	20	1, 1, −1, −1, 0, 0	5, −5, 5, −5, 0, 0	0, 1, −1, 0, 0	1, 0, 0, −1, 0
3	0.240	12	1, 0, −2, −2, 0, 0	4, −1, −1, −1, −1, 0	0, 0, −1, −1, 0	1, 0, −1, −1, 0
4	0.224	100	1, 0, −2, −2, 0, 2	4, −1, −1, −1, −1, 10	0, 0, −1, −1, 2	1, 0, −1, −1, 0
5	0.209	70	0, 0, 0, 0, 0, 4	0, 0, 0, 0, 0, 20	0, 0, 0, 0, 4	0, 0, 0, 0, 4
6	0.207	23	2, 1, −1, −2, 0, 0	0, 5, −5, 0, 0, 20	1, 0, 0, −1, 0	1, 1, −1, −1, 0
7	0.207	18	1, 1, −1, −1, 0, 4	5, −5, 5, −5, 0, 20	0, 1, −1, 0, 4	1, 0, 0, −1, 4
8	0.204	10	2, 0, −3, −3, 0, 0	6, −4, 1, 1, −4, 25	−1, 0, −1, −1, 4	1, 0, −2, −2, 4
9	0.190	12	2, 1, −1, −2, 0, 4	0, 5, −5, 0, 0, 20	1, 0, 0, −1, 4	1, 1, −1, −1, 4
10	0.175	14	3, 0, −3, −2, 2, 0	5, 0, −5, 0, 0, 0	0, −1, −2, −2, 0	1, −1, −3, −2, 0

Table 2
The peaks are identified on a diffraction pattern of the T6 decagonal phase $Al_{40}Mn_{25}Fe_{15}Ge_{20}$ (annealed at 1050 K for 100 h) from Yokoyama *et al.* (1997) (Fig. 3).

The fundamental reciprocal constants for the Frank scheme are chosen to be the same as in the LPC scheme.

Diffraction spots	d spacing (nm)	LPC indices	Frank indices	Steurer indices	Yamamoto indices
A	0.388	1, 0, −1, −1, 0, 0	−2, 3, −2, −2, 3, 0	1, 0, 0, 0, 0	0, 0, −1−1, 0
B	0.330	1, 1, −1, −1, 0, 0	5, −5, 5, −5, 0, 0	0, 1, −1, 0, 0	1, 0, 0, −1, 0
C	0.240	1, 0, −2, −2, 0, 0	4, −1, −1, −1, −1, 0	0, 0, −1, −1, 0	1, 0, −1, −1, 0
D	0.224	1, 0, −2, −2, 0, 2	7, −3, 2, −3, −3, 10	0, 1, −1, −1, 2	1, 0, −1, −1, 0
E	0.209	0, 0, −1, −1, 0, 5	6, −4, 1, 1, −4, 25	−1, 0, −1, −1, 5	1, 0, 0, 0, 5
F	0.207	1, 0, −2, −2, 0, 3	4, −1, −1, −1, −1, 15	0, 0, −1, −1, 3	1, 0, −1, −1, 3
G	0.207	0, 0, 0, 0, 0, 6	0, 0, 0, 0, 0, 30	0, 0, 0, 0, 6	0, 0, 0, 0, 6
H	0.204	2, 1, −1, −2, 0, 0	0, 5, −5, 0, 0, 0	1, 0, 0, −1, 0	1, 1, −1, −1, 0
I	0.190	1, 0, −2, −2, 0, 4	4, −1, −1, −1, −1, 20	0, 0, −1, −1, 4	1, 0, −1, −1, 4
J	0.175	1, −1, 1, −1, 0, 6	−15, 25, −25, 15, 0, 30	2, −3, 3, −2, 6	−1, 2, −2, 1, 6
K	0.148	2, 0, −3, −3, 2, 0	16, −4, −9, 11, −14, 0	−3, −2, −3, −5, 0	3, 0, −2, 0, 0
L	0.145	2, 1, −1, −2, 0, 6	0, 5, −5, 0, 0, 30	1, 0, 0, −1, 6	1, 1, −1, −1, 6
M	0.127	1, 3, 0, −4, −3, 5	4, 4, −1, −1, −6, 25	1, 2, 1, −1, 5	3, 4, 2, 0, 5
N	0.126	3, 2, −2, −3, 0, 0	5, 0, 0, −5, 0, 0	1, 1, −1, −1, 0	2, 1, −1, −2, 0
O	0.120	2, 0, −4, −4, 0, 0	8, −2, −2, −2, −2, 0	0, 0, −2, −2, 0	2, 0, −2, −2, 0
P	0.107	3, 2, −2, −3, 0, 6	5, 0, 0, −5, 0, 30	1, 1, −1, −1, 6	2, 1, −1, −2, 6

developed by Janssen (1988). These schemes are derived by projection from a five-dimensional non-orthogonal lattice onto a three-dimensional subspace in order to generate the real- and reciprocal-space structures. It is not at all straightforward, using these schemes, to understand the symmetry-related planes and directions and to interpret the experimental electron and X-ray diffraction patterns. The Frank indexing scheme we have proposed, being analogous to the hexagonal system, has the advantage of bringing out clearly the symmetry-related planes and directions and also providing a simple zone-axis rule which is not possible in other indexing schemes. It is, clearly, important to be able to convert indices between different schemes.

A five-index scheme of the kind employed by Yamamoto & Ishihara or by Steurer and co-workers can be converted to a six-index scheme by simply inserting an extra index, equal to zero, thus $(k_1, k_2, k_3, k_4, k_6) \rightarrow (k_1, k_2, k_3, k_4, 0, k_6)$. The purpose of this is to facilitate the various rules for translating between the different indexing schemes. We can now convert FG, five-index schemes or LPC indices to a Frank indexing scheme simply by multiplying by the matrix M shown in (47). An alternative statement of this rule is: calculate $m = (k_1 + k_2 + k_3 + k_4 + k_5)$, multiply the indices by 5 and then subtract m from the first five indices.

Since M is singular, there is no inverse matrix that can be used to translate from Frank indexing to LPC or to a five-index scheme. However, an index set satisfying the 'least path criterion' obtained from a Frank index set $(k_1, k_2, k_3, k_4, k_5, k_6)$ is $(k_1 - m, k_2 - m, k_3 - m, k_4 - m, k_5 - m, k_6)$, where m is the middle number when the integers k_1, k_2, k_3, k_4, k_5 are arranged in numerical order. *The resulting indices will then have a common factor 5*, which is to be divided out. Similarly, to convert from Frank indexing to a five-index scheme in which, say, the base vector $\mathbf{e}^5$ is missing, we choose $m = k_5$. Again, the resulting indices have a common factor 5, which is to be divided out.

A difficulty arises when comparing the indexing of X-ray diffraction patterns of quasicrystals given by different authors, over and above the question of different choices of base vectors. This is the phenomenon of inflation and deflation. The

Table 3
Indexing of pseudo-fivefold zone axis of T_6 decagonal phase {pattern I, zone axis [3, −8, −8, 3, 10, 1] of Choy *et al.* (1988)}.

Labels correspond to the diffraction spots marked in Fig. 4(*a*). Labels are the same as those of Choy *et al.* (1988). The fundamental reciprocal constants for the Frank scheme are chosen to be the same as in the Fitz Gerald scheme.

Rel-vector label	Fitz Gerald indices	Frank indices	LPC indices	Steurer indices	Yamamoto indices
9	1, −1, 1, −1, 0, 0	5, −5, 5, −5, 0, 0	1, 1, −1, −1, 0, 0	0, 1, −1, 0, 0	1, 0, 0, −1, 0
21	0, 1, −1, 0, 0, 0	10, 5, −5, 0, 0, 0	2, 1, −1, −2, 0, 0	1, 0, 0, −1, 0	1, 1, −1, −1, 0
10	0, 0, −1, 0, −1, 2	2, 2, −3, 2, −3, 10	1, 1, 0, −1, 0, 2	0, 0, 0, −1, 2	1, 1, 0, 0, 2
26	1, −1, 0, −1, −1, 2	7, −3, 2, −3, −3, 10	2, 2, −1, −2, 0, 2	0, 1, −1, −1, 2	2, 1, 0, −1, 2
7	0, −1, 1, −1, 0, 3	1, −4, 6, −4, 1, 15	−1, 0, 0, 0, −1, 3	0, 1, 0, 1, 3	0, 0, 1, 0, 3
8	−1, 1, −1, 0, 0, 3	−4, 6, −4, 1, 1, 15	0, 0, 0, −1, −1, 3	1, 0, 1, 0, 3	0, 1, 0, 0, 3
20	0, 0, 0, −1, 0, 3	1, 1, 1, −4, 1, 15	2, 2, 0, −1, 0, 3	1, 1, 0, 0, 3	1, 1, 0, −1, 3
17	0, 1, 0, 1, 0, 5	−2, 3, −2, 3, −2, 25	−1, 0, 1, 0, −1, 5	0, 0, 1, 0, 5	0, 1, 1, 1, 5
18	1, 0, 1, 0, 0, 5	3, −2, 3, −2, −2, 25	0, 1, 0, −1, −1, 5	0, 1, 0, 0, 5	1, 1, 1, 0, 5
42	1, 1, 0, 0, 0, 5	3, 3, −2, −2, −2, 25	3, 3, 0, −2, 0, 5	1, 1, 0, −1, 5	2, 2, 0, −1, 5
39	0, 0, 1, 0, 0, 8	−1, −1, 4, −1, −1, 40	−2, 0, 1, 0, −2, 8	0, 1, 1, 1, 8	0, 1, 2, 1, 8
40	0, 1, 0, 0, 0, 8	−1, 4, −1, −1, −1, 40	0, 1, 0, −2, −2, 8	1, 1, 1, 0, 8	1, 2, 1, 0, 8
Zone axis	3, −8, −8, 3, 10, 1	3, −8, −8, 3, 10, 1	1, −2, −2, 1, 2, 1	2, −5, −5, 2, 1	1, −3, −3, 1, 1

Table 4
Indexing of pseudo-threefold zone axis [8, −21, −21, 8, 26, 1] of Choy *et al.* (1988).

Labels correspond to the diffraction spots marked in Fig. 4(*b*). Labels are the same as those of Choy *et al.* (1988). The fundamental reciprocal constants for the Frank scheme are chosen to be the same as in the Fitz Gerald scheme.

Rel-vector label	Fitz Gerald indices	Frank indices	LPC indices	Steurer indices	Yamamoto indices
9	1, −1, 1, −1, 0, 0	5, −5, 5, −5, 0, 0	1, 1, −1, −1, 0, 0	0, 1, −1, 0, 0	1, 0, 0−1, 0
21	0, 1, −1, 0, 0, 0	0, 5, −5, 0, 0, 0	2, 1, −1, −2, 0, 0	1, 0, 0, −1, 0	1, 1, −1, −1, 0
2	2, −1, 1, 1, −1, 2	8, −7, 3, 3, −7, 10	−1, 0, 0, 0, 0, 2	−2, 0, −1, −1, 2	1, 0, 1, 1, 2
5	−1, 1, 0, 0, 1, 3	−6, 4, −1, −1, 4, 15	0, 0, 1, 1, 0, 3	1, 0, 1, 1, 3	−1, 0, 0, 0, 3
6	0, 0, 1, −1, 1, 3	−1, −1, 4, −6, 4, 15	0, 0, −1, −1, 1, 3	1, 1, 0, 1, 3	0, 0, 0, −1, 3
32	0, 1, 0, −1, 1, 3	−1, 4, −1, −6, 4, 15	3, 2, −1, −2, 0, 3	2, 1, 0, 0, 3	1, 1, −1, −2, 3
15	0, −1, 0, 0, −1, 5	2, −3, 2, 2, −3, 25	−1, 0, 1, 1, 0, 5	−1, 0, 0, 0, 5	0, 0, 1, 1, 5
16	0, 0, −1, 0, −1, 5	2, 2, −3, 2, −3, 25	1, 1, 0, −1, 0, 5	0, 0, 0, −1, 5	1, 1, 0, 0, 5
37	−1, 0, 0, 0, 0, 8	−4, 1, 1, 1, 1, 40	−1, 0, 2, 2, 0, 8	0, 0, 1, 1, 8	−1, 0, 1, 1, 8
29	0, −1, 1, −1, 0, 8	1, −4, 6, −4, 1, 40	−1, 0, 0, 0, −1, 8	0, 1, 0, 1, 8	0, 0, 1, 0, 8
30	−1, 1, −1, 0, 0, 8	−4, 6, −4, 1, 1, 40	0, 0, 0, −1, −1, 8	1, 0, 1, 0, 8	0, 1, 0, 0, 8
38	0, 0, 0, −1, 0, 8	1, 1, 1, −4, 1, 40	2, 2, 0, −1, 0, 8	1, 1, 0, 0, 8	1, 1, 0, −1, 8
Zone axis	8, −21, −21, 8, 26, 1	8, −21, −21, 8, 26, 1	2, −5, −5, 2, 6, 1	5, −13, −13, 5, 1	3, −8, −8, 3, 1

five planar base vectors in the systems mentioned here satisfy $\tau\mathbf{e}_1 = -\mathbf{e}_3 - \mathbf{e}_4$ *etc.*, where $\tau = (1 + \surd 5)/2$. Thus, for example, the indexing used by Yamamoto and that used by Steurer differ by τ-inflation. To convert Steurer indices to the corresponding Yamamoto indices, the τ-inflation matrix T given in equation (38) acts on the first five indices. Thus, a Steurer index $(k_1, k_2, k_3, k_4, 0, k_6)_{\rm S}$ becomes $(k'_1, k'_2, k'_3, k'_4, k'_5, k_6) = (-k_3 - k_4, -k_4, -k_1, -k_1 - k_2, -k_2 - k_3, k_6)$. If the new fifth index is not zero, it is to be subtracted out; $(k_1, k_2, k_3, k_4, 0, k_6)_{\rm Y} = (k'_1 - k'_5, k'_2 - k'_5, k'_3 - k'_5, k'_4 - k'_5, 0, k_6)$.

In the tables, LPC indices are obtained directly from the FG indices by τ^3 inflation followed by subtracting out the ‘middle index’. The Steurer indices are derived from FG by a τ inflation, followed by a subtracting out of one of the indices (for the sake of this demonstration, we have chosen k_5). From FG to the Yamamoto indices requires τ^2 inflation as the scaling constants in reciprocal space are related accordingly (*i.e.* the way the fundamental reciprocal-lattice vector is chosen).

The rules governing the various interconversions of the indices of reciprocal vectors displayed in the tables should now be clear. The interconversion of the *zone-axis* symbol involves, of course, a τ^{-1} deflation whenever a τ inflation is applied to the reciprocal indices. Conversion of a zone-axis symbol from a six-index scheme to a five-index scheme involves an additional complication because of the peculiar relation between the base vectors in direct space, for these two kinds of scheme. Let $\mathbf{e}_i$ ($i = 1, \ldots, 6$) be the base vectors in direct space in the FG scheme. Then the base vectors in a five-index scheme of the kind employed by Yamamoto and Steurer are

$$\mathbf{e}_1 - \mathbf{e}_5, \mathbf{e}_2 - \mathbf{e}_5, \mathbf{e}_3 - \mathbf{e}_5, \mathbf{e}_4 - \mathbf{e}_5, \mathbf{e}_6. \qquad (48)$$

On account of the identity $\mathbf{e}_5 = -\mathbf{e}_1 - \mathbf{e}_2 - \mathbf{e}_3 - \mathbf{e}_4$, it follows that, if $[u^1, u^2, u^3, u^4, u^5, u^6]$ is a zone-axis symbol in the FG, suitably deflated, the corresponding symbol in the five-index system will be $[w^1, w^2, w^3, w^4, w^6]$, where

$$\begin{pmatrix} u^1 - u^5 \\ u^2 - u^5 \\ u^3 - u^5 \\ u^4 - u^5 \end{pmatrix} = \begin{pmatrix} 2 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 2 & 1 \\ 1 & 1 & 1 & 2 \end{pmatrix} \begin{pmatrix} w^1 \\ w^2 \\ w^3 \\ w^4 \end{pmatrix} \tag{49}$$

and hence

$$\begin{pmatrix} 5w^1 \\ 5w^2 \\ 5w^3 \\ 5w^4 \end{pmatrix} = \begin{pmatrix} 4 & -1 & -1 & -1 \\ -1 & 4 & -1 & -1 \\ -1 & -1 & 4 & -1 \\ -1 & -1 & -1 & 4 \end{pmatrix} \begin{pmatrix} u^1 - u^5 \\ u^2 - u^5 \\ u^3 - u^5 \\ u^4 - u^5 \end{pmatrix}. \tag{50}$$

For example, to translate the FG zone-axis symbol [3, −8, −8, 3, 10, 1] to a Steurer symbol, first carry out the τ^{-1} deflation: [3, −8, −8, 3, 10] → [2, −5, −5, 2, 6]. Subtract out u^5, [2, −5, −5, 2, 6] → [−4, −11, −11, −4] and apply the matrix given in (50): [−4, −11, −11, −4] → [10, −25, −25, 10]. Finally, divide by the common factor 5; we get the zone-axis symbol [2, −5, −5, 2, 1].

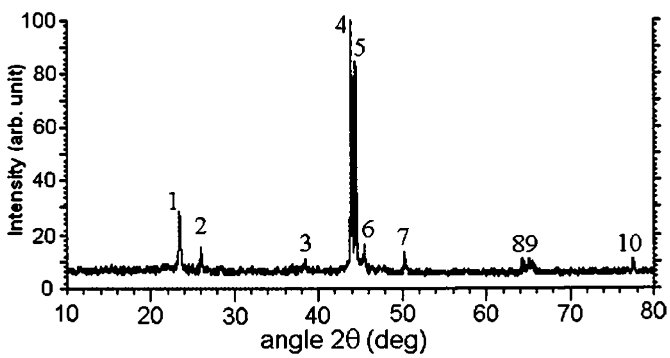

Figure 2
XRD pattern of the T4 DQC phase of Al–Cu–Co alloy. For indices of the labelled peaks refer to Table 1.

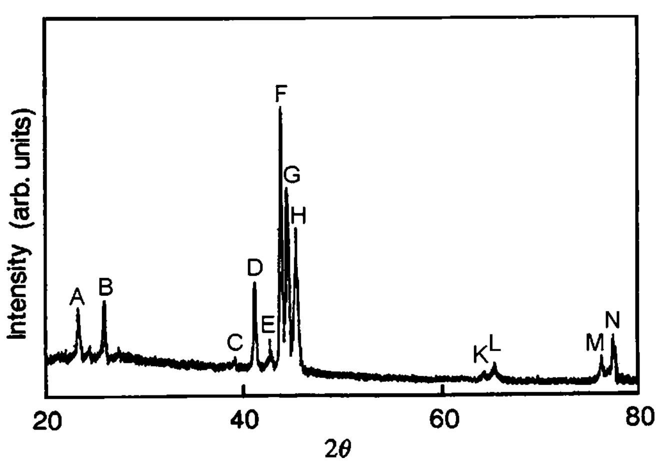

Figure 3
XRD pattern of the T6 DQC phase of $Al_{40}Mn_{25}Fe_{15}Ge_{20}$ alloy annealed at 1050 K for 100 h, from Yokoyama *et al.* (1997). Labelling of the peaks is in accordance with Takeuchi & Kimura (1987); the indices of these peaks are given in Table 2. Reprinted with permission from Yokoyama *et al.* (1997). Copyright (1997) Japanese Journal of Applied Physics.

4. Experimental results and discussions: diffraction patterns (XRD & EDP and ZAPM)

We have indexed the peaks of the T4 DQC phase of Al–Cu–Co (Fig. 2) and those of the T6 DQC phase of Al–Mn (Fig. 3). The labelling of the latter is from Takeuchi & Kimura (1987) [identified on an Al–Mn–Fe–Ge DQC pattern from

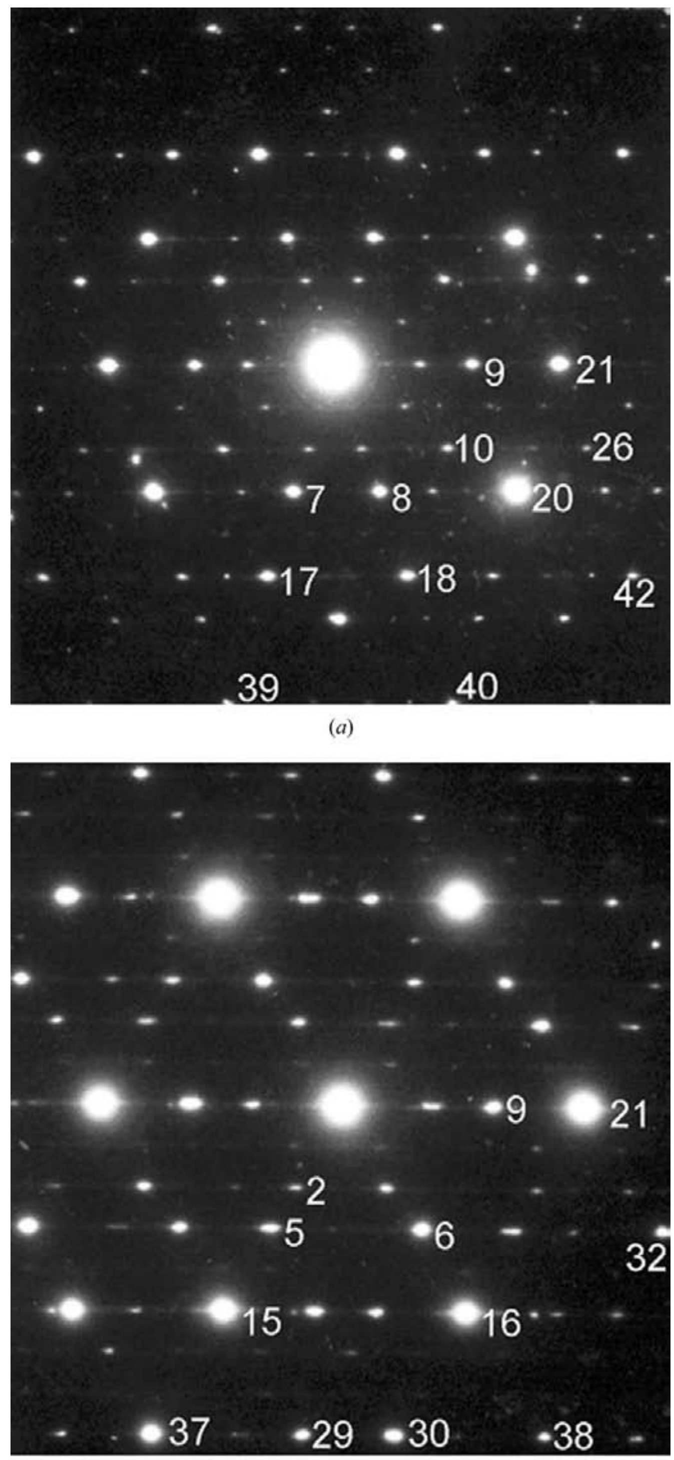

Figure 4
(*a*) Pseudo-fivefold pattern and (*b*) pseudo-threefold pattern from the Al–Mn system. For indices of the labelled spots refer to Tables 3 and 4.

Yokoyama *et al.* (1997) (Fig. 3)] based on both LPC and MB indices and displayed in Tables 1 and 2, respectively. Selected-area diffraction patterns displaying pseudo-fivefold and pseudo-threefold patterns (Figs. 4*a*, *b*) from a DQC of the Al–Mn system with 1.2 nm period are indexed. The corresponding indices are displayed in Tables 3 and 4. The same labels as those used by Choy *et al.* (1988) are used, for easy comparison of all indices.

5. Conclusions

Non-uniqueness of indices is a consequence of redundancy in a reference system and presents special problems. We have examined these problems in some detail in the case of decagonal quasicrystals, with particular emphasis on the analogy between hexagonal crystals and decagonal quasicrystals. The analogy naturally suggests a 'Frank indexing scheme' analogous to the Miller–Bravais indexing for hexagonal crystals as a way of dealing with the problem of non-uniqueness. As in the hexagonal case, the scheme arises naturally from a cubic lattice in higher-dimensional space. The analogy, however, fails to provide a simple zone law that is satisfied exactly by integer indices – the reason for this has been clarified. However, the simple approximate zone law used by Choy *et al.* is inherited by the Frank scheme. That different authors use different indexing schemes is an obstacle to the comparison of results. This is a problem of importance to experimentalists, which has not received much attention in the literature. Methods of translating between several important indexing schemes have been presented and the advantages of the six-index Frank scheme for indexing decagonal quasicrystals have been emphasized: it respects the symmetry of the structure it describes, it provides unique indices, and the simple approximate zone law is valid.

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