image may be regarded as the selection of a right-handed coordinate system compatible with a rotation.

These group-theoretical considerations justify the results of Jones (1986).

4. Practical procedure

In fact the ambiguities are handled by measuring a suitable physical property that specifies the allowed object as far as possible. As crystal structures are usually determined by diffraction experiments it is convenient to use properties derivable from X-ray diffraction data.

In the case of paramorphic merohedries the structure-factor moduli can be used for fixing the ambiguity of the description. The operation R_i (rotation 2 or mirror m) that is used for the construction of the characteristic coset correlates pairs of structure factors. The ratio q of their moduli changes to $1/q$ with the transformation to the other image.

In the case of non-centrosymmetric structures properties must be regarded that are sensitive to structure-factor phases. This can be done by comparing the moduli of Friedel pairs affected by anomalous dispersion or by measuring suitable triplet phases. For enantiomorphic merohedries this means the determination of the absolute configuration (for chiral species) or conformation (for achiral species). For hemimorphic and roto-inversional merohedries this means fixing the ambiguity in the description: The operation $\bar{1}$ correlates the sign of suitable triplet phases or the moduli of suitable Friedel pairs of structure factors; their values change with the transformation to the other image.

As a consequence of these considerations two types of absolute structures can be distinguished. An absolute structure can be determined by experiment in the case of enantiomorphic merohedries because left-handed coordinate systems are excluded. In the case of non-enantiomorphic merohedries an absolute structure is uniquely determined by the selection of one description among different equivalent possibilities. The difference in the two cases corresponds to the special role of chiral properties.

The transfer of these terms to space groups and crystal structures is proposed, because these considerations do not only affect problems of crystal structure determination but also problems in structure description and standardization. The extension on *klassengleiche* subgroup relations will, however, need further discussions.

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Penrose Patterns and Related Structures. I.
Superstructure and Generalized Penrose Patterns

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Abstract

The section method is applied to derive the Penrose pattern and related patterns with a ten- or fivefold axis. These are derived from a four-dimensional decagonal crystal or from a five-dimensional icosahedral crystal as a two-dimensional section. The two descriptions correspond to the three- and four-dimensional ones in the usual superstructure and the Penrose pattern can be regarded as the superstructure in the four-dimensional space. The diffraction intensities and symmetries of these patterns are dis-

cussed. The present study indicates that the point group in the quasicrystals is noncrystallographic but $(m+d)$-reducible similarly to that in incommensurate structures, where m and d are the dimension of the real space and the orthogonal complement to it.

1. Introduction

Since the discovery of the icosahedral quasicrystal in Al–Mn alloys (Schechtmann, Blech, Gratias & Cahn, 1984), much experimental and theoretical work has resulted in the discovery of a new type of quasicrystal found in Al–Mn and Al–Fe alloys (Bendersky, 1985; Chattopadhyay, Lele, Ranganathen, Subbana & Thangaraj, 1985; Fung, Yang, Zhou, Zhao, Zhan & Shen, 1986). This has a tenfold axis and the structure is periodic along the axis. In this so-called decagonal phase, the diffraction pattern normal to the tenfold axis is similar to that of the Penrose pattern (see Yamamoto & Ishihara, 1988). This suggests that the structure projected along the axis is closely related to the distribution of the vertices in the Penrose or generalized Penrose pattern. As is known for the icosahedral quasicrystal, the vertex model explains the characteristic feature of the diffraction pattern (Duneau & Katz, 1985; Katz & Duneau, 1986; Elser, 1986) but the real structure may not be obtained by simple decoration from the vertex model (Ishihara & Shingu, 1986). However, it plays an important role in the investigation of the structure of the icosahedral phase. Therefore, we consider the vertex model as a preliminary to the structure determination of the decagonal phase. In this paper, the theoretical insight of the two-dimensional (2D) Penrose pattern and related structures is given. Based on this consideration, the structure of the decagonal phase will be considered by Yamamoto & Ishihara (1988).

There are several methods of obtaining the Penrose pattern. We discuss two methods in this paper which are modifications of the projection method developed by de Bruijn (1981), Kramer & Neri (1984), Kalugin, Kitayev & Levitov (1985), Duneau & Katz (1985) and Elser (1986). In one method, the structure is obtained from a 4D decagonal crystal (Janssen, 1986), while in the other the same structure is obtained from a 5D icosahedral crystal (Henley, 1986). In both methods, the structure is given by a 2D section of a higher-dimensional crystal. We call this method the section method. This is convenient for considering the relation of the quasicrystal and the modulated structure because the latter is known to be given by a 3D section of a higher-dimensional crystal and the superspace approach is available to both cases on the same basis.

The symmetry of a quasicrystal is described by a superspace group. For the Penrose pattern, it is given by a 4D superspace group (Janssen, 1986). This is understandable from the fact that the 4D description is possible as mentioned above. On the other hand,

the 5D description makes us imagine the higher-dimensional description of the commensurately modulated structure (superstructure) (Yamamoto, 1982a, b). In this paper, we show that the two methods mentioned above are equivalent and the relation between these two corresponds to that of the usual description in the 3D space and the higher-dimensional one in the superstructure. Thus the situation is analogous to the superspace approach to the superstructure. From this and for other reasons mentioned later, we can recognize that the Penrose pattern is a superstructure in the 4D space. In the (usual) superstructure, even if we fix the modulation function, the structure depends on the phase of the modulation wave. In other words, it depends on the position of the section in the superspace. Consequently, its symmetry also depends on the section. A similar situation exists in the Penrose pattern and the peculiar properties appearing in this pattern and the related structures mentioned below are understandable by analogy with the superstructure.

The section method is convenient for calculating the structure factor of the Penrose pattern as in the projection method (Zia & Dallas, 1985; Duneau & Katz, 1985; Elser, 1986). The structure factor observed in real space is regarded as the projection of the Fourier spectra in the higher-dimensional space. The structure factor is easily obtained by this method. It is shown, however, that there are an infinite number of structures giving diffraction patterns similar to each other, which are called the generalized Penrose patterns. These are obtained from the same 5D crystal by taking different sections. We discuss why the generalized Penrose patterns give similar diffraction patterns in analogy with the superstructure and clarify the change of 4D symmetry with the selection of the section.

The arrangement of the paper is as follows. We discuss the relation between the usual and higher-dimensional descriptions in 1D superstructures in § 2. The derivation of the generalized Penrose patterns from a 5D crystal is described in § 3. In § 4, the 4D description and the relation with the 5D one are shown and the symmetry of the generalized Penrose pattern is discussed. The structure factor is easily obtained by both methods. The structure-factor formulas in 4D and 5D descriptions and their interrelation are discussed in § 5. The higher-dimensional description of the superstructure in the 3D space is extended to a more general case in § 6. Finally, the necessary condition for the superspace group describing the symmetry of quasicrystals is discussed in § 7.

2. Superspace approach to the superstructure

It is known that the incommensurately modulated structure is conveniently described in the superspace and its symmetry is specified by a superspace group

(de Wolff, 1974; Janner & Janssen, 1977, 1979). On the other hand the commensurately modulated structure (superstructure) is described in the 3D space. However, the superspace approach is also applicable to the superstructure and for some purposes this is more convenient than the ordinary treatment (Yamamoto, 1982a, b). We review the superspace approach to the superstructure in this section for latter discussions. Consider the superstructure in a 1D lattice for simplicity. This is described in the 2D space. An example is shown in Fig. 1. This has a sinusoidal modulation with wave vector $\mathbf{k} = \mathbf{a}^*/3$ (Fig. 1b). In the superspace approach the real structure is given as a section of a higher-dimensional crystal (Fig. 1a). The real space is called the external space and its orthogonal complement the internal space. The external and internal spaces are horizontal and vertical lines in this case. As is clear from the figure, the unit cell in the external space is triplicated owing to the existence of the displacive modulation. It is noted that the structure and its symmetry depend on the position of the section for a given modulation wave. For example, along the thick and dotted lines the 1D structure has an inversion point while any line between them breaks the inversion symmetry.

The 2D crystal in Fig. 1(a) gives the diffraction pattern shown in Fig. 1(b). The structure factor is given by the Fourier transformation of the crystal,

$$F(hk) = \int_0^1 \exp\left[2\pi i(hx + ky)\right] dt, \qquad (1)$$

where the coordinates of the string atom x and y are a sinusoidal function of t with amplitude u,

$$x = u \sin(2\pi t), \qquad y = (u/3) \sin(2\pi t) + t. \qquad (2)$$

On the other hand, the 1D section of this crystal gives the structure factor obtained from the 2D one by projection along the internal space. This is due to a property of the Fourier transformation. An infinite
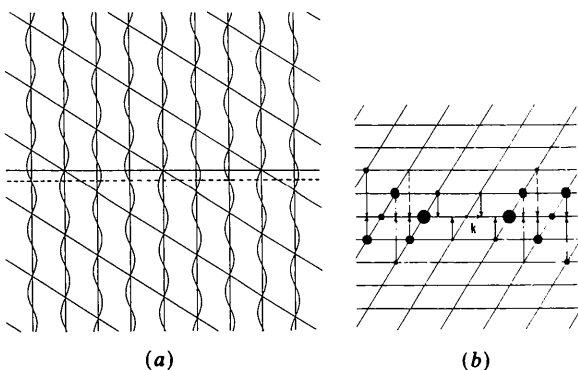

(a)   (b)

Fig. 1. Two-dimensional description of the superstructure in the one-dimensional lattice. (a) The superstructure is given as a section of the two-dimensional crystal, while the structure factor is obtained from (b) the Fourier spectra of the two-dimensional crystal by the projection normal to the external space.

number of reflections superimpose on the same point in the projection. For any integer n, hk and $h-n, k+3n$ are superimposed by the projection. The projected reflection is uniquely specified by hk within the range $-1 \le k \le 1$. The main reflection has $k = 0$ while the satellite reflection is specified by $k = \pm 1$. The structure factor of the 1D superstructure is given by the summation of the structure factor $F(h-n, k+3n)$ over n. Using the expression for the periodic δ function with period $\frac{1}{3}$, $\sum_n \exp(6\pi i n t) = \Delta(t)/3$, we have

$$\hat{F}(hk) = \frac{1}{3} \sum_{\nu=0}^{2} \exp\left[2\pi i(hx_\nu + ky_\nu)\right] \qquad (3)$$

for the hk $(-1 \le k \le 1)$ reflection in the 1D space, where x_ν, y_ν are the coordinates at $t = t_0 + \nu/3$. The position of the section is determined by t_0. The projected structure factor (3) depends on t_0. This reflects the fact that the real structure is different depending on the position of the section. Noting that $y_\nu = x_\nu/3 + t_0 + \nu/3$, we observe that (3) is the ordinary structure-factor formula for the superstructure. As is usually the case if the amplitude u is small, the structure factor $F(hk)$ for a reflection with large k gives a weak intensity. Then the main and satellite reflections, $\hat{F}(h0)$, $\hat{F}(h \pm 1)$, are well approximated by $F(h0)$ and $F(h \pm 1)$, which are independent of t_0. Therefore, when the amplitude u is small the structure factor of the commensurately modulated structure with a fixed modulation wave gives almost the same intensity for the structure at any section. A similar situation appears in the generalized Penrose patterns as shown below.

3. Derivation of generalized Penrose patterns from R^5

The mathematical derivation of quasi-periodic patterns has been introduced by de Bruijn (1981) and developed by several authors (Kramer & Neri, 1984; Kalugin et al., 1985; Duneau & Katz, 1985; Elser, 1986). This procedure, called the projection method, is briefly reviewed here for comparison with the section method used in this paper. When the cubic lattice in the n-dimensional space R^n is spanned by the orthogonal unit vectors $\mathbf{d}_i$ ($i = 1, 2, \ldots, n$) and the two subspaces R^m and R^{n-m} are given, the unit vectors $\mathbf{d}_i$ can be decomposed into two vectors $\mathbf{p}_i$ and $\mathbf{q}_i$ by the projection on the subspace R^m and its complementary subspace R^{n-m}. The quasiperiodic pattern in R^m is obtained by the following procedure. For the lattice point $\mathbf{r} = \sum_{i=1}^{n} h_i \mathbf{d}_i$ in R^n, we project $\mathbf{r}$ into R^m if its R^{n-m} components $\mathbf{t} = \sum_i h_i \mathbf{q}_i$ exist inside the volume $V = \{\sum_i \lambda_i \mathbf{q}_i | 0 < \lambda_i < 1\}$. We take $V = \{\sum_i \lambda_i \mathbf{q}_i | -\frac{1}{2} < \lambda_i - \gamma_i < \frac{1}{2}\}$ hereafter for the sake of comparison with the section method mentioned below, where γ_i are real numbers. Then the original V corresponds to the case of $\gamma_i = \frac{1}{2}$ for all i. The projected points $\mathbf{s} = \sum_i h_i \mathbf{p}_i$ form a quasi-periodic pattern in R^m

when the subspaces are appropriately chosen. The condition for the selection of subspaces giving rise to the quasi-periodic lattice has been discussed by Gahler & Rhyner (1986).

We introduce other orthogonal unit vectors a_i of which the first m vectors span R^m and the remaining $n - m$ ones span its orthogonal complement R^{n-m}. We call these two the external and internal spaces according to the terminology of the superspace group theory. The coordinates r_i referred to d_i are related to the new ones (x_i to a_i) by the orthogonal transformation $r_i = \sum_j M_{ij}x_j$. The unit vectors d_i are also related to a_i by the same relation because of the orthogonality of the matrix. The orthogonal matrix M defines the subspaces. The vectors p_i and q_i are then given by $\sum_{j=1}^{m} M_{ij}a_j$ and $\sum_{j=m+1}^{n} M_{ij}a_j$.

This method is equivalent to the section method mentioned here. In the latter, we place at $\sum_i \gamma_i q_i$ in the unit cell in R^n the 'atom' spreading only in the internal space R^{n-m}, the shape of which is given by $V = \{\sum_i \lambda_i q_i | -\frac{1}{2} < \lambda_i - \gamma_i < \frac{1}{2}\}$. The quasi-periodic pattern is given by an m-dimensional section of such a crystal in R^n.

An example of the equivalence of these two methods is given for a 1D quasi-crystal. In particular we consider the Fibonacci chain. This corresponds to the case of $n = 2$ and $m = 1$ in the projection method mentioned above. It is given by the matrix, M,

$$\frac{1}{(1+\tau^2)}\begin{pmatrix} \tau & -1 \\ 1 & \tau \end{pmatrix}, \qquad (4)$$

where τ is the golden ratio $(1+\sqrt{5})/2$ (Janssen, 1986). In this case, V is the vertical line within the range from $(1-\tau)/2\sqrt{(1+\tau^2)}$ to $(-1+\tau)/2\sqrt{(1+\tau^2)}$ provided that $\gamma_1 = \gamma_2 = 0$ for simplicity (see Fig. 2). The

projection method states that if lattice points exist between the two horizontal lines with interval V (A and B in Fig. 2), such points are projected along the vertical line. Thus we have a quasi-periodic pattern on the 1D space. On the other hand, the section method places the vertical bar with length V at each lattice point and takes a section on the horizontal line. This gives the same point configuration as that of the projection method when we take a section through the origin. It can be shown that the more general case with $\gamma_i \neq 0$ corresponds to the section through $\sum_i \gamma_i q_i$. If we call the volume V placed at each lattice point an atom and the structure obtained the crystal, we can say that the Fibonacci chain is given as a 1D section of the 2D crystal with a string atom at each lattice point of the square lattice. Hereafter we use the section method.

We consider the Penrose pattern. This is obtained from the rhombic–icosahedral atom defined by $V = \{\sum_i \gamma_i q_i | -\frac{1}{2} < \lambda_i < \frac{1}{2}\}$ located at the lattice point of the hypercubic lattice in R^5 (Henley, 1986) (see Fig. 3). The two subspaces are defined by the matrix M with elements

$$\sqrt{(2/5)}\begin{pmatrix} c_1 & s_1 & c_2 & s_2 & 1/\sqrt{2} \\ c_2 & s_2 & c_4 & s_4 & 1/\sqrt{2} \\ c_3 & s_3 & c_1 & s_1 & 1/\sqrt{2} \\ c_4 & s_4 & c_3 & s_3 & 1/\sqrt{2} \\ 1 & 0 & 1 & 0 & 1/\sqrt{2} \end{pmatrix}, \qquad (5)$$

where $c_j = \cos(2\pi j/5)$ and $s_j = \sin(2\pi j/5)$ ($j = 1, 2, \ldots, 5$). This corresponds to the case of $n = 5$ and $m = 2$ in the projection method. The 5D lattice has a period in the 3D internal space. All the lattice points are on the planes normal to a_5 with the interval $1/\sqrt{5}$. In this case the structure in the external space depends on the position of the section along a_5 as is inferred
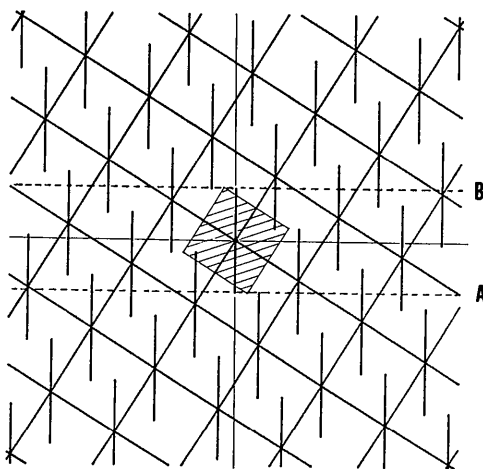

Fig. 2. Fibonacci chain. This is obtained from the two-dimensional square lattice by projecting along the internal space when a lattice point is between the two lines A and B (projection method) or by taking a section of the crystal with the string atom at the horizontal line (section method).
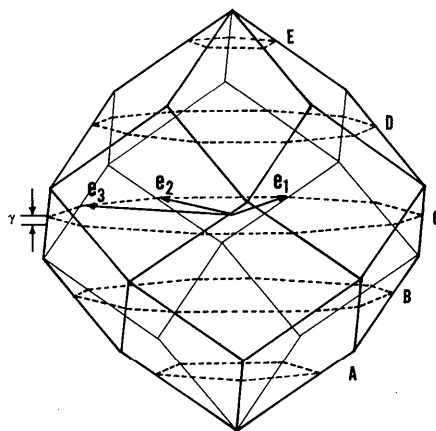

Fig. 3. Rhombic-icosahedral atom. The Penrose pattern is derived from the crystal in which the atom is placed at each lattice point of the five-dimensional hypercubic lattice. A, B, C, D, E correspond to $\nu = -2, -1, 0, 1, 2$. (See text.)

from the analogy with the superstructure discussed in the previous section. Consider the section through $r = \sum_i \gamma_i q_i$ in R^5. Then the a_5 component of r, x_5, is given by $\sum_i \gamma_i / \sqrt{5}$ from M. Thus x_5 specifies the position of the section.

For convenience, we introduce $\gamma = \sqrt{5} x_5 = \sum_i \gamma_i$. Then we have different structures for $0 \le \gamma \le \frac{1}{2}$ which are not superimposed by any translation, rotation or inversion to each other (Socolar, Lubensky & Steinhardt, 1986). In other words, these belong to the different local isomorphism classes (Levine & Steinhardt, 1986). In this way, we have an infinite number of patterns derived from the same 5D crystal. These are called the generalized Penrose patterns (Pavlovitch & Kleman, 1987; Conway & Knowles, 1986; Jaric, 1986) because one of these ($\gamma = \frac{1}{2}$) agrees with the Penrose pattern derived by Mackay (1982). Three examples are shown in Fig. 4. The generalized Penrose patterns are characterized by the appearance of the tenfold vertex. The density of tenfold vertices takes a maximum for $\gamma = 0$ and reduces with increasing γ. The Penrose pattern ($\gamma = \frac{1}{2}$) is the limiting case where the density becomes zero. Three tenfold vertices are found in Fig. 4(a) and one in (b).

As is clear from the above derivation, the point configuration given by this method is recognized as the section of the 5D crystal. It should be noted that the crystal does not have hypercubic symmetry but has icosahedral symmetry, since the internal space is not equivalent to the external space and the atom is icosahedral in the internal space.

4. Four-dimensional description of generalized Penrose patterns

The Penrose pattern is given as a 2D section of a 4D decagonal crystal (Janssen, 1986), which has four
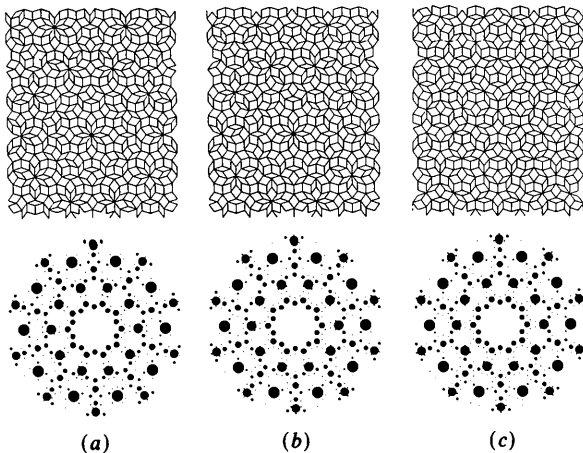

Fig. 4. Generalized Penrose patterns (upper) and their diffraction intensity (lower). The radius of the circle in the diffraction pattern is proportional to the structure factor. (a) $\gamma = 0$. (b) $\gamma = \frac{1}{4}$. (c) $\gamma = \frac{1}{2}$.

atoms in the decagonal unit cell. This crystal is obtained from the 5D icosahedral crystal discussed in the previous section as a 4D section perpendicular to the body-diagonal (11111) direction referred to d_i. Therefore the diffraction pattern (structure factor) is given by the projection of the 5D Fourier spectra along the axis. We first consider the following unit vectors instead of the orthogonal unit vectors d_i ($i = 1, 2, \ldots, 5$ and $d_i \cdot d_j = \delta_{ij}$). For the first four vectors we take $d'_i = d_i - d_5$ and as the fifth vectors we employ $d'_5 = \sum_{i=1}^{5} d_i$. The transformation matrix S defined by $d'_i = \sum_j S_{ij} d_j$ is written as

$$\begin{pmatrix} 1 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix}. \tag{6}$$

Because $\det(S) = 5$, the lattice is spanned by d'_i and five centering translations: $\nu(11111)'/5$ ($\nu = 0, 1, \ldots, 4$) where the prime means the quantity is referred to d'_i. The sublattice spanned by d'_i ($i = 1, 2, \ldots, 4$) constructs the icosahedral lattice in the 4D space as is clear from the metric tensor (Brown, Bülow, Neubüser, Wondratschek & Zassenhaus, 1978). The metric tensor has the form

$$\begin{pmatrix} A & B & B & B & 0 \\ B & A & B & B & 0 \\ B & B & A & B & 0 \\ B & B & B & A & 0 \\ 0 & 0 & 0 & 0 & C \end{pmatrix} \tag{7}$$

with $A = 2a^2$, $B = A/2$, $C = A/10$, where a is the length of the unit vector d_i. The decagonal point group is the subgroup of the icosahedral one in R^4. The above derivation implies that we do not need the hypercubic lattice to obtain the decagonal lattice as a 4D section. Even for the icosahedral lattice, the hypercubic is not necessary. For example, if we elongate the hypercubic lattice along the (11111) direction we also have the icosahedral lattice in R^4. Furthermore, the atoms spreading in the internal space reduce the symmetry of the crystal in R^4 from the icosahedral to the decagonal. This point will be discussed in § 7. The decagonal coordinates r'_i with respect to d'_i are related with the cubic ones r_i to d_i by $r'_i = \sum_j \tilde{S}_{ij}^{-1} r_j$, where the tilde means transposition. $\tilde{S}^{-1}$ is given by

$$\frac{1}{5} \begin{pmatrix} 4 & -1 & -1 & -1 & -1 \\ -1 & 4 & -1 & -1 & -1 \\ -1 & -1 & 4 & -1 & -1 \\ -1 & -1 & -1 & 4 & -1 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix}. \tag{8}$$

The unit vectors $\mathbf{d}_i^{*\prime}$ reciprocal to $\mathbf{d}_i'$ are also related to $\mathbf{d}_i^*$ by the same relation.

As is clear from (5) and (6) $\mathbf{d}_5'$ is parallel to $\mathbf{a}_5$ (see Appendix). In addition (7) shows that the $\mathbf{d}_i'$ $(i = 1, 2, \ldots, 4)$ are normal to it. Therefore the 2D external space through $\gamma \mathbf{d}_1'/5$ is the subspace of the 4D hyperplane through the same point and normal to the $\mathbf{d}_5'$ axis. From this fact we can obtain the generalized Penrose pattern from the 4D hyperplane as shown below.

Consider such a hyperplane. Then the atoms at the positions $\nu(11111)'/5$ $(\nu = 0, \pm 1, \pm 2)$ intersect with the hyperplane at the different positions shown in Fig. 3. The shape of the intersection is a pentagon or decagon centered at $\nu(1111)'/5$ in R^4. Their shape depends on ν because for different ν the plane intersects the rhombic-icosahedral atom at a different position. In the case of $\gamma = \frac{1}{2}$, four sections are regular pentagons but the remaining one corresponding to $\nu = 2$ reduces to a point. This agrees with the 4D description of the Penrose pattern (Janssen, 1986). The Penrose pattern is obtained by taking the 2D section. For other γ, we have a generalized Penrose pattern which consists of the same two unit rhombuses as those of the Penrose pattern.

We consider the symmetry of the generalized Penrose pattern. The decagonal lattice is invariant under the group generated by a fivefold rotation, a mirror and inversion. The action of these symmetry operators on the reciprocal unit vectors $\mathbf{d}_i^{*\prime}$ $(i = 1, 2, \ldots, 4)$ is given by a 4×4 matrix $\Gamma(R)$:

$$\Gamma(C_5^{-1}) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & -1 & -1 & -1 \end{pmatrix}$$

$$\Gamma(\sigma_v) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

$$\Gamma(I) = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \qquad (9)$$

The action to $\mathbf{a}_i^*$ is given by $\Gamma'(R) = (\tilde{M}\tilde{S})\Gamma(R)(\tilde{M}\tilde{S})^{-1}$. Therefore the atom spreading in the internal space is transformed by the matrices

$$\begin{pmatrix} c_2 & s_2 \\ -s_2 & c_2 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}. \qquad (10)$$

The matrix group is isomorphic to $D_5 \times C_2$ or D_{10}. The atoms are located at the Wyckoff positions $\nu(1111)'/5$ $(\nu = 0, \pm 1, \pm 2)$ in the decagonal coordinate system. The site symmetry for these is D_{10} for

$\nu = 0$ and D_5 for other ν when $\gamma = 0$. For other γ each atom has D_5 symmetry from its shape, as is clear from Fig. 3. This means that at least the structure has D_5 point symmetry. In two cases with $\gamma = 0$ and $\frac{1}{2}$, the structure is invariant for the inversion. In the former, the atom at the origin has inversion symmetry. The atoms at $\pm(1111)'/5$ are transformed to each other by the inversion and the same relation holds for atoms at $\pm(2222)'/5$. The structure has the inversion center at the origin. On the other hand, for $\gamma = \frac{1}{2}$ the four atoms are at $\nu(1111)'/5$ $(\nu = -2, -1, 0, 1)$. [The atom at $(2222)'/5$ shrinks to a point so that the atom intersects only at one point with the external space and is negligible.] In this case the inversion center is shifted to $(2222)'/5$. [When we take the origin on the inversion center, the above four atoms are at the Wyckoff positions $\nu(1111)'/5$ $(\nu = 1, 2, 3, 4)$ with the site symmetry of D_5.] For other γ, the inversion symmetry breaks down because each atom has neither the inversion symmetry nor a counterpart related to the inversion. Thus we have the tenfold axis for $\gamma = 0$ and $\frac{1}{2}$ and fivefold axis for the other γ. The number density of the vertices in the generalized Penrose pattern is independent of γ, as shown by Yamamoto & Ishihara (1988). This shows that only two cases have the tenfold axis among an infinite number of generalized Penrose patterns with the same density.

5. Structure factors

First we employ the 5D description of the generalized Penrose patterns. In this case, we consider the structure which is given by the rhombic-icosahedral atom at each hypercubic lattice point. The Fourier spectra have a finite value at the reciprocal-lattice points $\mathbf{h} = \sum_i h_i \mathbf{d}_i^*$, where $\mathbf{d}_i^*$ $(i = 1, 2, \ldots, 5)$ are the unit vectors reciprocal to $\mathbf{d}_i$. For these points the structure factor is given by

$$F_{\mathbf{h}} = \int_V \exp(2\pi i \mathbf{h} \cdot \mathbf{r}) \, dv, \qquad (11)$$

where $\mathbf{r} = \sum_i r_i \mathbf{q}_i$ and the integral is taken over the rhombic icosahedron in the internal space which is defined by $-\frac{1}{2} < r_i < \frac{1}{2}$.

The generalized Penrose pattern is also obtained from a hyperplane normal to the a_5 axis, as mentioned in § 4. Therefore we take the projection along this axis for the diffraction pattern. Then an infinite number of lattice points are projected on the same point in R^4. The reciprocal-lattice vector $\mathbf{h} = \sum_i h_i \mathbf{d}_i^*$ is expressed as $\sum_i h_i' \mathbf{d}_i^{*\prime}$ by using the decagonal unit vectors, where $h_i' = h_i - h_5$ for $i = 1, 2, \ldots, 4$ and $h_5' = \sum_{i=1}^5 h_i$. The decagonal indices have the reflection condition $\sum_{i=1}^4 h_i' + h_5' = 0 \pmod 5$ for general reflections because the centering translations exist. Since the unit vector $\mathbf{d}_5^{*\prime}$ is normal to $\mathbf{d}_j^*$ $(j \le 4)$, for any integer n reflections with $h_1' h_2' h_3' h_4' h_5' + 5n$ $(-2 \le h_5' \le 2)$ are projected on the same position in R^4. Therefore we

have to take a summation with respect to n to obtain the projected structure factor. For the reflection with $\mathbf{h}' = \sum_{i=1}^{4} h_i' \mathbf{d}_i'$ in R^4, we have

$$\hat{F}_{\mathbf{h}'} = \int_V \sum_n \exp \left\{ 2\pi i \left[\sum_{i=1}^{4} h_i' r_i' + (h_5' + 5n) \right. \right.$$

$$\left. \left. \times (r_5' - s) \right] \right\} \, \mathrm{d}v' \, \mathrm{d}r_5' \qquad (12)$$

where $s = \gamma/5$, r_i' $(i = 1, 2, \ldots, 5)$ are the $\mathbf{d}_i'$ components of $\mathbf{r}$ and $\mathrm{d}v$ is expressed by $\mathrm{d}r_5'$ and its complement $\mathrm{d}v'$. Using the expression for the periodic δ function with period $\frac{1}{5}$, $\sum_n \exp[10\pi i n(r_5' - s)] = \Delta(r_5' - s)/5$, we finally obtain

$$\hat{F}_{\mathbf{h}'} = \frac{1}{5} \sum_{\nu=0}^{4} \int_{V_\nu} \exp \left\{ 2\pi i \left[\sum_{i=1}^{4} h_i'(r_i' + \nu/5) \right] \right\} \, \mathrm{d}v' \qquad (13)$$

where V_ν is the section of the rhombic icosahedron at the plane through $(s + \nu/5)\mathbf{d}_5'$ and we have used the reflection condition, $\sum_{i=1}^{4} h_i' + h_5' = 0 \pmod 5$. The formula (13) agrees with the structure factor for five atoms at $\nu(1111)'/5$ $(\nu = 0, 1, \ldots, 4)$ in R^4. The analytical expression of the structure factor is given by

$$\hat{F}_{\mathbf{h}'} = \frac{1}{5} \sum_{\nu=0}^{4} \exp \left[2\pi i \left(\sum h_i' \nu/5 \right) \right] F^\nu(\mathbf{h}') \qquad (14)$$

where $F^\nu(\mathbf{h}')$ is the Fourier integral of the polyhedron corresponding to the νth plane in Fig. 3. Noting that each plane is in general decagonal, we can write this in the form

$$F^\nu(\mathbf{h}') = \sum_R \left[F_0(\mathbf{e}_1, \mathbf{e}_2, R^{-1}\mathbf{h}'^i) + F_0(\mathbf{e}_2, \mathbf{e}_3, R^{-1}\mathbf{h}'^i) \right], \qquad (15)$$

$$F_0(\mathbf{e}_1, \mathbf{e}_2, \mathbf{h}'^i) = e_1 e_2 \sin \theta_{12} \{ a_1[\exp(ia_2) - 1]$$

$$- a_2[\exp(ia_1) - 1] \}$$

$$\times [a_1 a_2 (a_1 - a_2)]^{-1}, \qquad (16)$$

where $\mathbf{e}_j$ $(j = 1, 2, 3)$ are edge vectors of two triangles constructing the decagon (Fig. 3), $e_j = |\mathbf{e}_j|$, $\mathbf{h}'^i$ is the internal component of the diffraction vector $\mathbf{h}'$, θ_{12} is the angle between two vectors $\mathbf{e}_1$ and $\mathbf{e}_2$, and $a_j = 2\pi \mathbf{e}_j \cdot \mathbf{h}'^i$ $(j = 1, 2)$. In (15) R runs over all the symmetry operators in the point group D_5. For a pentagonal plane the second term in (15) is dropped.

The diffraction patterns for three cases are shown in Fig. 4 and the structure factors are listed in Table 1. As shown in the figure, the diffraction patterns with different γ are similar to each other. This is considered as follows. The γ dependence of the diffraction pattern comes from the superposition of reflections in R^4. Therefore, if the structure factors $F_{\mathbf{h}}$ with $h_1' h_2' h_3' h_4' h_5' + 5n$ $(-2 \le h_5' \le 2)$ are all weak except for $n = 0$, the structure factor $\hat{F}_{\mathbf{h}'}$ for $h_1' h_2' h_3' h_4'$ in R^4 is approximated well by $F_{\mathbf{h}}$ for the case of $n = 0$ and

Table 1. *The normalized structure factors of the generalized Penrose patterns for three cases:* $\gamma = 0, \frac{1}{4}, \frac{1}{2}$

$h_1' - h_4'$	$\gamma = 0$	$\gamma = \frac{1}{4}$	$\gamma = \frac{1}{2}$
0 0 0 0	1·000	1·000	1·000*
0 1 1 0	0·057	0·059	0·061
1 1 2 1	0·053	0·056	0·060
0 1 2 0	0·020	0·047	0·063
1 2 2 1	0·392	0·387	0·382
0 2 2 1	0·460	0·462	0·463
0 2 2 0	0·089	0·089	0·090
1 2 3 1	0·070	0·086	0·100
1 3 3 2	0·097	0·095	0·091
1 3 3 1	0·012	0·012	0·012
0 3 3 1	0·046	0·085	0·111
1 3 4 2	0·759	0·759	0·759
1 3 4 1	0·046	0·046	0·046
2 4 4 2	0·069	0·077	0·085
1 4 4 2	0·257	0·253	0·249
1 4 4 1	0·323	0·324	0·327
2 4 5 3	0·098	0·092	0·084
2 4 5 2	0·062	0·076	0·088
1 4 5 2	0·044	0·046	0·047
2 5 5 3	0·088	0·091	0·095
2 5 5 2	0·493	0·488	0·481
1 5 5 3	0·072	0·067	0·061
1 5 5 2	0·071	0·079	0·087
2 5 6 3	0·151	0·149	0·146
2 5 6 2	0·214	0·216	0·219
3 6 6 3	0·051	0·066	0·078
1 5 6 3	0·902	0·902	0·902
1 5 6 2	0·021	0·020	0·019
2 6 6 3	0·063	0·067	0·072
2 6 6 2	0·337	0·332	0·327
3 6 7 3	0·093	0·091	0·088
1 6 6 3	0·089	0·080	0·069
2 6 7 4	0·069	0·068	0·067
2 6 7 3	0·026	0·026	0·026
2 6 7 2	0·040	0·074	0·098
3 7 7 3	0·679	0·679	0·680
1 6 7 3	0·071	0·079	0·086
2 7 7 3	0·213	0·209	0·205
2 7 7 2	0·060	0·090	0·113

the latter is independent of the section except for the phase factor common to all reflections, as is clear from (11). This is in fact true for strong reflections. Thus the section (or γ) dependence of the diffraction pattern is quite analogous to that of the usual superstructure discussed in § 2. From the analogy with the superstructure, we call reflections with $\sum_{i=1}^{4} h_i' = 0$, ± 1, $\pm 2 \pmod 5$ the main, the first-order satellite and second-order satellite reflections respectively. As shown in Table 1, the strong reflections are the main and the first-order satellites. From these facts we can recognize that the generalized Penrose patterns are the superstructures obtained from a different section of the same structure in R^5, though the first-order satellite reflections are strong in the present case. In order to clarify this point of view we introduce, in the next section, the 5D description of the superstructure of a 4D crystal, which is the extension of the higher-dimensional description of the 3D superstructure to the present case.

6. Superstructure in the four-dimensional space

In § 4 we showed that the generalized Penrose pattern is obtained from five kinds of atoms situated at

$\nu(1111)'/5$ ($\nu = 0, \pm 1, \pm 2$). If we place the same atom at these positions, we obtain a 4D lattice with shorter periods. This lattice is spanned by $\mathbf{d}_{0i} = \mathbf{d}'_i - \sum_{j=1}^4 \mathbf{d}'_j/5$ and is icosahedral. The unit-cell volume defined by $\mathbf{d}_{0i}$ is $\frac{1}{5}$ of that defined by $\mathbf{d}'_i$. Therefore we can consider that the generalized Penrose pattern is the superstructure in the 4D space. In analogy with the higher-dimensional description of the superstructure in the 3D space, we obtain this pattern from a 5D lattice. The 5D lattice is the same as that described in § 3 but the direct extension of the description leads to a different setting as shown below.

We consider a 4D crystal with 1D modulation. Then the diffraction vector $\mathbf{q}$ of the average structure is defined by four unit vectors $\mathbf{d}_{0i}^*$ ($i = 1, 2, 3, 4$), which are reciprocal to $\mathbf{d}_{0i}$ in the present case, and a 'wave vector' $\mathbf{k}$ as $\mathbf{q} = \sum_{j=1}^4 l_j \mathbf{d}_{0j}^* + l_5 \mathbf{k}$. The superstructure means that $\mathbf{k}$ is expressed by the rational multiple of $\mathbf{d}_{0i}^*$. The main reflection has the index $l_1 l_2 l_3 l_4 0$: l_5 gives the order of a satellite reflection. From $\mathbf{d}_{0i}$ we have $\mathbf{d}_{0i}^* = \sum_{j=1}^4 \mathbf{d}_j^{*\prime} + \mathbf{d}_i^{*\prime}$ ($i \le 4$) and $\mathbf{k}$ is given by $\sum_{j=1}^4 \mathbf{d}_j^{*\prime}/5$. Under the symmetry operations in D_{10}, the $\mathbf{d}_{0i}^*$ are transformed into integral linear combination of themselves and $\mathbf{k}$, into $\pm \mathbf{k} + \mathbf{K}$ similarly to the transformation properties of the unit vectors in the higher-dimensional description of the modulated structure, where $\mathbf{K}$ is a lattice vector (Janner & Janssen, 1979). According to the theory of modulated structures, the 5D unit vectors $\mathbf{b}_i^*$ are given by $\mathbf{b}_i^* = \mathbf{d}_{0i}^*$ ($i \le 4$) and $\mathbf{b}_5^* = \mathbf{k} + \mathbf{a}_5/\alpha$ (de Wolff, 1974). The corresponding unit vectors in the direct space are $\mathbf{b}_i = \mathbf{d}_{0i} - \alpha \mathbf{a}_5/5$ ($i \le 4$) and $\mathbf{b}_5 = \mathbf{a}_5$. In the above expressions α is an arbitrary scale factor for the internal space.

Now we compare the 5D lattice introduced above with that discussed in § 3. Consider the transformation matrix T which transforms $\mathbf{d}_i$ into $\mathbf{b}_i$. When we choose $\alpha = -\sqrt{5}$, we have

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix}. \tag{17}$$

Because $\det T = 1$, $\mathbf{b}_i$ and $\mathbf{d}_i$ span the same lattice. Therefore, if we place the icosahedral atom as shown in Fig. 3, we obtain the Penrose pattern. From T, we obtain $l_i = h_i$ ($i \le 4$) and $l_5 = \sum_{i=1}^5 h_i$. The last relation means that $l_5 = h_5'$ and $\sum_{i=1}^4 h_i' = -l_5$ (mod 5). This confirms that the reflections with $\sum_{i=1}^4 h_i' = 1, \pm 1, \pm 2$ (mod 5) are in fact the main, first-order satellite and second-order satellite reflections as stated in the previous section.

In the present description, the fundamental structure is given by a decagonal columnar atom situated at each lattice point. The decagonal column has the same height as that of the icosahedron in Fig. 3 and

the section perpendicular to the axis has the regular decagon with the average area of the five planes shown in the figure. In the fundamental structure the atom is continuous along the $\mathbf{b}_5$ axis because an atom contacts with another atom belonging to an adjacent lattice point sharing a plane normal to the decagonal axis.

The change of atom shape in the generalized Penrose pattern along the $\mathbf{b}_5$ axis causes a fivefold superstructure in the 4D space. Consequently satellite reflections appear in the fictitious diffraction pattern in the 4D space. The above discussion concludes that the Penrose pattern can be regarded as the superstructure in the 4D space and the two 5D descriptions are equivalent except for the trivial difference in the setting.

7. Superspace groups of the quasicrystals

The matrix representation of the point group describing the symmetry of the quasicrystals has to fulfil the necessary condition derived from the symmetry properties of the diffraction pattern. The symmetry operators included in the point group leave the diffraction pattern invariant. This means that the m-dimensional external space is invariant under the symmetry operator. Consequently, the $\mathbf{a}_i$ ($i = 1, 2, \ldots, m$) are transformed into a linear combination of themselves. In matrix notation, the rotation operator R is represented by an $n \times n$ matrix which has a form

$$\begin{pmatrix} R^e & 0 \\ 0 & R^i \end{pmatrix}, \tag{18}$$

where R^e is an $m \times m$ matrix with real entries and R^i is a $d \times d$ real matrix ($d = n - m$); 0 means an $m \times d$ or $d \times m$ zero matrix. The action of the rotation operator on the lattice basis $\mathbf{d}_i^*$ ($i = 1, 2, \ldots, n$) is expressed by an $n \times n$ integral matrix R and that of the orthogonal basis $\mathbf{a}_i^*$ is given by $\tilde{M} R \tilde{M}^{-1}$ from the transformation property of the basis vectors described in § 4. The matrix representation of the symmetry operator is transformed into the form of (18) by the similarity transformation with the matrix $\tilde{M}$. This is analogous to the situation in the modulated structure. For the modulated structure with a d-dimensional modulation in the m-dimensional space, the symmetry operator is reducible to the form of (18) by a similarity transformation. Therefore the point group describing the symmetry of the quasicrystal is $(m + d)$-reducible in the same way as that of the modulated structure.

As shown in §§ 3 and 4, the hypercubic lattice in R^5 and icosahedral lattice in R^4 are not necessary to obtain the generalized Penrose patterns. This is related to the reducibility mentioned above. The matrix representations are irreducible for the point

groups which leave these lattices invariant, so that these lattices are not necessary to describe the quasi-crystals.

8. Concluding remarks

It has been shown that the relation of the 4D description to the 5D one of the Penrose pattern corresponds to that of the 3D description with the 4D one in the usual superstructure. The higher-dimensional description is more convenient for some purposes, such as the derivation of the generalized Penrose pattern, though the symmetry is given by the space group in the lower-dimensional space. From this viewpoint, the generalized Penrose patterns and their structure factors have been derived based on the 5D description. The results of such calculations reveal why the diffraction patterns of these structures are not much different from each other, although the structures look very different.

From the analogy to the usual superstructure we can say that the Penrose pattern is the superstructure in the quasicrystal. The superspace group describing the symmetry of the quasicrystal is $(m + d)$-reducible. This is also analogous to the situation in the modulated structure.

APPENDIX

The unit vectors $\mathbf{d}_i'$ and $\mathbf{d}_i^{*\prime}$ in the decagonal system are related to $\mathbf{a}_i$ with $\mathbf{d}_i' = \sum_j (SM)_{ij} \mathbf{a}_j$ and $\mathbf{d}_i^{*\prime} = \sum_j (\tilde{M}\tilde{S})_{ij}^{-1} \mathbf{a}_j$, where SM is

$$\sqrt{(2/5)} \begin{pmatrix} c_1-1 & s_1 & c_2-1 & s_2 & 0 \\ c_2-1 & s_2 & c_4-1 & s_4 & 0 \\ c_3-1 & s_3 & c_1-1 & s_1 & 0 \\ c_4-1 & s_4 & c_3-1 & s_3 & 0 \\ 0 & 0 & 0 & 0 & 5/\sqrt{2} \end{pmatrix} \quad (A1)$$

and $(\tilde{M}\tilde{S})^{-1}$ is

$$\sqrt{(2/5)} \begin{pmatrix} c_1 & s_1 & c_2 & s_2 & 0 \\ c_2 & s_2 & c_4 & s_4 & 0 \\ c_3 & s_3 & c_1 & s_1 & 0 \\ c_4 & s_4 & c_3 & s_3 & 0 \\ 0 & 0 & 0 & 0 & 1/\sqrt{2} \end{pmatrix}. \quad (A2)$$

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