Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Received 3 September 2004
Accepted 27 October 2004

Generalized quasiperiodic patterns and superstructures in quasicrystals

Akiji Yamamoto

Advanced Materials Laboratory, NIMS, Tsukuba 305-0044, Japan. Correspondence e-mail: yamamoto.akiji@nims.go.jp

Patterns with octagonal and icosahedral symmetries obtained from periodic two-dimensional (2D) 8-grids and three-dimensional (3D) 12-grids by the dual method are shown to be superstructures of the Beenker pattern and the 3D Penrose pattern with the same edge length. The superstructures are described in the same spaces as those of the latter (4D for the Beenker and 6D for the 3D Penrose patterns) in the section method but their lattice constants are doubled. The occupation domains and the diffraction patterns for these cases are given.

1. Introduction

Since the discovery of an icosahedral Al–Mn quasicrystal (*i*-Al–Mn), extensive theoretical and structural studies have been performed. A quasicrystal is a quasiperiodic structure with non-crystallographic symmetry in contrast to modulated structures and composite crystals. Quasiperiodic patterns with non-crystallographic symmetry play an important role in structure analyses of quasicrystals (Yamamoto, 1996). It is known that there exist three distinct methods for the generation of quasiperiodic patterns, which are called the inflation–deflation method (IDM), the dual method (DM) and the projection method (PM). These methods were introduced by de Bruijn (1981) and applied to the Penrose pattern. The DM was extended to derive an icosahedral pattern (Kramer & Neri, 1984), and the so-called three-dimensional Penrose pattern (3DPP) was shown to be a special case of general icosahedral patterns. The PM was applied to general dihedral cases (Whittaker & Whittaker, 1988) to obtain generalized quasiperiodic patterns. This is equivalent to the DM (Gähler & Rhyner, 1986). Generalized octagonal and icosahedral patterns discussed in this paper are obtained from 8D and 12D lattices by the PM. The section method (SM) is a slight modification of the PM. It uses the minimal space that is necessary to describe the pattern (4D and 6D spaces for our cases) (Janssen, 1986). Furthermore, it is applicable to the calculation of diffraction patterns, which is essential for structure analysis (Yamamoto & Ishihara, 1988; Yamamoto, 1992). In crystallography, therefore, the SM is superior to the other methods. For generalized octagonal and icosahedral patterns, the PM is insufficient to obtain the diffraction pattern because it only needs the unit cell of the nD lattice ($n = 8$ or 12), while for the calculation of the diffraction patterns its projection onto the 2D or 3D internal (complementary, perpendicular) space called the occupation domain (atom surface, window) is necessary. In the SM, the patterns are obtained from the occupation domains (OD) by taking the crosspoint at the external (physical, parallel) space.

Many patterns obtained from the IDM and several patterns obtained from the DM or PM have not yet been obtained by the SM. In particular, generalized octagonal, decagonal, dodecagonal and icosahedral patterns derived from 8D, 10D and 12D space by the PM or the DM (Whittaker & Whittaker, 1988; Kramer & Neri, 1984) have not been derived yet using the SM and their diffraction patterns are not known. This paper reconsiders the generalized octagonal and icosahedral patterns obtained from periodic 8- and 12-grids by the DM with the SM and shows their ODs and diffraction patterns. They have the same symmetry (4D $p8mm$ and 6D $Pm\bar{3}\bar{5}$) as the patterns obtained from the periodic 4-grid (Beenker pattern, BP) and 6-grid (3DPP) and are generally regarded as superstructures of the BP or 3DPP as shown later. Their lattice constant is twice as large as that of the BP or 3DPP.

The arrangement of the present paper is as follows. In §2, the derivation of generalized quasiperiodic patterns by the DM is briefly summarized. The equivalent section methods are discussed in §3 and the occupation domains for the generalized quasiperiodic patterns are derived. In §4, their diffraction patterns are shown.

2. Dual method

The dual method is equally applicable to both generalized BPs in 2D space (Whittaker & Whittaker, 1988) and generalized 3DPPs. In this section, derivations of the generalized octagonal patterns in 2D space and the generalized 3DPPs in 3D space will be briefly described for discussion in the next section.

(*a*) *Generalized octagonal patterns*. The octagonal patterns with edge length a_0 can be derived from the periodic 8-grid, which is given by

$$\mathbf{e}_i^* \cdot \mathbf{x} = n_i + \gamma_i \quad (i \leq 8), \tag{1}$$

with an integer n_i and the unit vectors in the external (physical) space

$$\mathbf{e}_i^* = a_0^*\{\cos[2\pi(i-1)/8]\mathbf{a}_1 + \sin[2\pi(i-1)/8]\mathbf{a}_2\}, \quad (2)$$

where $a_0^* = 1/a_0$, γ_i is the shift of the ith grid along $\mathbf{e}_i^*$ and $\mathbf{a}_i$ $(i = 1, 2)$ are the unit vectors of 2D external space. The vectors $\mathbf{x}$ given by equation (1) are on parallel lines normal to the direction specified by $\mathbf{e}_i^*$. Note that there exists one line belonging to the $(i \pm 4)$th grid between two consecutive lines with the interval a_0 except for a singular case with $(\gamma_i + \gamma_{i+4})/2 = 0 \pmod{0.5}$ because $\mathbf{e}_{i\pm4}^* = -\mathbf{e}_i^*$. If $(\gamma_i + \gamma_{i+4})/2 = \pm 0.25 \pmod{0.5}$ for $i \le 4$, the grids are equivalent to 4-grids with a half interval, which leads to the well known BP (Beenker, 1982). In order to obtain a pattern with octagonal symmetry, $(\gamma_i + \gamma_{i+4})/2 = \gamma$ $(i \le 4)$ must be fulfilled while $\gamma_i' = (\gamma_i - \gamma_{i+4})/2$ can take an arbitrary value since it does not change the local isomorphism class of resulting patterns (Socolar, 1989). Let the intersection of the ith and jth grids with n_i and n_j be $\mathbf{y} = a_0[y_1\mathbf{a}_1 + y_2\mathbf{a}_2]$. Then we can assign 8 integers, $K_i = \lfloor \mathbf{e}_i^* \cdot \mathbf{y} - \gamma_i \rfloor$, where $\lfloor x \rfloor$ is the largest integer less than or equal to x. In particular, $K_i = n_i$ and $K_j = n_j$. Different sets of γ_i' lead to locally isomorphic structures. Corresponding to the intersection, we place a rhombus spanned by $\mathbf{e}_i$ and $\mathbf{e}_j$ at $\mathbf{r}_0 = \sum_{k=1}^{8} K_k \mathbf{e}_k$, which has corners at $\mathbf{r}_0$, $\mathbf{r}_0 + \mathbf{e}_i$, $\mathbf{r}_0 + \mathbf{e}_j$, $\mathbf{r}_0 + \mathbf{e}_i + \mathbf{e}_j$, where $\mathbf{e}_k = a_0^2\mathbf{e}_k^*$ for any k. Two cases are shown in Figs. 1(a) and 1(b), which correspond to $\gamma = 0.25$ and 0.1. As is clear from the figure, the former is equivalent to the BP and the other patterns with $\gamma \ne \pm 0.25 \pmod 1$ can be regarded as a superstructure of the BP as shown later. The characteristic feature of a generalized octagonal pattern is the appearance of a larger square and rhombus consisting of four tiles with the same orientation, which never appear in the BP.

(b) *Generalized icosahedral patterns*. These are derived from the 3D 12-grid,

$$\mathbf{e}_i^* \cdot \mathbf{x} = n_i + \gamma_i \quad (i \le 12), \quad (3)$$

by a similar method. The vectors $\mathbf{e}_i^*$ are given by

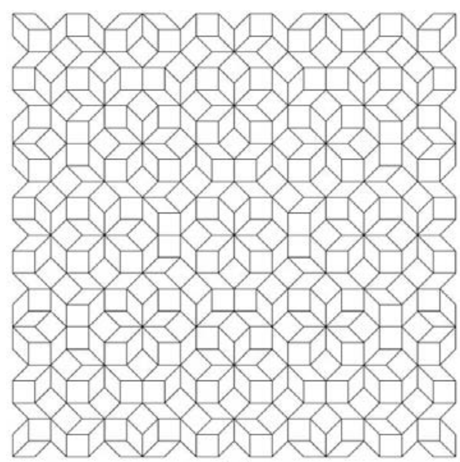
$$\begin{aligned} \mathbf{e}_1^* &= a_0^*\mathbf{a}_3, \\ \mathbf{e}_{i+1}^* &= a_0^*\{\cos(2\pi i/5)\mathbf{a}_1 + \sin(2\pi i/5)\mathbf{a}_2\}\sin\theta \\ &\quad + \cos\theta\mathbf{a}_3 \quad (1 \le i \le 5) \end{aligned} \quad (4)$$

with $\theta = \cos^{-1}(1/5^{1/2})$ and $\mathbf{e}_{6+i}^* = -\mathbf{e}_i^*$, where $\mathbf{a}_i$ $(i = 1, 2, 3)$ are the unit vectors in the 3D external space. In this case, the ith grid is a set of equidistant 2D planes normal to $\mathbf{e}_i^*$ and an intersection is given by three planes. Let the intersection of the ith, jth and kth grids with n_i, n_j and n_k be $\mathbf{y}$. Take $K_l = \lfloor \mathbf{e}_l^* \cdot \mathbf{y} - \gamma_l \rfloor$ for all l $(1 \le l \le 12)$. Then a rhombus spanned by $\mathbf{e}_i$, $\mathbf{e}_j$, $\mathbf{e}_k$ at $\sum_{l=1}^{12} K_l\mathbf{e}_l$ gives generalized icosahedral patterns. The projections of the patterns along the fivefold axis with $\gamma = (\gamma_i + \gamma_{i+6})/2 = 0.25$ and 0.1 are shown in Figs. 2(a) and 2(b). As shown by Kramer & Neri (1984), the former gives the 3DPP. It will be shown in the next section that the patterns with $\gamma \ne \pm 0.25 \pmod{0.5}$ are superstructures of the 3DPP. A generalized icosahedral pattern includes two consecutive rhombi with the same orientation in contrast to the 3DPP. A different $\gamma_i' = (\gamma_i - \gamma_{i+6})/2$ $(i \le 6)$ gives locally isomorphic patterns.

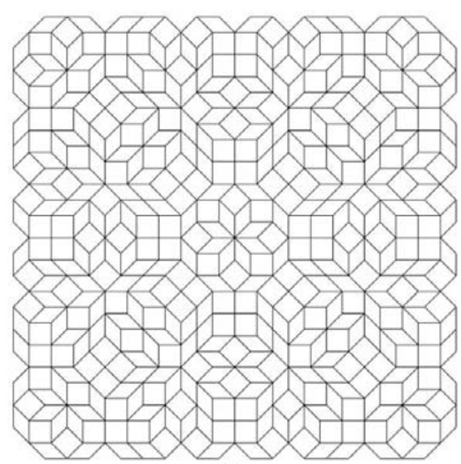
As shown in a case of quasi-periodic grids as in the Fibonacci hexagrid (Socolar & Steinhardt, 1986), if more than two lines or more than three planes cross at one point, we have a singular point where tiles formed by the aggregation of several rhombi or rhombohedra will appear. In the present case, however, the grid is periodic and just two different intervals of grids exist. In such a case, it can be shown that, even if singular points exist, their point density is zero as shown in Appendix A. The effect of such points can be recognized as point defects, which does not contribute to the diffraction intensity. Therefore almost everywhere the octagonal patterns consist of two rhombi and the icosahedral patterns of two rhombohedra, as shown in Figs. 1 and 2.

3. Section method

The patterns given in the previous section are also obtainable by the PM because this is shown to be equivalent to the dual method (Gähler & Rhyner, 1986). The octagonal (or icosahedral) patterns are obtained from 8D (or 12D) space by the PM but 4D (6D) space is sufficient to describe the structure. In



(a)



(b)

Figure 1
Octagonal patterns for (a) $\gamma = 0.25$ and (b) 0.1. The former is identical to the Beenker pattern ($\gamma_i' = 0$ for $i \le 4$). Four consecutive squares or rhombi appear in the latter.

the PM, we use a polytope which is the projection of the unit cell in the 8D (12D) space onto the 6D (9D) internal space. In order to obtain their diffraction patterns, it is necessary to obtain the ODs that are the projection of the polytope onto the minimal internal space, which is 2D (3D) space.

In the SM, the quasiperiodic structures are described as a crystal (periodic structure) in a higher-dimensional space with the minimal dimension (in contrast to the PM, where an additional dimension is necessary for the cases discussed in this paper). Then the quasiperiodic patterns are given as an intersection of the periodic structure in the higher-dimensional space with the external space and their diffraction pattern is regarded as the projection of the Fourier amplitudes of the structure in the higher-dimensional space onto the external space. In the previous section, we did not use the higher-dimensional space explicitly. However, as discussed by Kramer & Neri (1984) and Whittaker & Whittaker (1988), the vectors $\mathbf{e}_i^*$ in (2) and (4) can be regarded as the projection of the unit vectors of a higher-dimensional reciprocal lattice onto the external space. The higher-dimensional space is divided into the external and internal spaces by use of group theory.

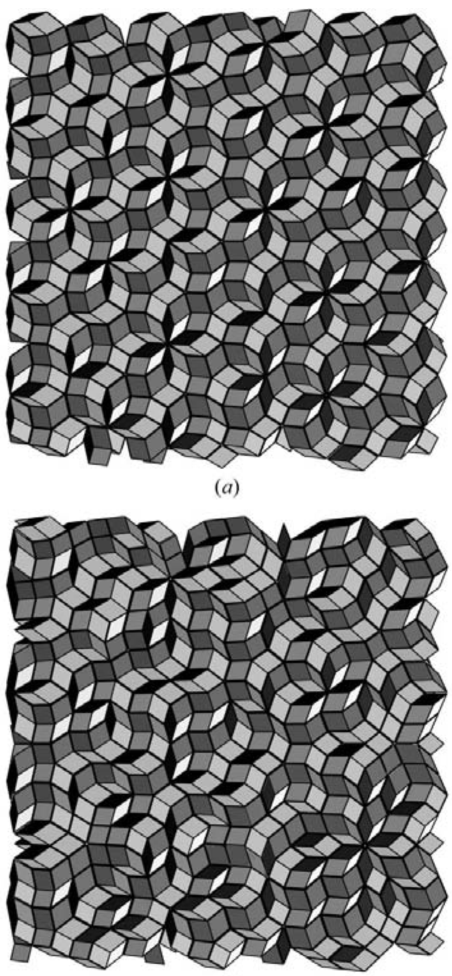


Figure 2
Puckered surfaces of icosahedral patterns normal to a fivefold axis for (*a*) $\gamma = 0.25$ and (*b*) 0.1. The former is identical to the 3DPP $[\gamma' = (0, 1, 2, 3, 4, 5)/10]$. Thick and thin lines represent the boundary of two rhombohedra and an edge of a rhombohedron, respectively. The characteristic feature in (*b*) is the appearance of two consecutive rhombohedra with the same orientation, which never appear in (*a*).

(*a*) *Octagonal patterns*. The octagonal group is generated by an eightfold rotation. On the basis of the unit vectors $\mathbf{e}_i^*$ of the octagonal lattice in the 8D space, the matrix representation of a rotation operator in the octagonal group can be expressed by an 8×8 integral matrix. The octagonal group is generated by the eightfold rotation around the body-diagonal direction, the matrix representation of which is given by the permutation matrix

$$\begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 2 & 3 & 4 & 5 & 6 & 7 & 8 & 1 \end{bmatrix}.$$

This is reducible into two one-dimensional and three two-dimensional irreducible representations. The two-dimensional irreducible representations of the eightfold rotation are given by

$$\mathrm{R}_k = \begin{bmatrix} \cos(2\pi k/8) & -\sin(2\pi k/8) \\ \sin(2\pi k/8) & \cos(2\pi k/8) \end{bmatrix} \quad (k = 1, 2, 3), \quad (5)$$

while the one-dimensional representations are $\mathrm{R}_4 = -1$ and $\mathrm{R}_5 = 1$. The basis vectors of the first two-dimensional representation span the external space, and the others span the internal space. The rank of the matrix is four in the octagonal case, so that the four-dimensional space is sufficient to describe the structure Janssen (1986). The internal space spanned by the basis vectors of the third two-dimensional representation is necessary but the other internal space is redundant. Therefore we can express all the patterns derived from the 8D space in the 4D space, which is spanned by the basis vectors of R_1 and R_3.

When the unit vectors in the 8D lattice are $\mathbf{e}_i^*$ and the basis vectors of the irreducible representations are $\mathbf{a}_i$ $(i \le 8)$, $\mathbf{e}_i^*$ are written in terms of $\mathbf{a}_i$ as

$$\mathbf{e}_i^* = a_0^* \sum_{j=1}^{8} \mathrm{M}_{ij} \mathbf{a}_j \quad (6)$$

with

$$\mathrm{M} = \begin{bmatrix} \mathrm{M}_1 & \mathrm{M}_2 \\ -\mathrm{M}_1 & \mathrm{M}_2 \end{bmatrix}, \quad (7)$$

where $\mathbf{a}_i$ $(i = 1, 2, 3, 4)$ are the basis vectors of the first and third two-dimensional representations $[k = 1, 3$ in equation (5)$]$. The vectors $\mathbf{a}_5$ and $\mathbf{a}_6$ are those of the second two-dimensional representation and $\mathbf{a}_7$ and $\mathbf{a}_8$ those of the two one-dimensional representations. The 4×4 matrices M_1 and M_2 are given by

$$M_1 = \frac{1}{2}\begin{bmatrix} c_0 & s_0 & c_0 & s_0 \\ c_1 & s_1 & c_3 & s_3 \\ c_2 & s_2 & c_6 & s_6 \\ c_3 & s_3 & c_1 & s_1 \end{bmatrix}, \qquad (8)$$

$$M_2 = \frac{1}{2}\begin{bmatrix} 1 & 0 & t & t \\ 0 & 1 & -t & t \\ -1 & 0 & t & t \\ 0 & -1 & -t & t \end{bmatrix}, \qquad (9)$$

where a_0^* is the lattice constant of the hypercubic (reciprocal) lattice, $c_i = \cos(2\pi i/8)$, $s_i = \sin(2\pi i/8)$ and $t = 1/\sqrt{2}$. The new vectors $\mathbf{e}_i^{*\prime} = (\mathbf{e}_i^* - \mathbf{e}_{4+i}^*)/2$ and $\mathbf{e}_{4+i}^{*\prime} = (\mathbf{e}_i^* + \mathbf{e}_{4+i}^*)/2$ $(i \leq 4)$ are given by

$$\mathbf{e}_i^{*\prime} = a_0^* \sum_{j=1}^{8} M'_{ij}\mathbf{a}_j \qquad (10)$$

with

$$M' = \begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix}. \qquad (11)$$

The vectors $\mathbf{e}_i^{*\prime}$ are obtained from $\mathbf{e}_i^*$ by $\mathbf{e}_i^{*\prime} = \sum_{j=1}^{8}(\tilde{S}^{-1})_{ij}\mathbf{e}_j^*$, where $(\tilde{S}^{-1}) = S/2$ with

$$S = \begin{bmatrix} 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{bmatrix}. \qquad (12)$$

The unit vectors $\mathbf{e}_i$ and $\mathbf{e}'_i$ reciprocal to $\mathbf{e}_i^*$ and $\mathbf{e}_i^{*\prime}$ are obtained from the right-hand side of equations (6)–(11) by replacing a_0^* with $a_0 = 1/a_0^*$, since M and M′ are orthogonal matrices. Similarly, we have $\mathbf{a}_i^* = \sum_{j=1}^{8}\tilde{M}_{ij}\mathbf{e}_j^*$ and $\mathbf{a}_i^* = \sum_{j=1}^{8}\tilde{M}'_{ij}\mathbf{e}_j^{*\prime}$. These show that $\mathbf{a}'_5$, $\mathbf{a}'_6$, $\sqrt{2}\mathbf{a}'_7$, $\sqrt{2}\mathbf{a}'_8$ are commensurable with $\mathbf{e}_i^*$ and $\mathbf{e}_i^{*\prime}$. The commensurability makes the 4D description possible.

The vectors $\mathbf{e}'_i$ reciprocal to $\mathbf{e}_i^{*\prime}$ are $\mathbf{e}'_i = \mathbf{e}_i - \mathbf{e}_{4+i}$ and $\mathbf{e}'_{4+i} = \mathbf{e}_i + \mathbf{e}_{4+i}$ $(i \leq 4)$. In the following, x_i stand for the coordinates with respect to $\mathbf{e}_i$ and x'_i stand for those to $\mathbf{e}'_i$ and vectors with coordinates x_i and x'_i are shown by $(x_1, x_2, \ldots, x_8)$ and $(x_1, x_2, \ldots, x_8)'$. The coordinates are transformed by $\tilde{S}^{-1} = S/2$ and the unit vectors $\mathbf{e}_i$ by S. The metric tensor has the form $\mathbf{e}_i \cdot \mathbf{e}_j = a_0^2\delta_{ij}$, indicating that the lattice is hypercubic, while $\mathbf{e}'_i \cdot \mathbf{e}'_j = 2a_0^2\delta_{ij}$ showing a hypercubic lattice with $a' = \sqrt{2}a_0$. [Rigorously speaking, we do not need a hypercubic lattice and can employ a lattice with lower symmetry which has lattice constants equal to the number of the irreducible representations (Janssen, 1986) but it is employed for simplicity.]

Since the determinant of the matrix S is $2^4 = 16$, the basis vectors $\mathbf{e}'_i$ span a sublattice of the original one which is spanned by $\mathbf{e}_i$. It should be noted that the sublattice is also a hypercubic lattice. There are 16 lattice points in the unit cell of the sublattice. If we consider them as the centering translations, the basis vectors give a different setting of the same lattice which has 16 centering translations. To obtain quasiperiodic patterns by the dual method, we need to place a polytope at each lattice point, which is the projection of the unit cell onto the internal space. Then the total symmetry is not hypercubic any more since the 16 points are not translationally equivalent and it is octagonal. Therefore, in the following, the 16 points are regarded as atom sites in 4D space, where the OD's are located and the lattice is regarded as the 2^4-fold superlattice. The 16 points in the unit cell of the superlattice are classified into six Wyckoff positions based on their site symmetry (see Table 1).

Table 1
The Wyckoff positions of the lattice points of the 8D hypercubic lattice in the superstructure cell.

The first column is the label used in Fig. 3. The second column stands for the order (number of equivalent positions). The third column is the site symmetry. The fourth and fifth columns show the first four coordinates of the position $\mathbf{x}$ in 8D space, which has the form $(\mathbf{0}, \mathbf{x}_0)$ and $(\mathbf{x}', -\mathbf{x}')$. The last column shows the $\mathbf{a}_8$ component of $\mathbf{x}$, $\mathbf{x} \cdot \mathbf{a}_8$, in units of $a_0/\sqrt{8}$.

Label	Order	Site symmetry	$\mathbf{x}_0$	$\mathbf{x}'$	γ
A	1	$8mm$	$(0,0,0,0)_0$	$(0,0,0,0)'$	0
B	4	mm	$(1,0,0,0)_0$	$(1,0,0,0)/2'$	1/2
C	4	mm	$(1,1,0,0)_0$	$(1,1,0,0)/2'$	1
D	2	$4mm$	$(1,0,1,0)_0$	$(1,0,1,0)/2'$	1
E	4	mm	$(0,1,1,1)_0$	$(0,1,1,1)/2'$	3/2
F	1	$8mm$	$(1,1,1,1)_0$	$(1,1,1,1)/2'$	2

In the SM, the lattice point $\mathbf{r}_0$ appears in the external space when the OD intersects with the external space. The OD is a convex polygon and is obtained from the polytope which is a projection of the unit cell in 8D space onto the 6D internal space. The unit vectors $\mathbf{e}'_{4+i}$ $(i \leq 4)$ have no $\mathbf{a}_1$ and $\mathbf{a}_2$ components, so that they are perpendicular to the external space. Therefore the two vectors with the same $\mathbf{e}'_i$ components $(i \leq 4)$ are projected at the same position in the external space even if their $\mathbf{e}'_{4+i}$ $(i \leq 4)$ components are different. The intersection of the polytope with the four-dimensional space spanned by $\mathbf{e}'_i$ $(i \leq 4)$ gives the OD. The ODs at the 16 points mentioned above are generally different. Those of the positions belonging to the same Wyckoff position are, however, related to each other by symmetry operations.

First we consider the simplest case, where the external space passes through the origin of the lattice. Then the external space passes through the origin or other corners of the polytope as shown below. Let the positions of each corner of the polytope be $\mathbf{y} = (y_1, \ldots, y_8)$, with $y_i = 0$ or 1 $(i \leq 8)$. The positions of the corners of the polytope at $\mathbf{x}$ are $\mathbf{x} + \mathbf{y}$. When these are on the external plane passing through the origin, their $\mathbf{a}_i$ $(i = 5, 6, 7, 8)$ components $\mathbf{x} \cdot \mathbf{a}_i + \mathbf{y} \cdot \mathbf{a}_i$ must be zero. This relation is fulfilled for some corners of the polytope. The 2^8 corners $\mathbf{y}$ of the polytope are classified into groups with their $\mathbf{a}_i$ $(i = 5, 6, 7, 8)$ components $\mathbf{y} \cdot \mathbf{a}_i$. The OD for the Wyckoff position $\mathbf{x}$ is defined by the groups with the $\mathbf{y} \cdot \mathbf{a}_i$ $(i = 5, 6, 7, 8)$, which are equal to $-\mathbf{x} \cdot \mathbf{a}_i$. This is a convex polygon consisting of the outermost points.

An infinite number of octagonal patterns is obtained by considering the external space passing through $\sqrt{8}\gamma a_0 \mathbf{a}_8$ with $0 \le \gamma \le 0.25$, since $\mathbf{a}_8$ is the basis vector of the identity representation. Consider the edge vector $\Delta\mathbf{y} = (\Delta y_1, \Delta y_2, \ldots, \Delta y_8)$ going out from the corner $\mathbf{y}$ of the unit cell. They are vectors $\Delta y_i = 1$ for $y_i = 0$ and zero for others. Therefore their number is equal to the number of zeros in $(y_1, y_2, \ldots, y_8)$. It depends on the corner $\mathbf{y}$. We remove the redundant internal space components from $\Delta\mathbf{y}$ except for $\mathbf{a}_8$ components, which is denoted by $\Delta\mathbf{y}'$. Then the points $\mathbf{x} + \mathbf{y} + (\sqrt{8}\gamma a_0/g)\Delta\mathbf{y}'$ are on the external space and define the ODs for the position $\mathbf{x}$, where g is the $\mathbf{a}_8$ component of $\Delta\mathbf{y}$. The ODs for $\gamma = 0.25$ and 0.1 are shown in Fig. 3. All the ODs are the same for $\gamma = 0.25$ and have octagonal symmetry. This means that all the Wyckoff positions are equivalent under the translations $(1, 0, 0, 0)'/2$ *etc.* and the structure has a smaller unit cell with half the lattice constant. This gives the BP with edge length $a_0/2$. The other cases can be regarded as superstructures of this as is clear from the diffraction patterns shown later. On the other hand, $\gamma = 0$ gives the BP with an edge length of a_0 in which each rhombus or square consists of four small rhombi or squares with an edge length of $a_0/2$. It is intuitively clear that this is a superstructure of the BP since the edge length is doubled. Direct calculations show that these ODs give the same pattern as that with the same γ derived from the dual method.

(*b*) *Icosahedral patterns*. The ODs of icosahedral patterns corresponding to those discussed in the previous section can be obtained by a similar method. The unit vectors of the 12D lattice $\mathbf{e}_i^*$ $(i \le 12)$ are given by the unit vectors $\mathbf{a}_i$ $(i \le 12)$ of the 3D space $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ and the 9D internal space $\mathbf{a}_4, \ldots, \mathbf{a}_{12}$. The transformation matrix M is obtained from the 12D representation of the icosahedral group based on the unit vectors $\mathbf{e}_i^*$ and its irreducible representations. In the present case, each 12×12 integral matrix is reduced to a $3 + 3 + 5 + 1$ block-diagonal matrix by the standard group-theoretical technique (Kramer & Neri, 1984; Janssen, 1986). In particular, the one-dimensional representation is the identity representation. When $\mathbf{a}_1, \ldots, \mathbf{a}_6$ are the basis vectors of the two 3D irreducible representations and $\mathbf{a}_7, \ldots, \mathbf{a}_{12}$ are those of the 5D and 1D irreducible representations, the matrix M has the form of equation (7) with the following 6×6 matrices M_1 and M_2.

$$\mathrm{M}_1 = \frac{1}{2}\begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 1 \\ c_1 s & s_1 s & c & c_2 s & s_2 s & -c \\ c_2 s & s_2 s & c & c_4 s & s_4 s & -c \\ c_3 s & s_3 s & c & c_1 s & s_1 s & -c \\ c_4 s & s_4 s & c & c_3 s & s_3 s & -c \\ c_5 s & s_5 s & c & c_5 s & s_5 s & -c \end{bmatrix}, \qquad (13)$$

Table 2
The Wyckoff positions of the lattice points of the 12D hypercubic lattice in the superstructure cell.

The first column is the label used in Fig. 4. The second and third columns give their order and site symmetry. The fourth and fifth columns show the first six coordinates of the position $\mathbf{x}$ in 12D space, which has the form $(\mathbf{0}, \mathbf{x}_0)$ and $(\mathbf{x}', -\mathbf{x}')$. The last column shows the $\mathbf{a}_{12}$ component of $\mathbf{x}$, $\mathbf{x}\cdot\mathbf{a}_{12}$ in units of $a_0/\sqrt{12}$.

Label	Order	Site symmetry	$\mathbf{x}_0$	$\mathbf{x}'$	γ
A	1	$m\bar{3}\bar{5}$	$(0, 0, 0, 0, 0, 0)_0$	$(0, 0, 0, 0, 0, 0)'$	0
B	6	$\bar{5}m$	$(1, 0, 0, 0, 0, 0)_0$	$(1, 0, 0, 0, 0, 0)/2'$	1/2
C	15	mmm	$(1, 1, 0, 0, 0, 0)_0$	$(1, 1, 0, 0, 0, 0)/2'$	1
D	10	$\bar{3}m$	$(1, 1, 1, 0, 0, 0)_0$	$(1, 1, 1, 0, 0, 0)/2'$	3/2
E	10	$\bar{3}m$	$(0, 0, 0, 1, 1, 1)_0$	$(0, 0, 0, 1, 1, 1)/2'$	3/2
F	15	mmm	$(1, 1, 1, 1, 0, 0)_0$	$(1, 1, 1, 1, 0, 0)/2'$	2
G	6	$\bar{5}m$	$(1, 1, 1, 1, 1, 0)_0$	$(1, 1, 1, 1, 1, 0)/2'$	5/2
H	1	$m\bar{3}\bar{5}$	$(1, 1, 1, 1, 1, 1)_0$	$(1, 1, 1, 1, 1, 1)/2'$	3

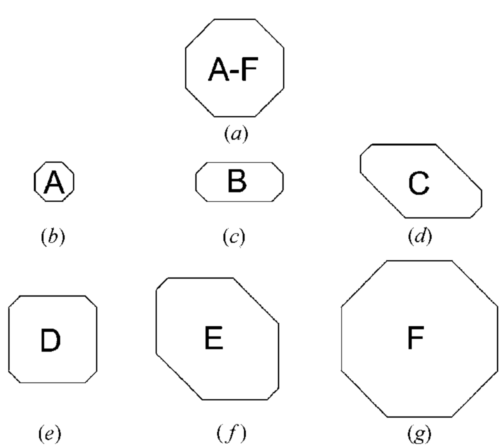


Figure 3
The occupation domains for the six independent Wyckoff positions of octagonal patterns given in Table 1. (*a*) $\gamma = 0.25$. (*b*)–(*g*) $\gamma = 0.1$.

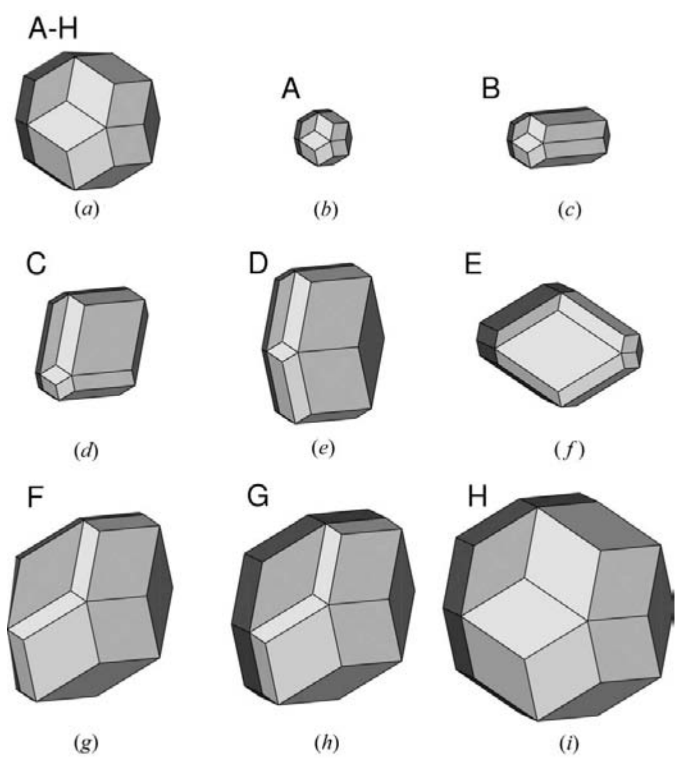


Figure 4
The occupation domains for the eight independent Wyckoff positions of icosahedral patterns shown in Table 2. (*a*) $\gamma = 0.25$. (*b*)–(*i*) $\gamma = 0.1$.

Table 3
The vectors defining the independent polygons in the occupation domains for generalized octagonal patterns.

The vectors $\mathbf{e}_j$ ($j = 1, 2, \ldots$) represent the corners of an occupation domain from its center. The superscript i means the internal space component. The two vectors defining a triangle are represented by (i,j) in the last line, where i and j represent the ith and jth vectors. The occupation domain is generated from the independent triangles by the site symmetry given in the heading. ($s = \frac{1}{2} - \gamma$ and $t = \gamma$.)

OD A $8mm$					
$\mathbf{e}_1 = (t, -t, 0, t)^i$	$\mathbf{e}_2 = (t, -t, -t, t)^i$				
(1,2)					
OD B mm					
$\mathbf{e}_1 = (s, -t, 0, t)^i$	$\mathbf{e}_2 = (s, -t, -t, t)^i$	$\mathbf{e}_3 = (s, t, -t, t)^i$	$\mathbf{e}_4 = (-s, t, -t, t)^i$	$\mathbf{e}_5 = (-s, t, -t, -t)^i$	$\mathbf{e}_6 = (-s, t, 0, -t)^i$
(1,2), (2,3), (3,4), (4,5), (5,6)					
OD C mm					
$\mathbf{e}_1 = (s, -s, t, t)^i$	$\mathbf{e}_2 = (s, -s, -t, t)^i$	$\mathbf{e}_3 = (s, s, -t, t)^i$	$\mathbf{e}_4 = (-s, s, -t, t)^i$	$\mathbf{e}_5 = (-s, s, -t, -t)^i$	
(1,2), (2,3), (3,4), (4,5)					
OD D $4mm$					
$\mathbf{e}_1 = (s, -t, 0, t)^i$	$\mathbf{e}_2 = (s, -t, -s, t)^i$	$\mathbf{e}_3 = (s, t, -s, t)^i$	$\mathbf{e}_4 = (0, t, -s, t)^i$		
(1,2), (2,3), (3,4)					
OD E mm					
$\mathbf{e}_1 = (s, -s, s, 0)^i$	$\mathbf{e}_2 = (s, -s, s, t)^i$	$\mathbf{e}_3 = (s, -s, -s, t)^i$	$\mathbf{e}_4 = (s, s, -s, t)^i$	$\mathbf{e}_5 = (-s, s, -s, t)^i$	$\mathbf{e}_6 = (-s, s, -s, 0)^i$
(1,2), (2,3), (3,4), (4,5), (5,6)					
OD F $8mm$					
$\mathbf{e}_1 = (s, -s, 0, s)^i$	$\mathbf{e}_2 = (s, -s, -s, s)^i$				
(1,2)					

where $c_i = \cos(2\pi i/5)$, $s_i = \sin(2\pi i/5)$, $c = \cos\theta$ and $s = \sin\theta$ with $\theta = \cos^{-1}(1/\surd 5)$ and

$$\mathrm{M}_2 = \frac{1}{2\surd 6}\begin{bmatrix} \surd 3 & -1 & \surd 2 & \surd 3 & -1 & \surd 2 \\ -\surd 3 & -1 & \surd 2 & -\surd 3 & -1 & \surd 2 \\ 0 & 2 & \surd 2 & 0 & 2 & \surd 2 \\ -\surd 3 & 1 & -\surd 2 & \surd 3 & -1 & \surd 2 \\ \surd 3 & 1 & -\surd 2 & -\surd 3 & -1 & \surd 2 \\ 0 & -2 & -\surd 2 & 0 & 2 & \surd 2 \end{bmatrix}. \qquad (14)$$

The 6D expression of the icosahedral patterns is obtained from the superlattice spanned by $\mathbf{e}'_i = \mathbf{e}_i - \mathbf{e}_{6+i}$ and $\mathbf{e}'_{6+i} = \mathbf{e}_i + \mathbf{e}_{6+i}$ $(i \le 6)$, which are reciprocal to $\mathbf{e}^{*\prime}_i = (\mathbf{e}^*_i - \mathbf{e}^*_{6+i})/2$ and $\mathbf{e}^{*\prime}_{6+i} = (\mathbf{e}^*_i + \mathbf{e}^*_{6+i})/2\,(i \le 6)$. The block-diagonal matrix in the present case is also given by equation (11) with M_1 and M_2 given above. The unit vectors $\mathbf{e}_i$ and $\mathbf{e}'_i$ span the hypercubic lattices with the lattice constants of $a = a_0$ and $a' = \surd 2 a_0$. It should be noted that $\surd 2\mathbf{a}^*_7$, $\surd 6\mathbf{a}^*_8$, $\surd 3\mathbf{a}^*_9$, $\surd 2\mathbf{a}^*_{10}$, $\surd 6\mathbf{a}^*_{11}$, $\surd 3\mathbf{a}^*_{12}$ are commensurable with $\mathbf{e}^*_i$ and $\mathbf{e}^{*\prime}_i$.

The transformation matrix S has a form similar to equation (12), the non-zero elements of which are $\mathrm{S}_{ii} = 1$ $(i \le 12)$, $\mathrm{S}_{i(i+6)} = -1$ $(i \le 6)$ and $\mathrm{S}_{(i+6)i} = 1$ $(i \le 6)$. The determinant of S is $2^6 = 64$. There are 64 lattice points of the original lattice in the unit cell of the superlattice. These positions are classified into eight Wyckoff positions shown in Table 2. In order to obtain the ODs located at these positions, we consider the edge vectors $\Delta\mathbf{y}$ going out from the corner $\mathbf{y}$. We remove the redundant internal space components from $\Delta\mathbf{y}$ and denote it as $\Delta\mathbf{y}'$. Then $\mathbf{x} + \mathbf{y} + (\surd 12\gamma a_0/g)\Delta\mathbf{y}'$ are on the external space passing through $\surd 12\gamma a_0\mathbf{a}_{12}$, where g is the $\mathbf{a}_{12}$ component of $\Delta\mathbf{y}$. The outermost points of them construct the ODs. Fig. 4 shows the ODs for $\gamma = 0.25$ and 0.1. Note that all the ODs are the same rhombic triacontahedron with an edge length of $a_0/2$ for $\gamma = 0.25$. Therefore this structure has a half period in the 6D space. Similarly to the octagonal case, the pattern with $\gamma = 0$ gives the 3DPP with the edge length of a_0, where each rhombohedron with an edge length of a_0 is divided into eight rhombohedra with the same shape but half the edge length. For the intermediate cases with $0 < \gamma < 0.25$, the consecutive rhombi with the same orientation appear sometimes as in the case of $\gamma = 0$. Their frequency becomes smaller with approaching $\gamma = 0.25$. As is well known, 3DPP has no such arrangement of rhombohedra.

Finally, we point out that the total area or volume of all occupation domains in a unit cell remains unchanged by the change of γ. This means that the point density of the pattern is the same and is independent of the different arrangements of points. Therefore, a slight change in γ causes a phason flip. γ changes continuously, so that we get an infinite number of octagonal and icosahedral patterns with the same point density.

4. Diffraction patterns

The diffraction pattern is obtained from the structure in the minimal dimension which is four in the octagonal structures and six in the icosahedral ones. The minimal spaces are the subspaces of the spaces spanned by $\mathbf{e}'_i$ $(i \le n/2)$, where n is 8 and 12 in the octagonal and icosahedral structures. Then the lattice constant is defined by $a' = \surd 2 a_0$. In the following sections, the projection of the positional vector onto this space is simply written as $\mathbf{x}$ and the prime is dropped for simplicity. The diffraction pattern is obtained from the Fourier integrals of the ODs obtained in the previous section. In the octagonal or icosahedral quasicrystal, the ODs are polygons or polyhedra. Then the structure factor is given by (Yamamoto & Ishihara, 1988; Yamamoto, 1992)

Table 4
The vectors defining the independent polyhedra in the occupation domains for generalized 3DPP.

The symbols are the same as in Table 2. Three vectors defining a tetrahedron are represented by (i,j,k) in the last line. The occupation domain is generated from the independent polyhedra by the site symmetry given in the heading. ($s = \frac{1}{2} - \gamma$ and $t = \gamma$.)

OD A $m\bar{3}\bar{5}$			
$\mathbf{e}_j = (-t, -t, -t, t, -t, t)^i$	$\mathbf{e}_j = (-t, -t, t, t, -t, t)^i$	$\mathbf{e}_j = (-t, 0, 0, t, -t, t)^i$	
(1,2,3)			
OD B $\bar{5}m$			
$\mathbf{e}_1 = (-s, -t, -t, t, -t, t)^i$	$\mathbf{e}_2 = (-s, -t, t, t, -t, t)^i$	$\mathbf{e}_3 = (-s, 0, 0, t, -t, t)^i$	$\mathbf{e}_4 = (0, -t, 0, t, -t, t)^i$
$\mathbf{e}_5 = (s, -t, -t, t, -t, t)^i$	$\mathbf{e}_6 = (-s, t, t, t, -t, t)^i$	$\mathbf{e}_7 = (-s, -t, t, -t, t, t)^i$	$\mathbf{e}_8 = (-s, -t, t, t, t, t)^i$
$\mathbf{e}_9 = (-s, 0, t, 0, t, t)^i$	$\mathbf{e}_{10} = (-s, t, t, t, t, t)^i$		
(1,2,3), (1,2,4), (1,5,4), (2,6,3), (7,8,9), (8,10,9)			
OD C mmm			
$\mathbf{e}_1 = (-s, -s, -t, t, -t, t)^i$	$\mathbf{e}_2 = (-s, -s, t, t, -t, t)^i$	$\mathbf{e}_3 = (-s, 0, 0, t, -t, t)^i$	$\mathbf{e}_4 = (-s, s, -t, t, -t, t)^i$
$\mathbf{e}_5 = (-s, s, t, t, -t, t)^i$	$\mathbf{e}_6 = (0, 0, -t, t, -t, t)^i$	$\mathbf{e}_7 = (-s, -s, t, -t, -t, t)^i$	$\mathbf{e}_8 = (-s, -s, t, -t, t, t)^i$
$\mathbf{e}_9 = (-s, -s, t, 0, 0, t)^i$	$\mathbf{e}_{10} = (0, -s, t, -t, 0, t)^i$	$\mathbf{e}_{11} = (s, -s, t, -t, -t, t)^i$	$\mathbf{e}_{12} = (s, -s, t, -t, t, t)^i$
$\mathbf{e}_{13} = (-s, s, -t, -t, t, -t)^i$	$\mathbf{e}_{14} = (-s, s, -t, t, t, -t)^i$	$\mathbf{e}_{15} = (-s, s, 0, 0, t, -t)^i$	$\mathbf{e}_{16} = (-s, s, t, -t, t, -t)^i$
$\mathbf{e}_{17} = (-s, s, t, t, t, -t)^i$	$\mathbf{e}_{18} = (-s, s, -t, t, t, t)^i$	$\mathbf{e}_{19} = (-s, s, 0, t, t, 0)^i$	
(1,2,3), (1,4,3), (2,5,3), (1,4,6), (4,5,3), (7,8,9), (7,8,10), (7,11,10), (8,12,10), (11,12,10), (13,14,15), (13,16,15), (14,17,15), (16,17,15), (14,18,19)			
OD D $\bar{3}m$			
$\mathbf{e}_1 = (-s, -s, -s, t, -t, t)^i$	$\mathbf{e}_2 = (-s, -s, s, t, -t, t)^i$	$\mathbf{e}_3 = (-s, 0, 0, t, -t, t)^i$	$\mathbf{e}_4 = (-s, s, s, t, -t, t)^i$
$\mathbf{e}_5 = (-s, -s, s, -t, -t, t)^i$	$\mathbf{e}_6 = (-s, -s, s, -t, t, t)^i$	$\mathbf{e}_7 = (-s, -s, s, 0, 0, t)^i$	$\mathbf{e}_8 = (0, -s, s, -t, 0, t)^i$
$\mathbf{e}_9 = (s, -s, s, -t, -t, t)^i$	$\mathbf{e}_{10} = (0, -s, s, 0, -t, t)^i$	$\mathbf{e}_{11} = (s, -s, s, t, -t, t)^i$	
(1,2,3), (2,4,3), (5,6,7), (5,2,7), (5,6,8), (5,9,8), (5,2,10), (5,9,10), (2,11,10), (9,11,10)			
OD E $\bar{3}m$			
$\mathbf{e}_1 = (t, -t, -t, -s, -s, -s)^i$	$\mathbf{e}_2 = (t, -t, t, -s, -s, -s)^i$	$\mathbf{e}_3 = (t, -t, 0, -s, -s, 0)^i$	$\mathbf{e}_4 = (t, -t, -t, -s, -s, s)^i$
$\mathbf{e}_5 = (t, -t, 0, -s, 0, -s)^i$	$\mathbf{e}_6 = (t, -t, -t, -s, s, -s)^i$	$\mathbf{e}_7 = (t, -t, t, -s, s, -s)^i$	$\mathbf{e}_8 = (t, -t, -t, 0, -s, 0)^i$
$\mathbf{e}_9 = (t, -t, -t, s, -s, s)^i$	$\mathbf{e}_{10} = (-t, -t, t, -s, s, -s)^i$	$\mathbf{e}_{11} = (-t, t, t, -s, s, -s)^i$	$\mathbf{e}_{12} = (0, 0, t, -s, s, -s)^i$
$\mathbf{e}_{13} = (t, t, t, -s, s, -s)^i$			
(1,2,3), (1,4,3), (1,2,5), (1,6,5), (2,7,5), (1,4,8), (4,9,8), (6,7,5), (10,11,12), (11,13,12)			
OD F mmm			
$\mathbf{e}_1 = (-s, -s, -s, s, -t, t)^i$	$\mathbf{e}_2 = (-s, -s, s, s, -t, t)^i$	$\mathbf{e}_3 = (-s, 0, 0, s, -t, t)^i$	$\mathbf{e}_4 = (-s, s, -s, s, -t, t)^i$
$\mathbf{e}_5 = (0, -s, 0, s, -t, t)^i$	$\mathbf{e}_6 = (-s, s, s, s, -t, t)^i$	$\mathbf{e}_7 = (-s, -s, s, -s, -t, t)^i$	$\mathbf{e}_8 = (-s, -s, s, -s, t, t)^i$
$\mathbf{e}_9 = (-s, -s, s, 0, 0, t)^i$	$\mathbf{e}_{10} = (0, -s, s, -s, 0, t)^i$	$\mathbf{e}_{11} = (s, -s, s, -s, -t, t)^i$	$\mathbf{e}_{12} = (-s, -s, s, s, t, t)^i$
$\mathbf{e}_{13} = (s, -s, s, -s, t, t)^i$	$\mathbf{e}_{14} = (-s, 0, s, 0, t, t)^i$	$\mathbf{e}_{15} = (-s, s, -s, s, -t, -t)^i$	$\mathbf{e}_{16} = (-s, s, -s, s, 0, 0)^i$
(1,2,3), (1,4,3), (1,2,5), (2,6,3), (4,6,3), (7,8,9), (7,2,9), (7,8,10), (7,11,10), (8,12,9), (8,13,10), (2,12,9), (11,13,10), (8,12,14), (15,4,16)			
OD G $\bar{5}m$			
$\mathbf{e}_1 = (-s, -s, -s, s, -s, t)^i$	$\mathbf{e}_2 = (-s, -s, s, s, -s, t)^i$	$\mathbf{e}_3 = (-s, 0, 0, s, -s, t)^i$	$\mathbf{e}_4 = (-s, s, -s, s, -s, t)^i$
$\mathbf{e}_5 = (0, 0, -s, s, -s, t)^i$	$\mathbf{e}_6 = (s, s, -s, s, -s, t)^i$	$\mathbf{e}_7 = (-s, -s, s, -s, s, -t)^i$	$\mathbf{e}_8 = (-s, -s, s, -s, s, t)^i$
$\mathbf{e}_9 = (-s, 0, s, -s, s, 0)^i$	$\mathbf{e}_{10} = (-s, s, s, -s, s, -t)^i$		
(1,2,3), (1,4,3), (1,4,5), (4,6,5), (7,8,9), (7,10,9)			
OD H $m\bar{3}\bar{5}$			
$\mathbf{e}_1 = (-s, -s, -s, s, -s, s)^i$	$\mathbf{e}_2 = (-s, -s, s, s, -s, s)^i$	$\mathbf{e}_3 = (-s, 0, 0, s, -s, s)^i$	
(1,2,3)			

$$F(\mathbf{q}) = \sum_{\{\mathrm{R}|\tau\}} \sum_{\mu} a^{\mu} f^{\mu}(\mathbf{q}^e) p^{\mu} \exp[-B^{\mu}(q^e)^2/4] \times \exp[2\pi i \mathbf{q} \cdot (\mathrm{R}\mathbf{x}^{\mu} + \tau)] F_0^{\mu}(\mathrm{R}^{-1}\mathbf{q}), \qquad (15)$$

where the multiplicity, position, temperature factor and occupancy of the μth independent ODs are represented by a^{μ}, $\mathbf{x}^{\mu}$, B^{μ} and p^{μ}. $F_0^{\mu}(\mathbf{q})$ and $f^{\mu}(\mathbf{q}^e)$ are the Fourier integral and atomic scattering factor of the μth OD at the diffraction vector $\mathbf{q}$ and its external space component $\mathbf{q}^e$. $F_0^{\mu}(\mathbf{q})$ is calculated by using the symmetry of the shape of ODs from the independent parts, which are decomposed into several triangles or tetrahedra. Thus the structure factor consists of the summation of Fourier integrals of triangles or tetrahedra which are given analytically. In the present cases, there exist six or eight independent sites in general as shown in the previous section. In order to calculate the Fourier integral of an OD, the site symmetry is applicable as shown in a previous paper (Yamamoto, 1996). This enables us to calculate the Fourier integral from that of a smaller independent part. Corner vectors of each independent part are listed in Tables 3 and 4. In Figs. 5 and 6, the diffraction patterns corresponding

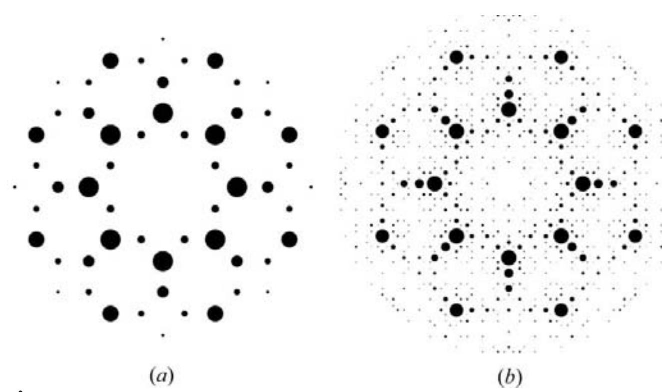


Figure 5
Diffraction patterns of octagonal patterns for (a) $\gamma = 0.25$ and (b) 0.1.

to the cases given in previous sections are shown. As is clear from the comparison between Figs. 5(*a*) and 5(*b*) or Figs. 6(*a*)–(*c*) and Figs. 6(*d*)–(*f*), there are satellite reflections in the latter that are absent in the former. In particular, it is noted that in the latter there exists a reflection at the midpoint of two reflections in the former. This clearly shows that the latter is a superstructure of the former.

5. Concluding remarks

The present paper shows that the octagonal and icosahedral patterns derived from 8 and 12 grids by the DM are superstructures of the Beenker pattern and the three-dimensional Penrose pattern. They can be expressed in four- and six-dimensional spaces with a larger unit cell. As a result, satellite reflections appear in their diffraction patterns. The derivation of the occupation domains for a general case was given.

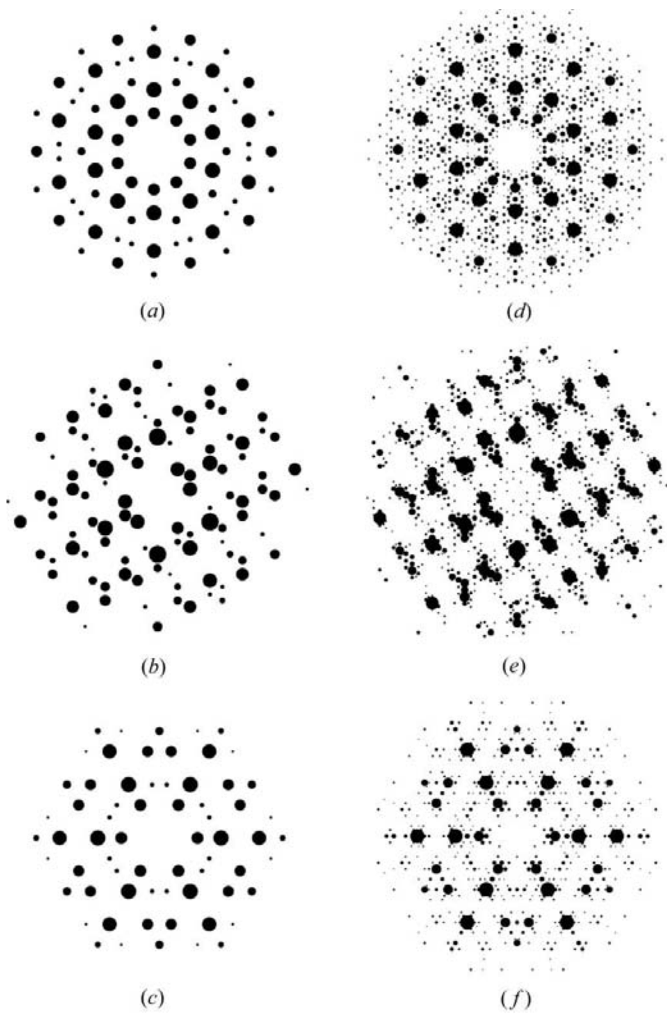


Figure 6
Diffraction patterns of icosahedral patterns for (*a*)–(*c*) $\gamma = 0.25$ and (*d*)–(*f*) $\gamma = 0.1$. Upper, middle and lower figures are fivefold, twofold and threefold patterns.

APPENDIX *A*

We show the distribution of singular points in the dual method discussed in §2. It is sufficient to consider the case with $\gamma_i' = 0$ since non-zero γ_i' leads to a locally isomorphic pattern (see text).

We consider first the octagonal patterns. Then $\gamma_i = \gamma_{i+4} = \gamma$ $(i = 1, 2, 3, 4)$. Let the three grid lines normal to $\mathbf{e}_i^*$, $\mathbf{e}_j^*$ and $\mathbf{e}_j^*$ $(i \neq j \neq k \bmod 4)$ cross at $\mathbf{y}$. Then from equation (1),

$$\begin{bmatrix} \mathrm{c}_i & \mathrm{s}_i \\ \mathrm{c}_j & \mathrm{s}_j \\ \mathrm{c}_k & \mathrm{s}_k \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} n_i + \gamma \\ n_j + \gamma \\ n_k + \gamma \end{bmatrix}, \tag{16}$$

where $\mathrm{c}_i = \cos(2\pi i/8)$ and $\mathrm{s}_i = \sin(2\pi i/8)$. The solution of the above equation exists if and only if the following condition is fulfilled.

$$\begin{vmatrix} \mathrm{c}_i & \mathrm{s}_i & n_i + \gamma \\ \mathrm{c}_j & \mathrm{s}_j & n_j + \gamma \\ \mathrm{c}_k & \mathrm{s}_k & n_k + \gamma \end{vmatrix} = 0. \tag{17}$$

We write the determinant of the 2×2 matrix $M(ij)$ formed by $(\mathrm{c}_i, \mathrm{s}_i)$ and $(\mathrm{c}_j, \mathrm{s}_j)$ as Δ_{ij}. Then the above equation becomes

$$\Delta_{jk} n_i - \Delta_{ik} n_j + \Delta_{ij} n_k = -(\Delta_{jk} - \Delta_{ik} + \Delta_{ij})\gamma. \tag{18}$$

$|\Delta_{ij}|$ represents the area of the rhombus (or square) with edge vectors with unit length, $\mathbf{e}_i^*/a_0^*$ and $\mathbf{e}_j^*/a_0^*$, which is similar to the rhombus or the square appearing in the octagonal pattern shown in Fig. 1. It is, therefore, $1/\sqrt{2}$ or 1.

Instead of solving the above equation for all possible triplets (i, j, k), we can solve it for topologically different cases. There are three such cases: $(1, 2, 3)$, $(1, 3, 4)$, $(1, 3, 6)$. Since $\Delta_{12} = \Delta_{23} = \Delta_{34} = 1/\sqrt{2}$ and $\Delta_{13} = 1$ and $\Delta_{14} = \Delta_{36} = -1/\sqrt{2}$, equation (18) for these three cases leads to

$$(n_i + n_k)/\sqrt{2} - n_j = -(\sqrt{2} - 1)\gamma \tag{19}$$

$$(n_i + n_j)/\sqrt{2} + n_k = -(\sqrt{2} + 1)\gamma \tag{20}$$

$$-(n_i + n_k)/\sqrt{2} + n_k = (-\sqrt{2} - 1)\gamma. \tag{21}$$

This means that, for a given γ $(0 < \gamma < 1/4)$, these have no solution in general, except for an accidental case where the right-hand sides are given by an integral linear combination of 1 and $1/\sqrt{2}$. In the trivial case with $\gamma = 0$, $n_i = n_j = n_k = 0$ is the solution. Except for such a point, there exists no singularity. This leads to the conclusion that, for a given triplet (i, j, k), these equations cross at one point at most.

Similarly, in the icosahedral patterns, if the four planes normal to $\mathbf{e}_i^*$, $\mathbf{e}_j^*$, $\mathbf{e}_k^*$ and $\mathbf{e}_l^*$ $(i \neq j \neq k \neq l \bmod 6)$ cross at one point, the equation

$$\begin{vmatrix} \mathrm{c}_i\mathrm{s} & \mathrm{s}_i\mathrm{s} & \mathrm{c} & n_i + \gamma \\ \mathrm{c}_j\mathrm{s} & \mathrm{s}_j\mathrm{s} & \mathrm{c} & n_j + \gamma \\ \mathrm{c}_k\mathrm{s} & \mathrm{s}_k\mathrm{s} & \mathrm{c} & n_k + \gamma \\ \mathrm{c}_l\mathrm{s} & \mathrm{s}_l\mathrm{s} & \mathrm{c} & n_l + \gamma \end{vmatrix} = 0 \tag{22}$$

should be fulfilled, where $\mathrm{c}_i = \cos(2\pi i/5)$, $\mathrm{s}_i = \cos(2\pi i/5)$, $\mathrm{c} = \cos(\theta)$ and $\mathrm{s} = \sin(\theta)$. This leads to the condition

$$\Delta_{jkl}n_i - \Delta_{ikl}n_j + \Delta_{ijl}n_k - \Delta_{ijk}n_l = -(\Delta_{jkl} - \Delta_{ikl} + \Delta_{ijl} - \Delta_{ijk})\gamma, \quad (23)$$

where Δ_{ijk} is the determinant of the 3×3 matrix $M(ijk)$ defined by ($c_i s, s_i s, c$), ($c_j s, s_j s, c$), ($c_k s, s_k s, c$), the absolute value of which gives the volume of the acute or obtuse rhombohedron similar to those appearing in Fig. 2 but with a unit edge length. It is, therefore, given by either $V_1 = (2\sqrt{2+\tau})/5$ or $V_2 = (2\sqrt{3-\tau})/5$. The ratio $V_1/V_2 = \tau = (1+\sqrt{5})/2$ is an irrational number.

There are three topologically different quartets (i,j,k,l): $(1,2,3,4)$, $(1,2,3,5)$, $(2,3,4,5)$. Since $\Delta_{123} = \Delta_{134} = -\Delta_{235} = -\Delta_{245} = V_1$ and $\Delta_{124} = \Delta_{234} = -\Delta_{125} = \Delta_{135} = \Delta_{345} = V_2$, equation (23) for these cases is given by

$$(-n_j - n_l)\tau + (n_i + n_k) = 2\tau^{-1}\gamma \quad (24)$$

$$-(n_i + n_l)\tau - (n_j + n_k) = 2\tau^2\gamma \quad (25)$$

$$(n_j - n_k)\tau + (n_i - n_l) = 0. \quad (26)$$

The first two have no solution in general, while the last one has a solution $n_i = n_l$, $n_j = n_k$. Note that, even in this case, the point density of such singular points is zero since such points have one-to-one correspondence to 2D lattice points and the point density of the 2D lattice points in 3D space is zero. All the singular points are on a plane normal to the vector defined by $(\mathbf{e}_2^* + \mathbf{e}_5^*) \times (\mathbf{e}_3^* + \mathbf{e}_4^*)$.

In the case where the five planes intersect at the same point, we need to consider the condition for a specified quintet (i,j,k,l,m). It is, however, sufficient to consider the case, where (i,j,k,l) has a solution, in order to find possible solutions. There is only one case $(i,j,k,l,m) = (2,3,4,5,6)$ which has a solution. In this case, in addition to the condition given by equation (23), another condition which is obtained from it by replacing the suffix l with m is imposed. Therefore, we consider the quintet $(i,j,k,l,m) = (2,3,4,5,6)$. In this case, in addition to equation (23), the other condition

$$\Delta_{346}n_i - \Delta_{246}n_j + \Delta_{236}n_k - \Delta_{234}n_m = -(\Delta_{346} - \Delta_{246} + \Delta_{236} - \Delta_{234})\gamma \quad (27)$$

should be fulfilled. Since $-\Delta_{246} = -\Delta_{346} = V_1$ and $\Delta_{236} = \Delta_{456} = V_2$, we have

$$(-n_i + n_j)\tau + (n_k - n_m) = 0. \quad (28)$$

Equations (27) and (28) lead to the solution $n_i = n_j = n_k = n_l = n_m$. This means that all the singular points are on a line parallel to $\mathbf{e}_2^* + \mathbf{e}_3^* + \mathbf{e}_4^* + \mathbf{e}_5^* + \mathbf{e}_6^*$ (or $\mathbf{e}_1^*$). The point density of such singular points is again zero since each singular point corresponds to a lattice point of a 1D lattice. The above consideration concludes that, even if there exist singular points where more than two lines or three planes intersect at the same point, their point density is zero.

This work is partially supported by 'Core Research for Evolutional Science and Technology'.

References

Beenker, F. P. M. (1982). Report 82-WSK-04, pp. 1–66. Eindhoven University of Technology.

Bruijn, N. G. D. (1981). *Proc. K. Ned. Acad. Wet. Ser. A*, pp. 39–66.

Gähler, F. & Rhyner, J. (1986). *J. Phys. A*, **19**, 267–277.

Janssen, T. (1986). *Acta Cryst.* A**42**, 261–271.

Kramer, P. & Neri, R. (1984). *Acta Cryst.* A**40**, 580–587.

Socolar, J. E. S. (1989). *Phys. Rev. B*, **39**, 10519–10551.

Socolar, J. E. S. & Steinhardt, P. J. (1986). *Phys. Rev. B*, **34**, 617–647.

Whittaker, J. W. & Whittaker, R. M. (1988). *Acta Cryst.* A**44**, 105–112.

Yamamoto, A. (1992). *Phys. Rev. B*, **45**, 5217–5227.

Yamamoto, A. (1996). *Acta Cryst.* A**52**, 509–560.

Yamamoto, A. & Ishihara, K. N. (1988). *Acta Cryst.* A**44**, 707–714.