AN ESSENTIALLY-THREE-DIMENSIONAL QUASICRYSTAL

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As the generator of an essentially-3-D quasicrystal, some detail of a 3-D Penrose transformation is given. The expansion rate $\tau^3 = 4.236$ is by far the larger than ever believed value $\tau = 1.618$. The features of this model agree rather well with those of high-resolution electron micrograph. The Penrose logic of hierarchic generation of patterns is summarized and a new expression is also given for 2-D Penrose transformation.

1. Introduction

Crystallography is now in an epoch of revolution. It has been believed as established in the last century as the general system of possible configurational order. In that system, periodicity is the most important nature and any ordered configuration without periodicity is out of scope. Also in the electronic theory of solids, whose basis is Bloch theorem, periodicity is a priori assumed.

The discovery of the sharp Bragg spots with icosahedral symmetry by Shechtman et al.\(^1\) is giving a shock to the system of configurational order in the above mentioned situation. It has long been known that icosahedral symmetry or, more generally, five-fold symmetry, is incompatible with periodicity. Some sensitive people felt some unsatisfaction in the classical crystallography excluding five-fold symmetry from rather aesthetic interest. For example, Husimi\(^2\) had an idea of filling the inevitable gaps in a nonperiodic packing with regular pentagons of equal size. Among such attempts, Penrose\(^3\) succeeded in a tessellation of a plane with two kinds of tiles closely connected with pentagon, basing on the logic of a recursive pattern-generation. His tessellation\(^3-6\) is essentially nonperiodic, homogeneous, isotropic and self-similar in a sense. Along this stream of interest, Mackay\(^7,8\) tried the generalization of this tiling to 3-D case. These efforts were paid before the exciting experiment by Shechtman.\(^1\)

After the experiment, many people explore the concept of quasicrystal
and its structural image.\textsuperscript{9,10} Most of them are based on the 2-D Penrose pattern. Very recently, the present author\textsuperscript{11} found a 3-D Penrose transformation and pointed out some difference between 2-D and 3-D. An essentially 3-D quasicrystal, as ideal as possible, can be generated by the infinite-time-recursion of this transformation. The main purpose of this paper is to give a detail of this transformation.

2. Penrose Logic

In this section, the basic logic of generating an ideal nonperiodic pattern is summarized. It was originally introduced by Penrose in 1972 for 2-D case.\textsuperscript{3}

Prepare a proper initial pattern. Explicitly, in 2-D case, it is composed of two kinds of elements and must fill a certain condition. A pattern is transformed by a certain transformation rule for elements into another pattern which is also composed of the same two kinds of elements. This transformation is applied again and again. After infinite-time-iteration of this procedure, a whole plane is tiled with two kinds of elements. The pattern thus obtained is essentially nonperiodic and has some self-similarity or some hierarchic structure. Suppose a tiling of a plane with two kinds of tiles with properly designed figures on their face so that they are composed of miniature tiles of the same two kinds. Nonperiodicity is proved by the fact that a finite unit cell and a proper Bravais lattice can not be chosen since the composition ratio of two elements are irrational.\textsuperscript{5}

Here, a new expression of the 2-D Penrose transformation is given. In this version, the elements are two kinds of arrows. These two are the same arrows as introduced by de Bruijn;\textsuperscript{6} red arrows and green arrows of unit length, which, in prints in black, are indicated respectively with single arrows and double arrows. A set of transformation and an example of iterative transformation are given in Fig. 1. The plane gets tesselated with two kinds of rhombus whose sides are two kinds of arrows. The expansion ratio of this transformation is $\tau$.

In the extension to 3-D, it is an easy way to imitate the 2-D pattern and to stack such layers in a sense. Isotropy, however, can not be expected in a 3-D pattern thus obtained. In order to find an essentially-3-D transformation if any, it is necessary to recognize the difference in nature of spaces in 2- and 3-D. For example, an $n$-gon has the same number of sides and vertices and generally an $n$-hedron has different numbers of vertices and faces. Such a difference of topological nature of space brings some hints to find an essentially-3-D transformation. What we should learn from the 2-D case is not the results but the spirit and the logic.
Fig. 1. New expression of a set of 2-D Penrose transformation and some results of its iterative operation. (a): The elements are two kinds of arrows, single (red) and double (green). (b): Their transformation. From (a) to (b) is the definition of the transformation. (c) and (d): Their next two generations.

3. Some Geometrical Preparations

A golden rhombus is a rhombus the ratio of whose two diagonals is the golden number \( \tau = (1 + \sqrt{5})/2 \) plays a key role in such problems as connected with five-fold symmetry. The rhombohedra whose faces are all golden...
rhombus are only two kinds $A_6$ and $O_6$. There acute vertices of three rhombi meets at a principal vertex in the former and three obtuse vertices in the latter.

It is noted that these rhombohedra are consistent with icosahedral symmetry and a whole solid angle $4\pi$ can be composed only with these rhombohedra. It is also noted that the projection of a rhombic face of a golden rhombohedron onto the face normal to the third direction of the rhombohedron is either of acute and obtuse rhombi, the two elements in rhombic version of 2-D Penrose tiling.

Some useful geometrical data on golden rhombus and these two golden rhombohedra $A_6$ and $O_6$ are summarized in Table 1. Any configuration constructed with only these two kinds of golden rhombohedra has bond orientational long range order since other nearest neighbour vectors never appear in a thus constructed “mono-quasicrystal” in the weakest sense than the twelves icosahedraly arranged.

As a preparation for the discussion below, it is useful to introduce some terms and to see some typical configurations constructed with only $A_6$ and $O_6$. Some properties of them were studied by Miyazaki. 12)

A zonogon is defined as a $2p$-gon with $p$ pairs of parallel edges. A zonohedron is a convex polyhedron made of zonogons. A golden isozonohedron is a zonohedron whose faces are all golden rhombus. There are altogether five golden isozonohedra; dodecahedron (12-hedron) $B_{12}$, icosahedron (20-hedron) $F_{20}$ and triacontahedron (30-hedron) $K_{30}$ besides two hexahedra (6-hedra) $A_6$ and $O_6$. All of them can be constructed with only $A_6$ and $O_6$ in multiple manners. This multiplicity is related with a kind of stereoisomer. $A_6$ and $O_6$ fill the condition as the 3-D tiles of quasicrystalline configuration in a weak sense. Some properties of them are given in Appendix A.

4. 3-D Penrose Transformation

Golden rhombohedra, acute $A_6$ and obtuse $O_6$ are chosen as the two quasi-unit-cells of 3-D Penrose tiling as by Mackay. 7,8) By the 3-D Penrose transformation to be introduced in this section, these two rhombohedra are transformed into two expanded rhombohedra which are composed of only the two kinds of rhombohedra. The expansion ratio is $\tau^3$ which is the ratio of the length of the principal diagonal of $A_6$ to that of $O_6$. An expanded $A_6$ is composed of 55 $A_6$'s and 34 $O_6$'s and an expanded $O_6$ of 34 $A_6$'s and 21 $O_6$'s. These three numbers {21, 34, 55} are successive terms of the Fibonacci sequence $\{f_n, f_{n+1}=f_{n-1}+f_n, f_1=f_2=1\} = \{1, 1, 2, 3, 5, 8, 13, 21, 34, 55, \ldots\}$. The corresponding three terms are respectively {1, 1, 2} in the original 2-D Penrose transformation and {1, 2, 3} in the 3-D version suggested by Mackay. 7,8) The following matrices related with Fibonacci sequence are useful,
**TABLE 1. Some useful geometrical data.**

<table>
<thead>
<tr>
<th><strong>Golden Rhombus</strong></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>minor angle</td>
<td>$\theta = \tan^{-1}\frac{1}{2} = 1.107 = 63.43$</td>
</tr>
<tr>
<td>major angle</td>
<td>$\pi - \theta = 2.034 = 116.57$</td>
</tr>
<tr>
<td>minor diagonal</td>
<td>$d = \sqrt{2-2t} = 1.052$</td>
</tr>
<tr>
<td>major diagonal</td>
<td>$D = \sqrt{2+2t} = 1.701$</td>
</tr>
<tr>
<td>area</td>
<td>$S = 2t$</td>
</tr>
<tr>
<td></td>
<td>($t = \cos \theta = (2\tau-1)/5 = 1/\sqrt{5}$)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Acute Rhombohedron A$_6$</strong></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>dihedral angles</td>
<td>$2\pi/5$ at 6 principal edges*</td>
</tr>
<tr>
<td></td>
<td>$3\pi/5$ at other 6 edges</td>
</tr>
<tr>
<td>solid angles</td>
<td>$\pi/5$ at 2 principal vertices*</td>
</tr>
<tr>
<td></td>
<td>$3\pi/5$ at other 6 vertices</td>
</tr>
<tr>
<td>minor diagonals</td>
<td>$d_A = \sqrt{3-2t} = 1.451$</td>
</tr>
<tr>
<td>major diagonal</td>
<td>$D_A = \sqrt{3+6t} = 2.384$ (principal)</td>
</tr>
<tr>
<td>interfacial distance</td>
<td>$l_A = \sqrt{(1+t)/2} = 0.851$</td>
</tr>
<tr>
<td>volume</td>
<td>$V_A = t/\sqrt{2+2t} = 0.761$</td>
</tr>
</tbody>
</table>

The point $a + \tau^{-1} \xi$ in the representation in Appendix B, dividing the principal diagonal in the golden ratio, is equidistant from nine among twelve midpoints of twelve edges. The distance is $\sqrt{(5-8t)/2} = 0.596$.

<table>
<thead>
<tr>
<th><strong>Obtuse Rhombohedron O$_6$</strong></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>dihedral angles</td>
<td>$4\pi/5$ at 6 principal edges</td>
</tr>
<tr>
<td></td>
<td>$\pi/5$ at other 6 edges solid angles</td>
</tr>
<tr>
<td></td>
<td>$7\pi/5$ at 2 principal vertices</td>
</tr>
<tr>
<td></td>
<td>$\pi/5$ at other 6 vertices</td>
</tr>
<tr>
<td>minor diagonals</td>
<td>$d_0 = \sqrt{3-6t} = 0.563$ (principal)</td>
</tr>
<tr>
<td>major diagonal</td>
<td>$D_0 = \sqrt{3+2t} = 1.973$</td>
</tr>
<tr>
<td>interfacial distance</td>
<td>$l_0 = \sqrt{(1-t)/2} = 0.526$</td>
</tr>
<tr>
<td>volume</td>
<td>$V_0 = t/\sqrt{2-2t} = 0.470$</td>
</tr>
</tbody>
</table>

**Some Useful Relations**

$$D = \tau d, \quad D_A = \tau^2 d_0, \quad V_A = \tau V_0, \quad l_A = \tau l_0$$

*1 A principal vertex of a rhombohedron is the vertex on the trigonal axis. A rhombohedron has two principal vertices. The principal diagonal joins them. An edge crossing a principal vertex is a principal edge. A rhombohedron has six principal edges.
\[ F_n \equiv \begin{pmatrix} f_{n+1} & f_n \\ f_n & f_{n-1} \end{pmatrix} = F_n^1, \]  
(1)

\[ F_n \begin{pmatrix} \tau \\ 1 \end{pmatrix} = \tau^n \begin{pmatrix} \tau \\ 1 \end{pmatrix}, \quad F_n \begin{pmatrix} 1 \\ -\tau \end{pmatrix} = (-\tau)^{-n} \begin{pmatrix} 1 \\ -\tau \end{pmatrix}. \]  
(2)

The expansion rate of Penrose transformation is equal to the larger eigenvalue \( \tau^n \) of the corresponding matrix \( F_n \) whose elements are \( \{ f_{n+1}, f_n, f_{n-1} \} \).

The present transformation consists of two parts; the skeleton part and other part. The transformation uniquely decides only the skeleton structure, leaving some degrees of freedom undecided in contrast with the completely deterministic 2-D Penrose transformation. One of the origins of this difference is the abundance of the symmetry operations in higher dimensions; 3-D rotation has more degrees of freedom than 2-D and there is the possibility of the so-called stereoisomer or the right- and left-hands freedom. All the rhombic faces have the identical skeleton structure. Therefore any two faces are fitting each other Reminisce of the 2-D case; the sides of a rhombus are not simple segments but two kinds of arrows and are differently transformed.

The coordinates of 102 quasi-lattice-points in the skeleton of an expanded \( A_6 \) and 86 quasi-lattice-points in the skeleton of an expanded \( O_6 \) are given in Appendix B in the form of six integer representation. The instruction for the model construction of the expanded \( A_6 \) and \( O_6 \) with sticks and ball joints is given in Ref. (11).

A skeleton of an expanded \( A_6 \) consists of two empty triacontahedral cages overlapping each other and some acute-rich parts near the eight vertices of the expanded rhombohedron. It has some missing part around each of twelve edges. A skeleton of an \( O_6 \) looks like a hexagonal snowflake, though the symmetry is trigonal as it should be. Around each of its edges, there is a missing part as in the former case.

The following discussion generally holds. Suppose the situation that the symmetry of the outside of a zonohedron is rather high and that of its internal structure low. A configuration with the same internal structure and with a different direction is also available without affecting the surroundings. In other words, it is the freedom to choose an axis. Moreover, there is another freedom of the rotation around the axis. Both are the case now.

The inside of each triacontahedral cages can be treated independently of any other parts. Each of them has 104 different configurations of 9 internal quasi-lattice-points constructing 10 \( A_6 \)'s and 9 \( O_6 \)'s besides the central \( O_6 \) which partitions the two cages off. The derivation of the number 104 is given in Appendix B. The missing parts around an edge compose an \( F_{20} \) when the angle is closed. It is mentioned in the last section and Appendix A that \( F_{20} \) and \( K_{30} \) can be constructed only with some \( A_6 \)'s and \( O_6 \)'s.

After all, the number of possible configurations in an expanded
rhombohedron is $10^4 \cdot 10^3$ for 89 quasi-lattice-points in the acute case and $10^3$ for 55 quasi-lattice-points in the obtuse case.

It is noted that these numbers should be understood as lower bounds since there are some other less symmetrical configurations. The counting of the exact number is rather troublesome and is still an open question. It depends on the details of the definition of Penrose transformation. Here the author tried to find the one most highly symmetrical as possible.

5. 3-D Penrose Patterns

Starting with any configuration constructed with only $A_6$ and $O_6$, a 3-D Penrose pattern is generated by the infinite time recursive operation of the 3-D Penrose transformation mentioned in the previous section. In each operation in this recursion, the redundant part of the transformation may be chosen arbitrarily. Therefore, the meaning of self-similarity in this case is in a generalized sense. Any way, the composition $[A_d]/[O_6]$ tends to $\tau$ in the limit of infinite operations, as seen from the former of Eq. (2).

The system has a kind of residual entropy due to the multiplicity of the redundancy in the transformation. The structure of the redundancy in the whole recursive transformation is also hierarchic and it brings a geometric-series-like enhanced factor.

In the limit of infinitely large system, the value of the residual entropy per quasi-lattice-point is given by

$$S_0 = [\tau^2 \cdot (\tau^9 - 1)]^{-1} \cdot [\tau \cdot \ln (164^2 \cdot 10^3) + \ln 10^3] = 0.176 = \ln 0.193. \quad (3)$$

In this respect, a quasicrystal is more closely related with an amorphous configuration than ever thought on a base of incomplete knowledge on 3-D Penrose transformation.

6. Concluding Remarks

There are many common features to the projection of the present 3-D pattern (Fig. 2) to some symmetry axes and some experimental results. In the projection along a pentagonal axis, one of the six quasi-basic-vectors is reduced to a point and other five are vectors of length $2t=0.894$ pointing five vertices of a regular pentagon of side length $\sqrt{2(1-t)}=1.05$ from its center. These fives are the bases of 2-D Penrose pattern.

A striking feature of the projection of a skeleton along a pentagonal axis is the presence of regular decagons and its portions surrounded by a ring of regular pentagons. For example, in the case of Fig. 2(b), two overlapping decagons are surrounded with 14 pentagons after four points are properly supplied outside the rhombus. This pentagon in the present case is actually a
Fig. 2. The projection of the expanded rhombohedra $A_5$ and $O_5$ along five-fold axes. 
(a) and (b): $A_5$, (c) and (d): $O_5$. 
pentagram in the projection. It means that the concerned five points are not on a plane as the stars in a constellation are not. It is noted that the above mentioned decagon surrounded with pentagons are also regarded as a double ring of decagons.

Hiraga et al.\textsuperscript{13} pointed out the similar feature about their high-resolution electron micrograph along a pentagonal axis. The bright dots surrounded by decagonal double ring are distributed all over their image. If one marks such decagons then the marked regions are rather dominant and almost percolated. Figures 2(a) and 2(b), which are the projection of the skeleton of an expanded \textit{A}_6 along two five-fold axes, respectively correspond to Figs. 4(a) and 4(b) of Ref. (13).

Furthermore, the followings should be noted. The smallest decagons in the original version of 2-D Penrose tiling have six quasi-lattice-points in their inside. The same pattern is obtained from the whole configuration of \textit{F}_{20} and \textit{K}_{30} with all of their inner quasi-lattice-points by projection along a pentagonal axis. Bursill and Lin\textsuperscript{14} relates their experimental images to the original version of 2-D Penrose tiling.

According to Mackay,\textsuperscript{15} the self-similarity of linear factor $\tau^3$ is observed in electron micrograph by Portier \textit{et al.}\textsuperscript{16}

As for the composition of Al and Mn in the realized alloys, Kimura \textit{et al.} concluded to be nearly Al\textsubscript{13}Mn ($\sim$20.5at\%Mn).\textsuperscript{17} Compare with Al\textsubscript{6}Mn ($\sim$14.3at\%Mn) originally reported by Shechtman \textit{et al.}\textsuperscript{1} Two ideas are proposed for the atomic location by two experimentalist groups; Hiraga \textit{et al.}\textsuperscript{18} and Kimura \textit{et al.}\textsuperscript{19} Mn atoms are at the vertices of rhombohedra in both of them. Then each of \textit{A}_6 and \textit{O}_6 contains a manganese atom. The centers of every edges of them are occupied by an aluminum atom. That corresponds to three Al’s a rhombohedron. The difference between two assignments concerns the inside of \textit{A}_6. Two Al’s according to Hiraga \textit{et al.} and one according to Kimura \textit{et al.} are on a principal diagonal of \textit{A}_6. Therefore an \textit{A}_6 corresponds to Al\textsubscript{13}Mn in the former and to Al\textsubscript{6}Mn in the latter, while an \textit{O}_6 to Al\textsubscript{3}Mn in both. After all, two proposed values of the Mn-composition are $(2-\tau)/3 = 19.1\text{at}\%\text{Mn}$ and $(4-\tau)/11 = 21.7\text{at}\%\text{Mn}$ respectively by Hiraga \textit{et al.} and Kimura \textit{et al.} Though the value is open question, such a situation may be referred to as quasistoichiometry in that the composition of the stoichiometric quasi-unit-cells is irrational.

The author is indebted to Professor A. L. Mackay, Professor T. Ninomiya, Professor S. Hitotsumatsu, Professor K. Miyazaki, Professor S. Takeuchi, Professor K. Hiraga, Professor M. Hirabayashi, Professor M. Tanemura, Dr. K. Kimura, Dr. H. Aoki and Mr. K. Senba for valuable discussion.
Appendix A. Golden Isozonohedra; A₆, O₆, B₁₂, F₂₀, K₃₀

The definitions of zonohedron and golden isozonohedron are given in the text. Five golden isozonohedra are A₆, O₆, B₁₂, F₂₀ and K₃₀.

These are two golden rhombohedra A₆ and O₆. The angle of two edges at a principal vertex is acute in A₆ and obtuse in O₆.

Golden dodecahedron B₁₂, discovered by Bilinski, can be regarded as the locus of an A₆ or that of O₆. It is composed of 2 A₆’s and 2 O₆’s. Among 4 quasi-lattice-points altogether, three are on the surface and the other one inside. The one inside is chosen of 2 equivalent possibilities. The whole configuration of B₁₂ is four dimensional in the sense that only four kinds of nearest neighbour vectors are used among allowed six.

Golden icosahedron F₂₀, discovered by Fedrov, can be regarded as the locus of a B₁₂. It has a five-fold symmetry axis. It is composed of 5 A₆’s and 5 O₆’s. Among 10 quasi-lattice-points altogether, six are on the surface and the other four inside. The four inside are chosen of 10 equivalent possibilities. The whole configuration of F₂₀ is five-dimensional in the sense that only five kinds of nearest neighbour vectors are used among allowed six and the one parallel to the pentagonal axis is excluded.

Golden triacontahedron K₃₀, discovered by Kepler, can be regarded as the locus of an F₂₀. It has icosahedral symmetry. It is composed of 10 A₆’s and 10 O₆’s. Among 20 quasi-lattice-points altogether, ten are on the surface and the other ten inside. The ten inside are chosen of 400 equivalent possibilities. It is the minimum convex region where all of the allowed six nearest neighbour vectors appear.

It is noted that the same number of A₆’s and O₆’s are contained in three golden isozonohedra B₁₂, F₂₀, and K₃₀.

Appendix B. The Coordinates in the Six-Integer Representation

The configurations with bond orientational perfect long range order of icosahedral symmetry can be expressed in a form of six-integer-set. It is useful to introduce proper representation suitable for the purpose. For example, sometime trigonal and sometime pentagonal.

(1) The trigonal representation

The six quasi-bases, α-β-γ-ζ-η-ζ are taken so that

\[(\alpha, \beta) = (\beta, \gamma) = (\gamma, \alpha) = (\alpha, \eta) = (\alpha, \zeta) = (\beta, \zeta) = (\beta, \zeta) = (\gamma, \zeta) = (\gamma, \eta) = t\]

\[(\xi, \eta) = (\eta, \zeta) = (\zeta, \xi) = (\alpha, \xi) = (\beta, \eta) = (\gamma, \zeta) = -t\]

where \(t = \cos \theta = 1/\sqrt{5}\).
For example, they can be taken as follows;

\[ \alpha = (p, q, 0), \quad \xi = (-q, 0, p), \]
\[ \beta = (0, p, q), \quad \eta = (p, -q, 0), \]
\[ \gamma = (q, 0, p), \quad \zeta = (0, p, -q), \]

where \( p = \sqrt{(1 + i)/2} \) and \( q = \sqrt{(1 - i)/2} \).

There are following relations among them,

\[
\begin{align*}
p &= \tau q, \quad pq = p^2 - q^2 = \tau, \quad \alpha + \beta + \gamma = \tau^3 (\xi + \eta + \zeta), \\
\zeta &= -\alpha + \tau^{-1}(\beta + \gamma), \quad \eta = -\beta + \tau^{-1}(\gamma + \alpha), \quad \xi = -\gamma + \tau^{-1}(\alpha + \beta).
\end{align*}
\]

A representation by these bases is expressed as \((i, j, k, l, m, n)\).

(2)  **The pentagonal representation**

The six quasi-bases, \(A-B-C-D-E-Z\) are taken so that

\[
\begin{align*}
(A, B) &= (B, C) = (C, D) = (D, E) = (E, A) = (A, Z) \\
&= (B, Z) = (C, Z) = (D, Z) = (E, Z) = \tau, \\
(A, C) &= (B, D) = (C, E) = (D, A) = (E, B) = -\tau.
\end{align*}
\]

For example, they can be taken as follows;

\[ A = \alpha, \quad B = \beta, \quad C = \xi, \quad D = -\xi, \quad E = \eta \text{ and } Z = \gamma. \]

A representation by these bases is expressed as \([i, j, k, l, m, n]\).

(3)  **The coordinates**

The coordinates of quasi-lattice-points are listed in either of these representations.

In these three choices, if all of three formers or all of three latters are chosen, then the internal configuration has trigonal symmetry. There are twenty possibilities in the choice of the trigonal axis. In other six cases among \(2^3\) choices, there are three-times more possibilities for the direction of axis.

Therefore, there are altogether \(2^3 \times 20 = 160\) configurations for ten inner quasi-lattice-points for a fixed surface configuration. It is useful for the following discussion to note that seven trigonal surface quasi-lattice-points among twenty are occupied by the principal vertices of the inner \(O_6\)’s and one among the seven can be on a trigonal axis.

In the case of a triacontahedral cage in the skeleton of an expanded \(A_6\), an \(O_6\), which separate the cage into two parts, is already fixed. Then, only nine inner quasi-lattice-points have freedom and the number of configurations is reduced to as \(2^3 \times (1 + 3 + 3 \times 3) = 104\).
An Expanded Acute Rhombohedron: $A_6$

The Coordinates of 102 Quasi-Lattice-Points in the Skeleton of an Acute Rhombohedron

\[
\begin{align*}
(000000), & (100000), (010000), (001000), (011000), (101000), (110000), (111000), \\
(220000), & (222000), (222010), (222001), (222011), (222101), (222110), \\
(333111), & (433111), (343111), (334111), (434111), (443111), (444111), \\
(111100), & (111010), (211001), (121001), (112001), (122010), (222010), \\
(111010), & (111100), (211010), (121010), (112010), (122100), (222100), \\
(111001), & (111101), (211001), (121001), (112001), (122010), (222010), \\
(333110), & (333001), (233100), (323010), (332001), (322001), (232001), \\
(333101), & (333010), (233101), (323011), (332011), (322011), (232011), \\
(333011), & (333100), (233110), (323100), (332100), (322100), (232100), \\
(222201), & (222200), (222200), (222200), (222200), (222200), \\
(222201), & (222200), (222200), (222200), (222200), (222200). \\
\end{align*}
\]

An Expanded Obtuse Rhombohedron: $D_6$

The Coordinates of 86 Quasi-Lattice-Points in the Skeleton of an Obtuse Rhombohedron

\[
\begin{align*}
(000000), & (100000), (010000), (001000), (011000), (101000), (110000), (111000), \\
(000010), & (000100), (010100), (001100), (011100), (101000), (110000), (111000), \\
(000010), & (000100), (010100), (001100), (011100), (101000), (110000), (111000), \\
(000010), & (000100), (010100), (001100), (011100), (101000), (110000), (111000), \\
(100100), & (100100), (110100), (101100), (111100), (101000), (110000), (111000), \\
(100100), & (100100), (110100), (101100), (111100), (101000), (110000), (111000), \\
(100100), & (100100), (110100), (101100), (111100), (101000), (110000), (111000), \\
(100100), & (100100), (110100), (101100), (111100), (101000), (110000), (111000), \\
(100100), & (100100), (110100), (101100), (111100), (101000), (110000), (111000), \\
(100100), & (100100), (110100), (101100), (111100), (101000), (110000), (111000). \\
\end{align*}
\]

A Golden Dodecahedron: $B_{12}$

The Coordinates of 14 Surface Quasi-Lattice-Points

\[
\begin{align*}
(000000), & (100000), (010000), (001000), (000100), \\
(110000), & (101000), (010100), (001100), (000100), \\
(111000), & (110100), (101000), (010000), (001000). \\
\end{align*}
\]

The Coordinate of an Internal Quasi-Lattice-Point

\[
(100100) \text{ or } (011000)
\]

A Golden Icosahedron: $F_{20}$

The Coordinates of 22 Quasi-Lattice-Points

\[
\begin{align*}
(000000), & (111110), \\
(000000), & (010000), (001000), (000100), (000010), \\
(001100), & (000110), (100010), (100000), (101000), \\
(110100), & (111010), (011010), (010110), (001110), \\
(110110), & (111100), (011100), (101100), (100110), \\
(111110), & (110110), (101110), (100110), (101100), \\
(011110), & (001110). \\
\end{align*}
\]
The Coordinates of 4 Internal Quasi-Lattice-Points

There are ten possibilities

(1) [101000], [101100], [100100], [110100];
(2) [101000], [101100], [100100], [110100];
(3) [101000], [101100], [100100], [110100];
(4) [101000], [101010], [100100], [110100];
(5) [010010], [011010], [001010], [010100];
(6) [010010], [011010], [001010], [010100];
(7) [010010], [001100], [010100], [010100];
(8) [010010], [011010], [010100], [010100];
(9) [100100], [110100], [010100], [011010];
(10) [100100], [110100], [010100], [101000].

A Golden Triacountahedron: $K_{30}$

The Coordinates of 32 Surface Quasi-Lattice-Points

[000000], [111111],
[100000], [011100], [001000], [100100], [000100], [000000],
[001100], [000110], [100010], [110000], [011000],
[101010], [111100], [011100], [011010], [100110],
[000101], [000011], [100111], [110101], [100101],
[110001], [111001], [001101], [001011],

The Coordinates of 10 Internal Quasi-Lattice-Points

For example, [100100], [010100], [000101], [010101], [100101], [110100], [110101],
and for fixed these seven, the other three are chosen among the following six,
either of [110110] or [101001],
either of [010001] or [111100],
either of [011011] or [011111].

REFERENCES

long-ranged orientational order and no translational symmetry, Phys. Rev. Lett., 53,
1951–1953.
irregularity or aperiodicity), Sugaku Seminar, 8, June p. 40–46 (in Japanese).
[3] Penrose, R. (1974): The role of Aesthetics in pure and applied mathematical research,
rapidly cooled metals, Science, 229, 233–238. See references therein.
Note added in proof

Two numerical values 104 appearing in Section 4 and 160 appearing in Section 4 and Appendix B (3) are the corrected ones respectively from the original incorrect 164 and 400, which were reported in the talk at the Seminar and written in Ref. (11).

In the text, the Penrose transformation is described as an expansion or structuration of two rhombohedra A₀ and O₀ so that the logical structure map be clearly seen. The obtained structure may be more clearly seen by noting that a point is transformed into a flower dodecahedron Fl₀₆ consisting of 20 A₀'s (exactly speaking, a concave 60-hedron which looks like a dodecahedron each of whose 12 faces is a five-petalous flower). In this point of view, the tiling elements should not be regarded as A₀ and O₀ but as Fl₀₆, F₂₀, C=2K₃₀—O₀ and O₀.

Though the concept of self-similarity is useful, it may be better regarding it as a result of some local rule. Self-similarity, as a basic principle of a growing process, is a little curious: The situation may remind one a horoscope. If self-similarity is really the basic rule, an atom may have to know the position of its own star in deciding its position to attach. Therefore, it is expected that the basic rule is replaced by some local rule which leads the equivalent result.

In the discussion, Bennema gave a comment about the higher-dimensional crystallography. After that a very similar three-dimensional structure to the present model has been obtained as the projection of certain selected points of a six-dimensional simple cubic lattice to the three dimensional space. The relation between the two models have not been known until the author figured.
it out.22)

Some two-dimensional Penrose-like tilings are obtained by similar hierarchical transformations. Some of them have pentagonal symmetry and some others have octahedral symmetry.20)


DISCUSSION

Chernov
1. Physical meaning of elementary figures?
2. Elastic energy of the construction and its stability?
A: 1. We have some arbitrariness in the choice of a unit cell in conventional crystallography. A rhombohedron is the most convenient in many cases. In order to keep icosahedral symmetry, the present two elementary figures are at least convenient. Rigorously speaking, I don’t know whether these two are necessary or not. In 2-D, the rhombic version is the easiest to understand or the most familiar to physicists and crystallographers than any other versions essentially without any difference; pentagon-and-some-others, dirt-and-kite, etc.
2. Of course, energetical discussions are necessary as physics or material science. Crystallography as a system of possible arrangements is a kind of geometry. The problems can be separated. My work belongs to the latter category in the present stage. I, however, have an idea that this 3-D Penrose tiling may be preferable because of configurational entropy due to the degeneracy. It is sure that some idealized concepts are necessary apart from the problems as material science.

Kirkpatrick
Is it a requirement that each atom have 12 nearest regions.

Bennema
Up till 15 years ago the 230 three dimensional space groups were the basis for the crystallography. Then modulated structures were discovered and the three dimensional symmetry of the 230 space groups was “destroyed”. Prof. Janner and Prof di Wolff from Holland who met each other in Kyoto developed the idea of using four dimensional (on higher) space group and considering modulated crystal as three dimensional cut
through higher dimensional space groups. Is such a cut also possible here?

A: Though I am not familiar to their idea, a similar viewpoint, I guess, is already used in this field. Any Penrose site in 2-D is represented by a set of five integers since it is a certain sum of five kinds of unit vectors. They are six in 3-D. These unit vectors, being a set of nonorthogonal overcomplete bases in the original dimension, can be orthogonalized in higher dimensions. Some people (Duneau and Katz, for example) regard the quasicrystals as some section or some projection of a normal lattice in higher dimension. This point of view can be useful but I am afraid that it is only a restatement and nothing new is added. Our intuition works only on lower dimensions. Even a 3-D image can be composed only by combining 2-D images and it is impossible to get it directly. It is also precisely what I had to pay efforts to in this talk.