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Three-dimensional Penrose Transformation and the Ideal Quasicrystals

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Keywords: quasicrystal, Penrose tiling, self-similarity, five-fold symmetry, icosahedral symmetry

Crystallography is now in an epoch of revolution. Since some configurational long range order with icosahedral symmetry and without translational symmetry was experimentally observed in Al-Mn system in 1984, the general framework of configurational order has been required to include such a kind of order. Translational symmetry is no more the most important property in the coming generalized scheme.

The purpose of this paper is to propose a three-dimensional Penrose transformation explicitly and to discuss the difference due to the dimensionality. There are several categories in the concepts of quasicrystal. The ideal one is, in a sense, homogeneous, isotropic, self-similar and connected with golden ratio. Some degrees of freedom remain in three-dimensional case in contrast with deterministic two-dimensional case.

§1. INTRODUCTION

As Mendeleev's periodic table predicted the existence of some never discovered atomic elements, some aesthetically motivated researches on nonperiodic tiling effectively predicted the atomic arrangement with new type of long range order. The discovery of the diffraction patterns with icosahedral symmetry in some Al-Mn alloy system was reported by Shechtman et al(1984). It was a really shocking affair. The experiment suggests the existence of some icosahedral long range order of new type and then the defect of the classical crystallography as a general system of ordered arrangements was revealed (See, for example, Mackay:1986). Penrose tiling (Penrose:1974 & 1977, Gardner:1977), being nonperiodic, self-similar and pentagonally symmetric, is the prototype of the concept of quasicrystals (Mackay:1981 & 1982, Levine & Steinhardt :1984) to understand such a kind of ordered structure. Almost nobody had dreamed that there are some inorganic materials with such a structure. Now the problem is one of the most important ones in physics and also in Science on Form.

It has long been known that pentagonal or five-fold rotational symmetry can not coexist with periodicity. A crystal is defined as a periodic arrangement of atoms. The rotational symmetry which can compatible with the translational periodicity is only four kinds; 2-, 3-, 4- and 6-fold. Pentagonal or 5-fold symmetry, being the elements of the most symmetrical point group, icosahedral group I_h, is out of scope in classical crystallography (see, for example, Kittel:1971).

Therefore the discovery of some long range order with icosahedral symmetry and without periodicity in a material system was really shocking. However, nonperiodic long range order has been already studied by some sensitive people before the experiment. The tessellation of a plane with regular pentagons were tried independently by Husimi(1969) and by Penrose(1974). They both noticed some self-similarity contained in a pentagon and classified the shapes of gaps which necessarily appear when a plane is systematically packed by equal pentagons and/or the pentagonal aggregates consisting of six pentagons. Penrose succeeded in the nonperiodic tiling with only two kinds of elements (Fig. 1). Being recursively generated, the Penrose tiling has a kind of self-similarity. The concept of quasicrystal is the generalization of the essence of the Penrose tiling. It also suggests the possibility of solving the problem of conflict between long range order and short range order (Ogawa & Tanemura: 1974, Ogawa:1983).

The purpose of this paper is to extend the Penrose's logic of generating nonperiodic ordered patterns into three-dimensional case. The concept of quasicrystal has not been established yet. There may be various grades of order in quasicrystal, for example, with or without self-similarity. The present model concerns with the ideal quasicrystal in the sense that it is considered to be symmetrical as high as possible.

§2. THE PENROSE'S LOGIC OF HIERARCHIC GENERATION OF PATTERNS

The Penrose's logic of systematic generation of infinite patterns is described as follows. We are concerning the patterns onsisting of only some kinds of basic elements. Suppose there is

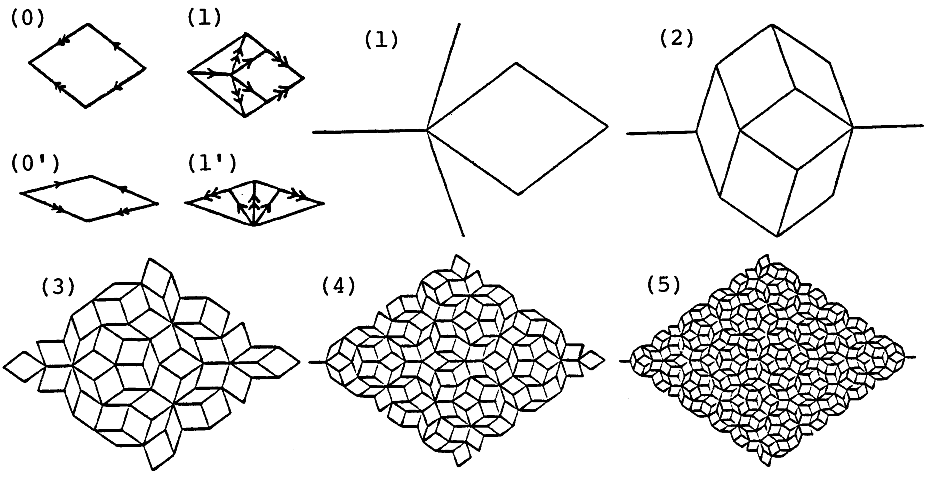


Fig. 1 The Original Penrose Transformation of Two Arrowed Rhombi; Arrows are omitted in higher generations. Side length should be always regarded as 1. The limiting figure is the Penrose tiling.

a transformation of each of these elements into some other pattern consisting of these basic elements. If the transformation is proper, some patterns of these elements can be transformed again and again. Therefore, an infinite pattern, which can be nonperiodic, is generated after the infinite recursive operations of the same transformation. Penrose actually found such a transformation which is referred to as the Penrose tiling.

The Penrose tiling of rhombic version, consist of two kinds of rhombi, A (acute rhombus with an angle of 72°) and O (obtuse rhombus of 144°) of edge length 1. A and O are respectively transformed into A^* and O^* of edge length $\tau=(\sqrt{5}+1)/2=1.618$ (golden mean). The numerical relation there is given by

$$A \rightarrow A^* = 2\ A + O, \qquad O \rightarrow O^* = A + O. \tag{1}$$

It is noted that the existence of a special arrangement of these rhombi is essential for the above mentioned logic can be applied. The transformation is shown in Fig. 1. It is noted that the edges of these rhombi should be regarded as not simple segments but two kinds of arrows (De Bruijn:1981b-c) so that all the rhombi on the edge should be completed and any triangles should not remain. Only the edges of the same kind of arrow and the same direction fit each other.

§3. THREE-DIMENSIONAL PENROSE TRANSFORMATION

In order to keep icosahedral symmetry as a whole, it is convenient to use six basic vectors icosahedrally chosen as five vectors pentagonally chosen are used in two-dimension. The angles between the twelve (twice of six) vectors are either of θ, $\pi-\theta$, or π, where $\theta=\text{atan}2=61.43°$. Therefore, two of the twelve vectors construct only one kind of rhombus, which is referred to as the golden rhombus since the ratio of the diagonals is the golden mean τ. Three of the twelve vectors construct two kinds of rhombohedra A_6 and O_6 (Fig. 2). In A_6, three vertices of angle θ meet at a principal vertex on the principal diagonal and three of $\pi-\theta$ in O_6. A_6 is rather long and O_6 is rather thin. The ratio of their principal diagonal lengths is $d_A/d_O=\tau^3=4.236$.

The basic elements of three-dimensional Penrose tiling are these two rhombohedra A_6 and O_6. It is noted that the quasi-lattice point on a trigonal axis can be expressed with integer M and N in the form of Md_A+Nd_O. In the rhombic version of the original Penrose tiling, all the vertices of rhombi transformed

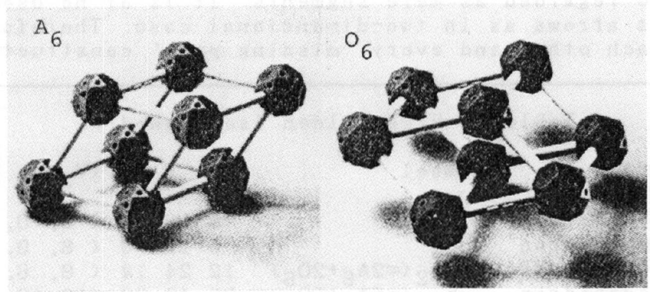


Fig. 2 The Basic Elements A_6 and O_6 in Three-Dimension.

into some vertices. Therefore this condition is imposed to the three-dimensional extension of the Penrose transformation. Then the expansion ratio can not be less than τ^3 in order to keep the principal diagonal of O_6^*.

This value corresponds to the following numerical relation

$$A_6 \rightarrow A_6^* = 55\ A_6 + 34\ O_6, \qquad (2a)$$
$$O_6 \rightarrow O_6^* = 34\ A_6 + 21\ O_6. \qquad (2b)$$

It is noted that the Penrose's logic can not be applied unless a set of proper arrangements is found as in two-dimensional case.

The author (1985) succeeded in finding some sets of proper arrangements. The way is essentially multiple in the sense that the only way can not be uniquely chosen in principle. Some freedom inevitably remain, while the translation in two-dimension is completely deterministic. As will be discussed in §5, there is no deterministic transformation in three-dimension.

In this transformation, only the skeleton parts of A_6^* and O_6^* are uniquely determined (Fig. 3-4). A skeleton of A_6^* consists of the overlapping two K_{30}'s which share an O_6 in common and some A_6-rich parts near the eight vertices of the expanded rhombohedron. It has a 'missing part' at the mid-part of each edge, which will be treated later. Here, K_{30}, Kepler triacontahedron, is one of five golden isozonohedra listed in Table 1, all of whose faces are golden rhombi. Their naming is due to Coxeter and Miyazaki (Miyazaki & Takada: 1980, Miyazaki: 1983). In Table 1, F, E and V are respectively number of faces, edges and vertices, V_k that of k-edged vertices, N_o and N_i 'atomic numbers' inside the zonohedron respectively on the surface and in the inner part.

An skeleton of an O_6^* looks like a hexagonal snowflake, though the symmetry is trigonal as it should be. At the mid-part of their edges, there is a 'missing part' again. The shape of these missing parts is some parts of F_{20}. The edge coincides with the pentagonal axis of F_{20}. The instruction for the construction of the ball and stick model of A_6^* and O_6^* in Ogawa (1985) and the coordinates in the six-integer representation of the quasilattice points in Appendix [in more details in Ogawa (1986c)].

The most striking feature of A_6^* and O_6^* is that the skeleton structure of the face is common to all the faces of A_6^* and O_6^*. In Fig. 5, A is a rhombic face of A_6^*, A' its section at a mirror plane, KF a rhombic face of K_{30} in A_6^* and F_{20} in O_6^*, and F' a section of F_{20} through the pentagonal axis. Another important fact is that the structure is so symmetrical that the edges can be regarded as mere segments. It is of no use to regard the edges as arrows as in two-dimensional case. Therefore any two faces fit each other and every 'missing part' construct an F_{20}.

Table 1 Five Golden Isozonohedra

Zonohedron	symbol	F	E	V	(V_3	V_4	V_5)	N_o	N_i
Acute rhombohedron	A_6	6	12	8	(8,	0,	0)	1	0
Obtuse rhombohedron	O_6	6	12	8	(8,	0,	0)	1	0
Bilinski dodecahedron	B_{12} (=$2A_6$+$2O_6$)	12	24	14	(8,	6,	0)	3	1
Fedorov icosahedron	F_{20} (=$5A_6$+$5O_6$)	20	40	22	(10,	10,	2)	6	4
Kepler triacontahedron	K_{30} (=$10A_6$+$10O_6$)	30	60	32	(20,	0,	12)	10	10

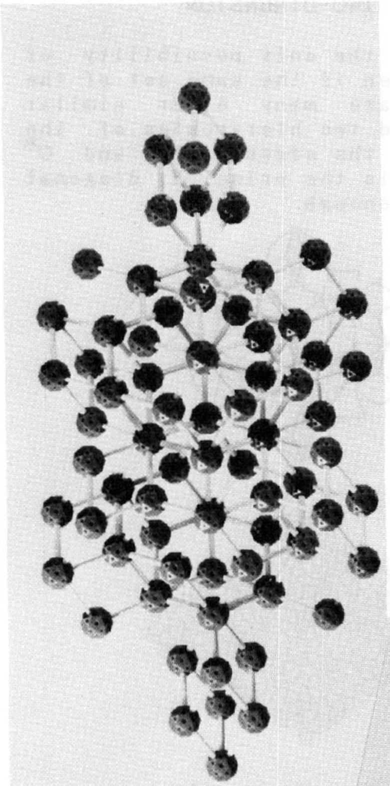
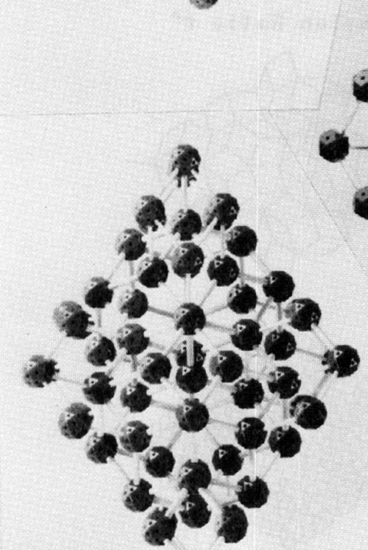


Fig.3 A Skeleton of A_6^*; views along two five-fold axes where four points inside each triacontahedral cage are omitted



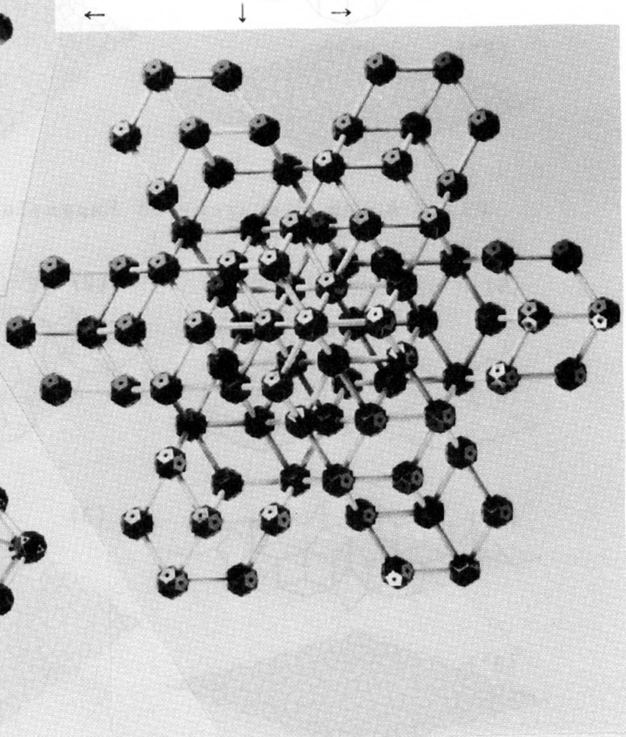


Fig.4 A Skeleton of O_6^*; a view along the principal axis

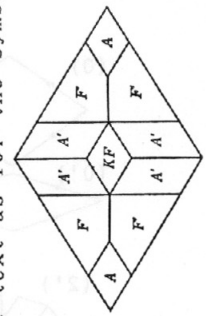


Fig.5 The Structure of a Section at a Rhombic Face of Expanded Rhombohedra; see text as for the symbols

§4. THE OTHER HIERARCHIES IN TWO-DIMENSION

The original penrose tiling is not the only possibility of the hierarchic generation of patterns even if the same set of the basic elements A and O concern. There are many other similar possibilities. Actually the author found two hierarchies of the expansion ratio τ^2=2.618 (Fig. 6-7). All the edges of A^* and O^* are of the same structure; $1+\tau$, where τ is the principal diagonal of A. Now the arrow of only one kind is enough.

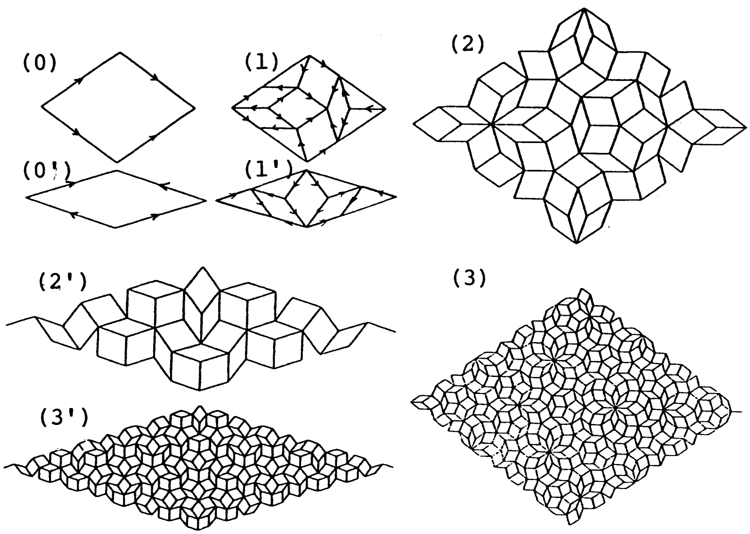


Fig. 6 A New Hierarchy of Expansion Ratio τ^2

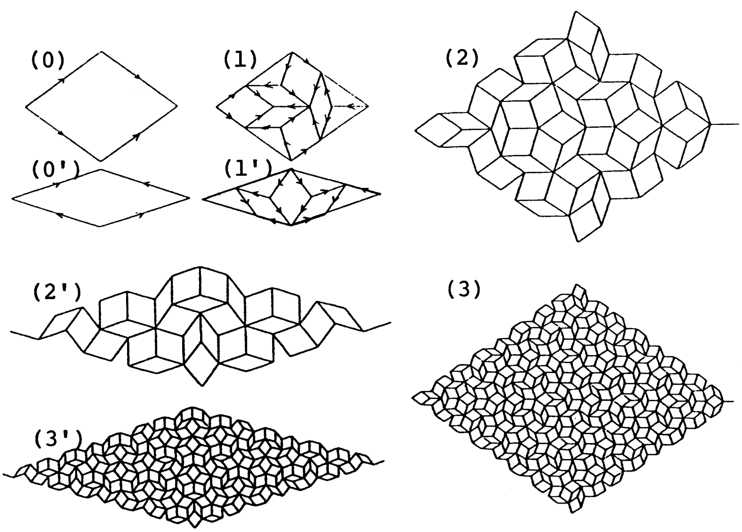


Fig. 7 Another New Hierarchy of Expansion Ratio τ^2

There is a two-dimensional case where the edges can be regarded as mere segments (See Fig. 8). The expansion ratio in this case is $\sqrt{5}\tau$=3,618. Generally in the case of such a large expansion ratio, there are inevitably some highly symmetrical region where the inner structure is less symmetrical than the outline (see, for example, marked parts in Fig. 8). It is noted that the inner structure can be reconstructed in such a highly symmetrical region without disturbing any other parts when the edges are mere segments. This property yields the residual degree of freedom. It is also the case in the inner part of A_6^* in three-dimensional case.

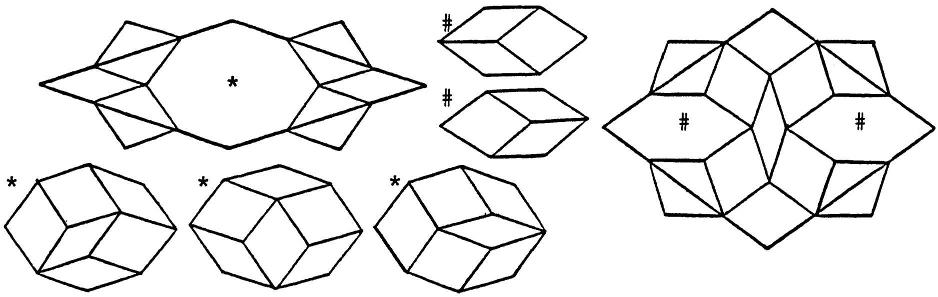


Fig. 8 A Hierarchy of Expansion Ratio $\sqrt{5}\tau$

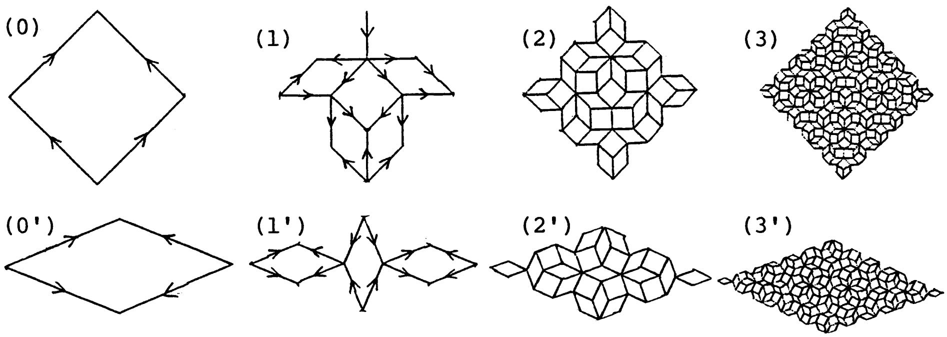


Fig. 9 Hierarchy of Expansion Ratio $1+\sqrt{2}$ in the Octahedral case

§5. ESSENTIAL DEGENERACY IN THREE-DIMENSIONAL CASE

The residual degrees of freedom at the edges of A_6^* and O_6^* should be distinguished from the general case mentioned above. The freedom in the inner part can be arbitrarily fixed. The different way of fixing corresponds to the different hierarchy.

The case at the edges of A_6^* and O_6^* is different. Each of the two ends of a edge consists of the common edge of five A_6's and between them is an F_{20} coinciding its five-fold axis to the concerned edge. There are only four inner quasilattice-points inside an F_{20}. The contradiction between the symmetry of the outlook and that of the inner structure does not allow the division of F_{20}. If one dare to divide them, extremely large number of basic elements, whose shape are common and whose edges are differently colored, are necessary. The interpretation that only the skeleton is determined seems more beautiful as a logical structure. Such a case of degeneracy may be referred to as an essential degeneracy.

§6. A CLASSIFICATION OF HIERARCHIES

A number of hierarchies appeared in this paper. They can be classified by some difference of the logical structure. They are summarized in Table 2.

In column [E] of Table 2, 'unique' means that the transformation is fully deterministic. Generally, the old vertices at the corner of the basic elements transformed into vertices of different form and a new points are born in some form. The number of ways of birth is small for small expansion ratio and large for large expansion ratio. In the course of recursive transformation, they change their forms. In some

Table 2 Summary of Hierarchies

Hierarchy	[A]		[B]	[C]	[D]	[E]	[F]	[G]
Pentagonal cases in 2-D								
(1) Penrose	A	O	(2-1-1-1)	τ	2	u	c	h
(2) Fig. 6	A	O	(5-3-3-2)	τ^2	1	u	c	p
(3) Fig. 7	A	O	(5-3-3-2)	τ^2	1	u	f	p
(4) Fig. 8	A	O	(10-5-5-5)	$\sqrt{5}\tau$	0	d	c, f	p
Octahedral cases in 2-D								
(5) Fig. 9	S	R	(3-4-2-3)	$1+\sqrt{2}$	1	u	f	h
(6) Watanabe et al	S	R	(6-8-4-8)	$2+\sqrt{2}$	0	d	f	p
Icosahedral Case in 3-D								
(7) Ogawa	A_6	O_6	(55-34-34-21)	τ^3	0	e	f	p

Column [A]; the basic elements, S is square and R rhombus of 45.
[B]; a set of number of elements which correspond the coefficients in the r.h.s. of Eqs. (1) and Eq. (2).
[C]; the expansion ratio.
[D]; the number of varieties of arrows.
[E]; 'u' stands for 'unique',
'd' for 'degenerate'
'e' for 'essentially degenerate'.
[F]; the type of the limitting behavior of a vertex in the course of recursive transformation;
'c' stands for 'cyclic',
'f' for 'fixed pattern'.
[G]; 'h' means the existence of 'half-mirror pattern' as shown in Fig. 10,
'p' means that some periodic arrangements of basic elements are allowed as operand of transformation.

hierarchies, they go into some limit cycle of changing form and take a fixed limiting form in the other. For the latter case, there exists a center of self-similarity in a sense. Column [F] describes such a kind of nature.

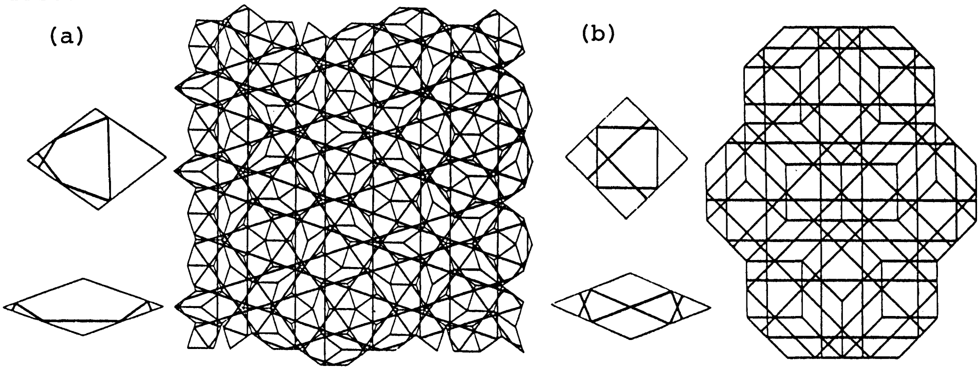


Fig. 10 "Half-Mirror Patterns" (a) in the pentagonal case
(b) in the octahedral case

For hierarchy (1) and (5), a set of 'half-mirror patterns' shown in Fig. 10 consistently exists on each of two kinds of tiles. It is noted that what looks as a straight line consists of the pieces of segments on every tiles. The lines obey the law of reflection at every edges of tiles. Such a pattern seems to exist only in the primitive cases for a given set of tiles. In these patterns, the arrangement of each set of parallel lines is of a one-dimensional quasilattice. The dual of the pattern is the tiling of the next generation. The pattern looks something very suggestive.

§7. CONCLUDING REMARKS

The origin of one of the important differences due to dimensionality is in that a sum of two of five basic vectors in two-dimension directs to another basic vector and all of the other five vectors are necessary to point the direction of a basic vector in three dimension. This property, together with that the ratio of the diagonal lengths of A_6 and O_6 is τ^3, makes the expansion ratio of the three-dimensional Penrose transformation large. Accordingly, some regions with high symmetry appear in three-dimensional case. After all, the property of three-dimensional Penrose transformation necessarily differs from the original one in two-dimension. The model corresponds to the ideal 'quasi-Bravais-lattice' with the highest symmetry in 3-D.

The A_6-rich parts in A_6^* and O_6^* compose a 'flower dodecahedron' shown in Fig. 11. It also corresponds to the limiting form in [G] in Table 2. Twenty A^6's arrange icosahedrally with their principal vertices at the center. From physical point of view, this structure is supposed to be the origin of stability of a quasicrystal (Ogawa: 1977, Ogawa & Nara: 1979).

The comparison of the present model with the experiments in Al-Mn alloys are given in Hiraga $ Hirabayashi (1986) and Takeuchi & Kimura (1986).

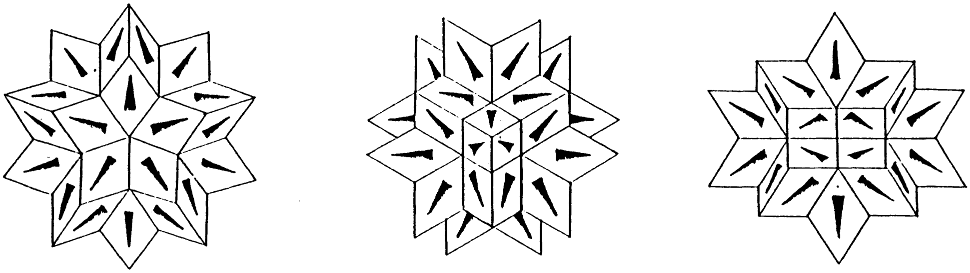


Fig. 11 'Flower Dodecahedron'; views along 5-, 3- and 2-fold axis, where the wedges are outward from the center of a 'flower'.

ACKNOWLEDGMENTS

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APPENDIX THE COORDINATES IN SIX-INTEGER REPRESENTATION

The Cartesian coordinates of six quasibases α-β-γ-ξ-η-ζ are

$\alpha=(p, q, 0), \beta=(0, p, q), \gamma=(q, 0, p), \xi=(-q, 0, p), \eta=(p, -q, 0), \zeta=(0, p, -q)$

where $p=\sqrt{(1+t)/2}$ and $q=\sqrt{(1-t)/2}$ with the relations,

$$p=\tau q, \quad pq=p^2-q^2=t, \quad \alpha+\beta+\gamma=\tau^3(\xi+\eta+\zeta),$$
$$\xi=-\alpha+\tau^{-1}(\beta+\gamma), \quad \eta=-\beta+\tau^{-1}(\gamma+\alpha), \quad \zeta=-\gamma+\tau^{-1}(\alpha+\beta).$$

The Coordinates of Quasilattice-Points in A Skeleton of A_6^*

(000000) (100000) (010000) (001000) (011000) (101000) (110000) (111000)
(222000) (222100) (222010) (222001) (222011) (222101) (222110) (222111)
(333111) (433111) (343111) (334111) (344111) (434111) (443111) (444111)
(111100) (111011) (211001) (121001) (112100) (122100) (212010) (221001)
(111010) (111101) (211010) (121100) (112010) (122110) (212011) (221101)
(111001) (111110) (211011) (121101) (112110) (122101) (212110) (221011)
(211000) (121000) (112000) (122000) (212000) (221000)
(233111) (323111) (332111) (322111) (232111) (223111)
(333110) (333001) (233100) (323010) (332001) (322010) (232001) (223100)
(333101) (333010) (233101) (323011) (332101) (322001) (232100) (223010)
(333011) (333100) (233110) (323110) (332011) (322011) (232101) (223110)
(111$\bar{1}$11) (1111$\bar{1}$1) (11111$\bar{1}$) (222200) (222020) (222002)
(211$\bar{1}$11) (1211$\bar{1}$1) (11211$\bar{1}$) (232200) (223020) (322002)
(221$\bar{1}$11) (1221$\bar{1}$1) (21211$\bar{1}$) (223200) (322020) (232002)
(212$\bar{1}$11) (2211$\bar{1}$1) (12211$\bar{1}$) (233200) (323020) (332002)
(222$\bar{1}$11) (2221$\bar{1}$1) (22211$\bar{1}$) (333200) (333020) (333002)

together with either of the following for sets,

[(122010) (212001) (221100) (223011) (232110) (322101)]
[(122001) (212100) (221010) (223101) (232011) (322110)],
[(122010) (212001) (221100) (223101) (232011) (322110)],
or [(122001) (212100) (221010) (223011) (232110) (322101)].

The Coordinates of Quasilattice-Points in A Skeleton of O_6^*

(000000)	(100000)	(010000)	(001000)	(011000)	(101000)	(110000)	(111000)
(000100)	$(100\bar{1}00)$	(010100)	(001100)	(011100)	$(101\bar{1}00)$	$(110\bar{1}00)$	$(111\bar{1}00)$
(000010)	(100010)	$(0100\bar{1}0)$	(001010)	$(0110\bar{1}0)$	(101010)	$(1100\bar{1}0)$	$(1110\bar{1}0)$
(000001)	(100001)	(010001)	$(00100\bar{1})$	$(01100\bar{1})$	$(10100\bar{1})$	(110001)	$(11100\bar{1})$
	$(100\bar{1}10)$	$(0100\bar{1}1)$	$(00110\bar{1})$	$(0111\bar{1}0)$	$(10110\bar{1})$	$(110\bar{1}10)$	
	$(100\bar{1}01)$	$(0101\bar{1}0)$	$(00101\bar{1})$	$(01110\bar{1})$	$(101\bar{1}10)$	$(1100\bar{1}1)$	
	$(100\bar{1}11)$	$(0101\bar{1}1)$	$(00111\bar{1})$	$(0111\bar{1}\bar{1})$	$(101\bar{1}1\bar{1})$	$(110\bar{1}\bar{1}1)$	
	$(200\bar{1}10)$	$(0200\bar{1}1)$	$(00210\bar{1})$	$(\bar{1}111\bar{1}0)$	$(1\bar{1}101\bar{1})$	$(11\bar{1}\bar{1}01)$	
	$(200\bar{1}01)$	$(0201\bar{1}0)$	$(00201\bar{1})$	$(\bar{1}1110\bar{1})$	$(1\bar{1}1\bar{1}10)$	$(11\bar{1}0\bar{1}1)$	
	$(200\bar{1}11)$	$(0201\bar{1}1)$	$(00211\bar{1})$	$(\bar{1}111\bar{1}\bar{1})$	$(1\bar{1}1\bar{1}1\bar{1})$	$(11\bar{1}\bar{1}\bar{1}1)$	
	$(200\bar{2}10)$	$(0200\bar{2}1)$	$(00210\bar{2})$	$(\bar{1}112\bar{1}0)$	$(1\bar{1}102\bar{1})$	$(11\bar{1}\bar{1}02)$	
	$(200\bar{2}01)$	$(0201\bar{2}0)$	$(00201\bar{2})$	$(\bar{1}1120\bar{1})$	$(1\bar{1}1\bar{1}20)$	$(11\bar{1}0\bar{1}2)$	
	$(200\bar{2}11)$	$(0201\bar{2}1)$	$(00211\bar{2})$	$(\bar{1}112\bar{1}\bar{1})$	$(1\bar{1}1\bar{1}2\bar{1})$	$(11\bar{1}\bar{1}\bar{1}2)$	

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