Prediction of the external shape of ideal icosahedral quasicrystals

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In this work the problem of the prediction of the external shapes (habits) of icosahedral quasicrystals is addressed in terms of geometrical considerations. The cut and projection method is used to find the densest family of quasilattice planes that, according to the Bravais rule, are the most significant from the morphological point of view. The three kinds of six-dimensional cubic lattices are worked out, namely, primitive (P), face centered (F), and body centered (I). Algebraic methods are proposed to find the densest sublattices of the six-dimensional lattices projecting onto a given quasilattice plane. The results are compared with experimental observations.

I. INTRODUCTION

It is well known that crystals frequently grow with polyhedral external shapes (habits). This fact can be understood on the basis that crystals consist of identical units that are repeated according to a lattice. The lattice periodicity also explains why the various facets (flat faces of the polyhedra) of crystals form always the same angles among themselves (law of constancy of angles) and why the directions of the normals to the facets can be indexed (Miller indices) with small integers (law of rational indexes).

The name "morphologically important planes" comes from the fact that the observed facets tend to correspond to the densest lattice planes (Bravais rule), which at the same time are those with the largest distances among themselves to keep constant lattice volume. The densest lattices planes have small values of the Miller indices h,k,l.[1]

Quasicrystals, although noncrystalline, behave in a similar way. They also present polyhedral habits, a law of constancy of angles is obeyed, and can be indexed, in the Fourier module, with small integers.[2]

In the present study the assumption is made that the morphologically significant quasilattice planes in quasicrystals are also those with the highest densities and largest separations. Advantage is taken of the fact that quasicrystals can be thought of as projections of a subset of a six-dimensional lattice. Thus the hypothesis is formulated as indicating that the relevant planes in R^3 are those that correspond (via projection) to the densest lattice hyperplanes in R^6. Kupke and Trebin[3] have addressed similar questions in the case of a six-dimensional P lattice. These authors compare their results with numerical simulation of heavy ion channeling of perfect icosahedral quasilattices. To some extent the present study is an alternative algebraic approach that is extended to the cases of F and I lattices.

At the same time several algebraic aspects of six-dimensional lattices are treated. It is shown that most of the time the best tool is the time-honored Gauss-Jordan reduction of matrices to row reduced echelon form.

Within this geometrical and methodological framework, the likely facets in quasicrystals projecting from P, F, and I lattices in R^6 are derived. We obtain that considering only the densest quasilattice planes, the most likely external form of the ideal icosahedral quasicrystals are the triacontahedron and the pentagonal dodecahedron, for the P and F cases, respectively, in agreement with experimental observations.[4-6] The I phase, yet unobserved, should prefer the shape, according to our results, of a triacontahedron.

II. PRELIMINARY CONSIDERATIONS

The starting point of the present approach is the fact that the quasicrystals can be regarded as projections of a subset of a lattice in the six-dimensional space R^6. We shall review briefly this approach in order to state the notation. Let us consider the space R^6 equipped with the canonical basis $\{e_1,e_2,e_3,e_4,e_5,e_6\}$. The connection with the "physical space" $E^{\parallel}=R^3$ is achieved by projecting R^6 onto $E^{\parallel}$ by means of the projector $\pi:R^6\to R^3$ whose matrix relative to the canonical basis is given by[7]

$$\pi=\begin{pmatrix} b & a & -a & -a & a & a \\ a & b & a & -a & -a & a \\ -a & a & b & a & -a & a \\ -a & -a & a & b & a & a \\ a & -a & -a & a & b & a \\ a & a & a & a & a & b \end{pmatrix},$$

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where $a = 1/\sqrt{20}$ and $b = \frac{1}{2}$. The projector onto perpendicular space $E^{\perp}$ (the orthogonal complement of $E^{\parallel}$ in R^6) is given by $\pi^{\perp} = 1 - \pi$, where 1 is the 6×6 identity matrix.

From this the quasicrystal is defined in the usual way. First one considers the six-dimensional P lattice

$$L_P = \left\{ \sum_{i=1}^{6} n_i e_i \,|\, n_i \in Z \right\}, \tag{1}$$

and then a strip S is selected in the way described by Katz and Duneau.[7] The structure resulting from projecting onto $E^{\parallel}$ all the points of L_P inside the strip is the quasilattice Q_P. That is

$$Q_P = \pi(L_P \cap S) .$$

The projection of all points inside the strip onto $E^{\perp}$ defines the acceptance domain $K = \pi^{\perp}(L_P \cap S)$, that in this case is a rhombic triacontahedron.[7]

In six dimensions there are there Bravais lattices consistent with icosahedral symmetry: P, F, and I cubic lattices.[8,9] Most of the experimentally observed icosahedral quasicrystals are of the P type, however F icosahedral quasicrystals have been obtained in some alloys in the system Al-Cu-R (R = Fe, Os, Ru, Mn) (Refs. 5, 10, and 11) and Al-Pd-TM (TM = transition metal).[12] The last case (I) has not yet been observed experimentally. These lattices will be described in detail in Secs. IV and V.

III. PRIMITIVE SIX-DIMENSIONAL LATTICE

The method used to find the densest family of quasilattice planes is proposed by Katz and Duneau,[7] which relates quasilattice planes and their normal to sublattices of L_P. Our procedure to find these sublattices in each of the three lattices in six dimensions is described below. We present in detail only the case of planes invariant under fivefold rotations (fivefold planes). Similar algebraic techniques apply in all the other cases including F and I lattices.

The primitive six-dimensional lattice of lattice parameter one is generated by a canonical basis as in (1). Upon projecting from R^6 onto R^3 the unit hypercubic cell, a tricontahedron is obtained that is formed by ten prolate rhombohedra and ten oblate rhombohedra whose edge lengths are $1/\sqrt{2}$. Consider a plane (facet) in a quasilattice whose normal points in the direction of one of the fivefold axes; by a plane in a quasilattice we mean a plane that contains at least three noncollinear quasilattice points. Using the numbering shown in Fig. 1 for the vectors pointing to the vertices of an icosahedron, it can be readily seen that two vectors in this plane are

$$\varepsilon_3 - \varepsilon_2 = \pi(e_3) - \pi(e_2)$$

and

$$\varepsilon_1 - \varepsilon_2 = \pi(e_1) - \pi(e_2) .$$

The kernel of the procedure can be stated briefly: (i) Find the sublattice Λ_W of L_P that projects onto the space spanned by the vectors that determine a plane of the quasilattice ($\varepsilon_3 - \varepsilon_2$ and $\varepsilon_1 - \varepsilon_2$ in this case); the occupation density of this plane is directly related with the density of Λ_W. (ii) Find the average density of the family of planes defined by the same normal (fivefold in this case). The denser this family of planes is, the more likely the facet is to appear and develop.

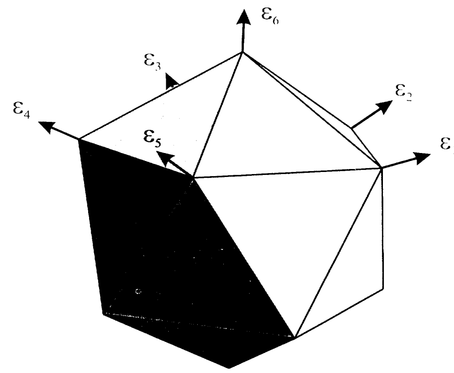


FIG. 1. The projected basis vectors ε_i of L_P are six vertices of an icosahedron.

The sublattice Λ_W of L_P that projects onto a given plane is known to be a four-dimensional lattice.[7] This can also be seen directly as follows: Consider the subspace generated by the set

$$\{ \varepsilon_3 - \varepsilon_2, \varepsilon_1 - \varepsilon_2, \varepsilon_3^{\perp} - \varepsilon_2^{\perp}, \varepsilon_1^{\perp} - \varepsilon_2^{\perp}, \varepsilon_6^{\perp} \} , \tag{2}$$

where $\varepsilon_1, \varepsilon_2$ are as before and $\varepsilon_i^{\perp} = \pi^{\perp}(e_i)$, $i = 1,2,3,6$. This set is linearly independent and since $\pi(\varepsilon_i) = \varepsilon_i$ and $\pi(\varepsilon_i^{\perp}) = 0$, it projects onto the space spanned by $\{\varepsilon_3 - \varepsilon_2, \varepsilon_1 - \varepsilon_2\}$. Then the (five-dimensional) subspace spanned by (2) projects onto the fivefold plane of the quasilattice. The sublattice Λ_W is then the intersection of this subspace and L_P. There is a very simple (yet elegant) way of obtaining a basis for Λ_W. Write a matrix M whose rows are the components of the vectors (2) (with respect to the canonical basis $\{e_1, e_2, e_3, e_4, e_5, e_6\}$, these components in turn are to be obtained from the projection matrices π and $\pi^{\perp}$). Then bring M to the reduced row echelon form M'. The rows of M' form another basis for Λ_W that has many zeros and ones as components. Explicitly,

$$M' = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & -1/\sqrt{5} \\ 0 & 1 & 0 & 0 & 0 & -1/\sqrt{5} \\ 0 & 0 & 1 & 0 & 0 & -1/\sqrt{5} \\ 0 & 0 & 0 & 1 & 0 & -1/\sqrt{5} \\ 0 & 0 & 0 & 0 & 1 & -1/\sqrt{5} \end{bmatrix} .$$

Then a linear combination of the rows of M'

$$x_1(1,0,0,0,0,-1/\sqrt{5}) + x_2(0,1,0,0,0,-1/\sqrt{5})$$
$$+ x_3(0,0,1,0,0,-1/\sqrt{5})$$
$$+ x_4(0,0,0,1,0,-1/\sqrt{5})$$
$$+ x_5(0,0,0,0,1,-1/\sqrt{5})$$

TABLE I. Generators and volumes of the primitive cells of lattices Λ_W projecting onto the tree planes of a P quasilattice generated by the vectors in column 2.

Direction	Generators in 3D	Generators of Λ_W	$V(\Lambda_W)$
twofold	$\{\varepsilon_1,\varepsilon_2\}$	$\{e_1,e_2,e_3-e_5,e_4-e_6\}$	2
threefold	$\{\varepsilon_1+\varepsilon_2,\varepsilon_2+\varepsilon_3\}$	$\{e_1-e_3,e_2+e_3,e_4-e_6,e_5-e_6\}$	3
fivefold	$\{\varepsilon_3-\varepsilon_2,\varepsilon_1-\varepsilon_2\}$	$\{e_1-e_5,e_2-e_5,e_3-e_5,e_4-e_5\}$	$\sqrt{5}$

will also lie in L_P if and only if x_1,x_2,x_3,x_4,x_5 are all integer and $\sum_{i=1}^{5} x_i=0$, so a basis for Λ_W is given by

$$\{(1,0,0,0,-1,0),(0,1,0,0,-1,0),(0,0,1,0,-1,0)\ (0,0,0,1,-1,0)\}\ , \tag{3}$$

confirming that the dimension of Λ_W is four indeed.

Let W be the four-dimensional space containing the lattice Λ_W, such that

$$\Lambda_W=W\cap L_P\ .$$

One can obtain the pattern of projected points onto the fivefold plane spanned by $\{\varepsilon_3-\varepsilon_2,\varepsilon_1-\varepsilon_2\}$ by the cut and projection method in Λ_W, with the strip $S_W=(S\cap W)$.

Orthogonal to Λ_W, there is a two-dimensional lattice $\Lambda_{W^\perp}$, which projects onto an one-dimensional space orthogonal to the quasilattice plane, i.e., projects onto a space spanned by the normal to the fivefold plane. A subspace $W^\perp$ orthogonal to W is obtained calculating the null space of the matrix whose rows are the components of the vectors (3). This procedure gives

$$W^\perp=\mathrm{Span}\{(0,0,0,0,0,1),(1,1,1,1,1,1)\}\ . \tag{4}$$

The pattern of vertices along the normal to the fivefold plane, that gives the sequence of separations between planes, is derived similarly by the cut and projection method but in the two-dimensional lattice

$$\Lambda_{W^\perp}=\pi_{W^\perp}(L_P)\ ,$$

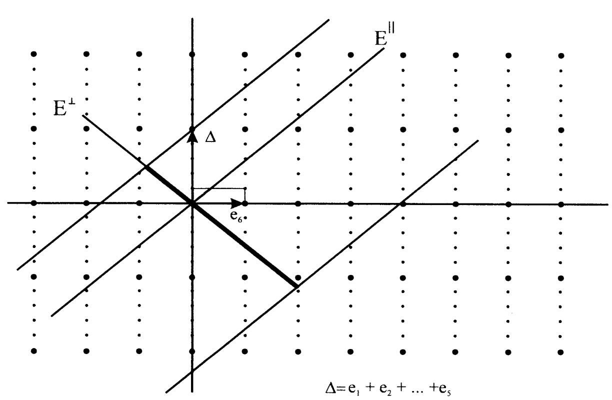


FIG. 2. Cut and projection method in $\Lambda_{W^\perp}$. Small points come from the projection $\pi_{W^\perp}(L_P)$. $E^\|$ and $E^\perp$ are indeed $\pi_{W^\perp}(E^\|)$ and $\pi_{W^\perp}(E^\perp)$. The strip is generated by translating the acceptance domain $\pi_{W^\perp}(K)$ (strong line along $E^\perp$) onto $E^\|$. The primitive cell of $\Lambda_{W^\perp}$ is dashed.

with a strip $S_{W^\perp}=\pi_{W^\perp}(S)$,[7] where $\pi_{W^\perp}$ denotes the orthogonal projection onto the subspace $W^\perp$. From the projection $\pi_{W^\perp}(L_P)$ we can obtain a basis for $\Lambda_{W^\perp}$, that reads

$$\{e_6,(e_1+e_2+e_3+e_4+e_5)/5\}\ .$$

The cut and projection method in this lattice is depicted in Fig. 2.

In the derivation of Λ_W and $\Lambda_{W^\perp}$, attention was paid to the question of whether the basis obtained for the lattices were the smallest or primitive or, in other words, if all lattice points in the four-dimensional lattice could be obtained as integer combinations of these basis vectors. Frequently all that had to be done to check this was to extend the basis for Λ_W (or $\Lambda_{W^\perp}$) to a basis for L_P and to check that its volume was 1. This would ensure that no points of L_P were missed.

Calculations were made to assess the morphological importance of high symmetry planes, i.e., fivefold, threefold, and twofold facets; the assumption being made that the densest planes are those that would contribute most to the equilibrium habits. Tables I and II show the results for the lattice L_P. Table I gives the generators of the three different quasilattice planes in three dimensions, the basis for the four-dimensional lattices Λ_W associated with each plane, and the volume of the smallest (primitive) cell of Λ_W which is denoted by $V(\Lambda_W)$. Table II gives the basis for the lattices $\Lambda_{W^\perp}$ that projects onto the normal to each quasilattice plane in Table I. The area $A(\Lambda_{W^\perp})$ of the primitive cell of $\Lambda_{W^\perp}$ is also given.

IV. FACE-CENTERED LATTICE

A face-centered-cubic lattice in R^6 is defined as

$$L_F=\left\{\sum_{i=1}^{6} n_i e_i\ \middle|\ \sum_{i=1}^{6} n_i=0(\mathrm{mod}\ 2)\right\}\ ,$$

TABLE II. Generators and areas of the primitive cells of the two-dimensional lattices $\Lambda_{W^\perp}$ projecting onto the normal to quasilattice planes in Table I.

Direction	Generators of $\Lambda_{W^\perp}$	$A(\Lambda_{W^\perp})$
twofold	$\{(e_4+e_6)/2,(e_3+e_5)/2\}$	1/2
threefold	$\{(e_4+e_5+e_6)/3,(e_1-e_2+e_3)/3\}$	1/3
fivefold	$\{e_6,(e_1+e_2+e_3+e_4+e_5)/5\}$	$1/\sqrt{5}$

TABLE III. Generators and volumes of the primitive cells of lattices Λ_W projecting onto the tree planes of a F quasilattice generated by the vectors in column 2.

Direction	Generators in 3D	Generators of Λ_W	$V(\Lambda_W)$
twofold	$\{-\varepsilon_1-\varepsilon_2,\varepsilon_1-\varepsilon_2\}$	$\{-e_1-e_2,e_1-e_2,$ $e_3-e_4-e_5+e_6,e_4-e_6\}$	4
threefold	$\{-\varepsilon_1-\varepsilon_2,\varepsilon_5-\varepsilon_6\}$	$\{-e_1-e_2,e_1-e_3,e_4-e_5,e_5-e_6\}$	3
fivefold	$\{\varepsilon_1-\varepsilon_2,\varepsilon_2-\varepsilon_3\}$	$\{e_1-e_2,e_2-e_3,e_3-e_4,e_4-e_5\}$	$\sqrt{5}$

and in this case a basis for the lattice is given by the rows of the generator matrix[13]

$$F=\begin{bmatrix} -1 & -1 & 0 & 0 & 0 & 0\\ 1 & -1 & 0 & 0 & 0 & 0\\ 0 & 1 & -1 & 0 & 0 & 0\\ 0 & 0 & 1 & -1 & 0 & 0\\ 0 & 0 & 0 & 1 & -1 & 0\\ 0 & 0 & 0 & 0 & 1 & -1 \end{bmatrix} . \quad (5)$$

Note that $\mathrm{Det}(F)=2$ and that in six dimensions this is a lattice with lattice parameter 2. The lattice L_F is also known as the checkerboard lattice and is identical with the root lattice D_6,[13] which has been studied in great detail in Refs. 14 and 15. The quasilattice Q_F is obtained from cut and projection method with the lattice L_F and the acceptance domain K which is the same as for the lattice L_P: a rhombic tricontahedron.[14,15] This implies that the vertices of Q_F are just the even vertices of the quasilattice Q_P projected from the lattice L_P.

Tables III and IV show the counterpart results of Tables I and II for the case of the lattice L_F. Results are shown in the canonical basis but calculations are made simpler using the primitive basis given by the rows of (5).

V. BODY-CENTERED LATTICE

A body-centered-cubic lattice in R^6 is defined as the lattice dual (reciprocal) to L_F and is given explicitly by

$$L_I=\left\{ \sum_{i=1}^{6} \frac{n_i}{2} e_i \,|\, n_i=n_j (\mathrm{mod}\ 2) \right\} ,$$

and a basis can be given in terms of the generator matrix[13]

TABLE IV. Generators and areas of the primitive cells of the two-dimensional lattices $\Lambda_{W\perp}$ projecting onto the normal to quasilattice planes in Table III.

Direction	Generators of $\Lambda_{W\perp}$	$A(\Lambda_{W\perp})$
twofold	$\{(e_4+e_6)/2,(e_3+e_5)/2\}$	1/2
threefold	$\{(e_1-e_2+e_3+e_4+e_5+e_6)/3,$ $(-e_1+e_2-e_3+e_4+e_5+e_6)/3\}$	2/3
fivefold	$\{(e_1+e_2+e_3+e_4+e_5)/5+e_6,$ $(e_1+e_2+e_3+e_4+e_5)/5-e_6\}$	$2/\sqrt{5}$

$$I=\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0\\ 0 & 1 & 0 & 0 & 0 & 0\\ 0 & 0 & 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 0 & 1 & 0\\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{bmatrix} . \quad (6)$$

with $\mathrm{Det}(I)=\frac{1}{2}$. A primitive basis for L_I is given by the rows of the matrix I. The I quasilattice Q_I can be also obtained by the cut and projection method in L_I with the rhombic triacontahedron as the acceptance domain.

The relationship between the three lattices L_P, L_F, and L_I is given as

$$L_I(a)\to L_P(a)\to L_F(2a) ,$$

where a is the lattice parameter. L_F is a sublattice of L_P of index 2 and L_P is a sublattice of L_I of index 2.

Tables V and VI show the results for the lattice L_I. These are shown in the canonical basis but calculations were worked out using the primitive basis given by the rows of (6).

VI. AVERAGE DENSITY OF A FAMILY OF PLANES

For a given type of lattice (L_P, L_F, or L_I) and for a given type of facet (twofold, threefold, fivefold or any other) the four-dimensional lattice Λ_W, that projects onto the space containing the facet, can be calculated. The occupation density (number of vertices per unit area) of the particular plane under consideration is inversely proportional to the volume $V(\Lambda_W)$. We have to take into account that not all the lattice points in Λ_W are projected but only those inside the strip S_W. The acceptance domain in this case is just a section of the triacontahedron K, given by $\pi^{\perp}(S_W\cap L_m)$, where $m=P$, F, or I, as depicted in Fig. 3 for the case of a plane normal to a fivefold axis.

With the above considerations, the density of vertices (quasilattice points) in a given quasilattice plane can be calculated as follows. Let us consider a square domain, of area A_S, in the quasilattice plane. If N is the number of vertices inside the square, then the density is given by

$$\rho=\frac{N}{A_S} . \quad (7)$$

All the N vertices in the square domain are projections of vertices of Λ_W contained in a four-dimensional region whose volume $V_{4\mathrm{D}}$ is A_S times the "height" of the strip.

TABLE V. Generators and volumes of the primitive cells of lattices Λ_W projecting onto the three planes of a I quasilattice generated by the vectors in column 2.

Direction	Generators in 3D	Generators of Λ_W	$V(\Lambda_W)$
twofold	$\{\varepsilon_1,\varepsilon_2\}$	$\{e_1,e_2,e_3-e_5,$ $(-e_1-e_2-e_3+e_4+e_5-e_6)/2\}$	1
threefold	$\{\varepsilon_1+\varepsilon_2,\varepsilon_2+\varepsilon_3\}$	$\{-e_2-e_3-e_4+2e_5-e_6,$ $e_1+2e_2+e_3+e_4-2e_5+e_6,$ $-e_1-e_2-e_4+2e_5-e_6,e_4-e_5\}$	3
fivefold	$\{\varepsilon_3-\varepsilon_2,\varepsilon_1-\varepsilon_2\}$	$\{e_1-e_5,e_2-e_5,e_3-e_5,e_4-e_5\}$	$\sqrt{5}$

Since the acceptance domain is the planar section of the triacontahedron $\pi^\perp(S_W\cap L_m)$, whose area we denote by $|\pi^\perp(S_W\cap L_m)|$, we have $V_{4D}=A_S\times|\pi^\perp(S_W\cap L_m)|$. On the other hand, this same volume is equal (up to small boundary corrections) to the number of enclosed unit cells of Λ_W times the volume of the unit cell, that is, $V_{4D}=N\times V(\Lambda_W)$. Consequently $N=A_S|\pi^\perp(S_W\cap L_m)|/\ V(\Lambda_W)$ and, by substituting in (7), we obtain

$$\rho=\frac{|\pi^\perp(S_W\cap L_m)|}{V(\Lambda_W)}\ . \tag{8}$$

The complete family of planes along one direction are obtained by translating the lattice Λ_W over $\Lambda_{W^\perp}$. In each translation we have to cut and project, and the acceptance domains will be different parallel sections of the triacontahedron. From Eq. (8), since $V(\Lambda_W)$ is fixed for each family, the density of each plane depends only on the corresponding section of the triacontahedron. The average density of the family is therefore

$$\bar{\rho}=\frac{1}{V(\Lambda_W)}\left[\frac{\sum_{i=1}^{N}A_i}{N}\right],$$

where A_i is the area of the section of the triacontahedron corresponding to a plane i, and N is the number of planes considered. In the limit, we have

$$\bar{\rho}=\frac{1}{V(\Lambda_W)}\left[\frac{V(K)}{l_K}\right], \tag{9}$$

where $V(K)=2^{1/2}\tau^2(3-\tau)^{1/2}\approx 4.3525$ is the volume of the triacontahedron and l_K is the diameter of the triacontahedron measured along the normal to the planes. These diameters are 1.9465, 2.0836, and 2.2882 for, respectively, the twofold, threefold, and fivefold directions. Note that the average density from one family to another is carried by $V(\Lambda_W)$ and l_K. In the particular case of the family of fivefold planes of a P quasilattice, $V(\Lambda_W)$ is given in Table I and $l_K=2.2882$ is twice the circumradius of the triacontahedron K. Since the triacontahedron has minor variations from family to family, oversimplifying we can write

$$\bar{\rho}\propto\frac{1}{V(\Lambda_W)}\ ,$$

which means that *the morphological importance of a family of planes varies inversely with the volume of the primitive cell of the four-dimensional lattice* Λ_W *that projects onto the space containing one of the planes of that family.*

Following the same reasoning that led to Eq. (8), we can see that the average separation between planes in a given family varies directly with the area of the primitive cell of the two-dimensional lattice $\Lambda_{W^\perp}$ that projects onto the normal to that family of planes, and is given by

$$\bar{d}=\frac{A(\Lambda_{W^\perp})}{l_K}\ . \tag{10}$$

Therefore, we can write

$$\bar{d}\propto A(\Lambda_{W^\perp})\ .$$

TABLE VI. Generators and areas of the primitive cells of the two-dimensional lattices $\Lambda_{W^\perp}$ projecting onto the normal to quasilattice planes in Table V.

Direction	Generators of $\Lambda_{W^\perp}$	$A(\Lambda_{W^\perp})$
twofold	$\{(e_4+e_6)/2,(e_3+e_5)/2\}$	1/2
threefold	$\{(e_1-e_2+e_3+e_4+e_5+e_6)/6,$ $(-e_1+e_2-e_3+e_4+e_5+e_6)/6\}$	1/6
fivefold	$\{(e_1+e_2+e_3+e_4+e_5)/10+e_6/2,$ $(e_1+e_2+e_3+e_4+e_5)/10-e_6/2\}$	$1/2\sqrt{5}$

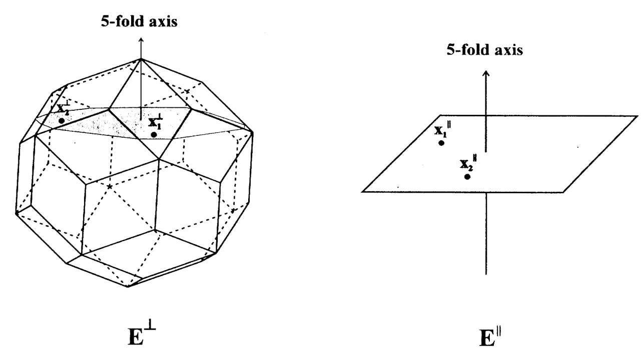


FIG. 3. The acceptance region for the cut and projection method in Λ_W is a section of the triacontahedron K. This section has the same symmetry as the quasilattice plane where the accepted points of Λ_W are projected. If $X_1^\parallel$ and $X_2^\parallel$ are points on the given plane, then their counterparts in perpendicular space are $X_1^\perp$ and $X_2^\perp$ that lie on a planar section of the triacontahedron.

TABLE VII. Average densities of planes and average separations between themselves for the three different families of each one of the three kinds of six-dimensional lattices studied in this work.

6D Lattice	Direction	$\bar{\rho}$	$\bar{d}$
	twofold	1.1180	0.2568
P	threefold	0.6963	0.1600
	fivefold	0.8507	0.1954
	twofold	0.5590	0.2568
F	threefold	0.6963	0.3199
	fivefold	0.8507	0.3909
	twofold	2.2360	0.2568
I	threefold	0.6963	0.0799
	fivefold	0.8507	0.0977

Observe that since the volume of the unit cell of the lattices L_P, L_F, or L_I is fixed, quantities $V(\Lambda_W)$ and $A(\Lambda_{W^\perp})$ are related in such a way that, as in crystals, the larger the average density of a family of planes, the larger the average separation between themselves. We have therefore a generalization of the Bravais rule in crystallography that states that the habit faces are the faces with the highest reticular density or, equivalently, the faces with planes with the largest separation.[1]

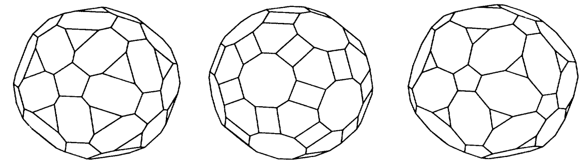
VII. RESULTS AND DISCUSSION

Average densities and separations between planes were calculated for the three families of planes of the three quasilattices Q_P, Q_F, and Q_I, using formulas (9) and (10). Results are shown in Table VII.

From Table VII, the density of each of the three quasilattices can be calculated for $\bar{\rho}/\bar{d}$. This gives $\rho_P = 4.353$, $\rho_F = 4.353/2$, and $\rho_I = 4.353 \times 2$. But most importantly, from the information about average densities of planes, the following predictions about the ideal shape of the icosahedral quasilattice can be made:

(1) In the case P, the largest occupation density is carried by the planes with normal along the twofold axis of the icosahedron. If we take into account only these planes, the polyhedral shape should have big twofold facets resembling a rhombic triacontahedron. By considering the influence of threefold and fivefold planes, the shape should be a polyhedron as shown in Fig. 4(a), where the facets have ratios of areas approximately similar to the ratios of densities in Table VII.

(2) In the case F, the densest planes are those of the fivefold family so in this case, we have a polyhedron with big fivefold facets. The ideal shape is therefore a pentagonal dodecahedron. Figure 4(b) shows the polyhedron obtained considering also the influence of twofold and threefold facets.



(a) (b) (c)

FIG. 4. Polyhedral shapes of icosahedral P, F, and I quasicrystals. The facets of each polyhedron have ratios of areas approximately similar to the ratios of densities in Table VII.

(3) In the yet unobserved case I we have the same results as in the P case but with bigger twofold facets. This resembles also a rhombic triacontahedron. Figure 4(c) shows the polyhedron with facets with areas of approximately the same ratio as the densities.

The ideal external shape, according to the most important facets, for P and F cases (triacontahedron and dodecahedron, respectively) coincides with experimental observations.[4–6] More careful experiments have shown that facets of F quasicrystals are not perfect dodecahedra but twofold and threefold facets also appear with small areas,[6] this is expected since twofold and threefold planes have a minor, but nonzero, importance in the facet formation.

There exist theoretical approaches to the equilibrium shapes of perfect quasiperiodic structure models and of random tilings[16] and of cluster-based quasicrystals.[17] These works entail qualitative consideration of bond energies that, since quasicrystal growth is a physical process, will probably play a more important role than geometrical quantities like density of planes. We show however, that based on an entirely geometric approach, we obtain an answer that matches experimental observations and energetical predictions. We have also shown how geometrical crystallography rules such as the Bravais rule, can be applied to quasicrystals and phrased in terms of the six-dimensional lattice associated with the quasilattice.

The cut and projection method and the procedure proposed here to find the four-dimensional lattices associated with quasilattice planes have the advantage of being completely algebraic so that it can be easily mechanized using software for doing mathematics. In addition, it is also possible to study the possible morphology of rational approximants that can be obtained by a modification of the cut and projection method.[18,19] This work is under way.

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[1] B. K. Wainshtein, in *Modern Crystallography I, Symmetry of Crystals, Methods of Structural Crystallography*, edited by M. Cardona, P. Fulde, and H.-J. Queisser, Springer Series in Solid-State Sciences Vol. 15 (Springer-Verlag, Berlin, 1981), Chap. 3.
[2] T. Jansen, A. Janner, and P. Bennema, Philos. Mag. B **59**, 233 (1989).
[3] T. Kupke and H. R. Trebin, J. Phys. I (France) **3**, 1629 (1993).

[4]B. Dubost, J. M. Lang, M. Tanaka, P. Sainfort, and M. Audier, Nature (London) **324**, 48 (1986).

[5]A. P. Tsai, A. Inoue, and T. Masumoto, Jpn. J. Appl. Phys. **26**, L1505 (1987).

[6]C. Beeli and H.-U. Nissen, Philos. Mag. B **68**, 487 (1993).

[7]A. Katz and M. Duneau, J. Phys. I (France) **47**, 181 (1986).

[8]D. Martinais, C.R. Acad. Sci. **305**, 509 (1987).

[9]D. S. Rokhsar, N. D. Mermin, and D. C. Wright, Phys. Rev. B **35**, 5478 (1987).

[10]A.P. Tsai, A. Inoue, and T. Masumoto, Jpn. J. Appl. Phys. **27**, L1587 (1988).

[11]A. P. Tsai, A. Inoue, and T. Masumoto, J. Mater. Sci. Lett. **7**, 322 (1988).

[12]A. P. Tsai, Y. Yokoyama, A. Inoue, and T. Masumoto, Jpn. J. Appl. Phys. **29**, L1161 (1990).

[13]J. H. Conway and N. A. Sloane, *Sphere Packings, Lattices and Groups* (Springer-Verlag, New York, 1988).

[14]P. Kramer, Z. Papadopoulous, and D. Zeidler, in *Proceedings of the Symposium Symmetries in Science V: Algebraic Structures, their Representations, Realizations and Physical Applications, Schloss Hofen, Austria,* edited by B. Gruber (Plenum, New York, 1991).

[15]P. Kramer, Z. Papadopolous, and D. Zeidler, in *Group Theory in Physics,* edited by A. Frank, T. H. Seligman, and K. B Wolf, AIP Conf. Proc. No. 266 (AIP, New York, 1992), p. 179.

[16]T. L. Ho, J. A. Jaszczak, Y.-H. Li, and W. F. Saam, Phys. Rev. Lett. **59**, 1116 (1987).

[17]T. Lei and C. L. Henley, Philos. Mag. B **63**, 677 (1991).

[18]M. Torres, G. Pastor, I. Jiménez, and J. Fayos, Philos. Mag. Lett. **59**, 181 (1989).

[19]J. L. Aragón and M. Torres, Europhys. Lett. **15**, 203 (1991).

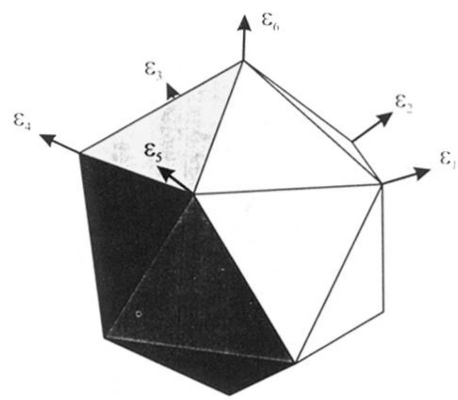

FIG. 1. The projected basis vectors ε_i of L_P are six vertices of an icosahedron.

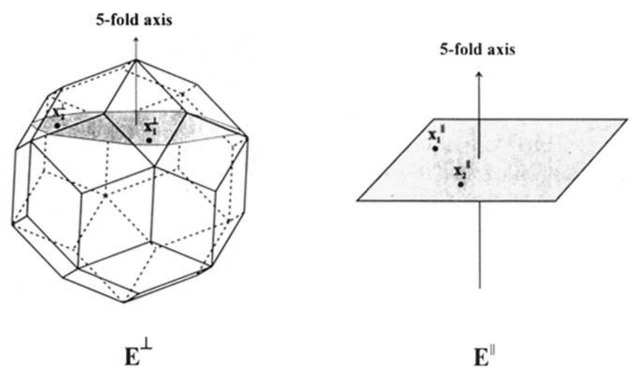

FIG. 3. The acceptance region for the cut and projection method in Λ_W is a section of the triacontahedron K. This section has the same symmetry as the quasilattice plane where the accepted points of Λ_W are projected. If $X_1^{\parallel}$ and $X_2^{\parallel}$ are points on the given plane, then their counterparts in perpendicular space are $X_1^{\perp}$ and $X_2^{\perp}$ that lie on a planar section of the triacontahedron.