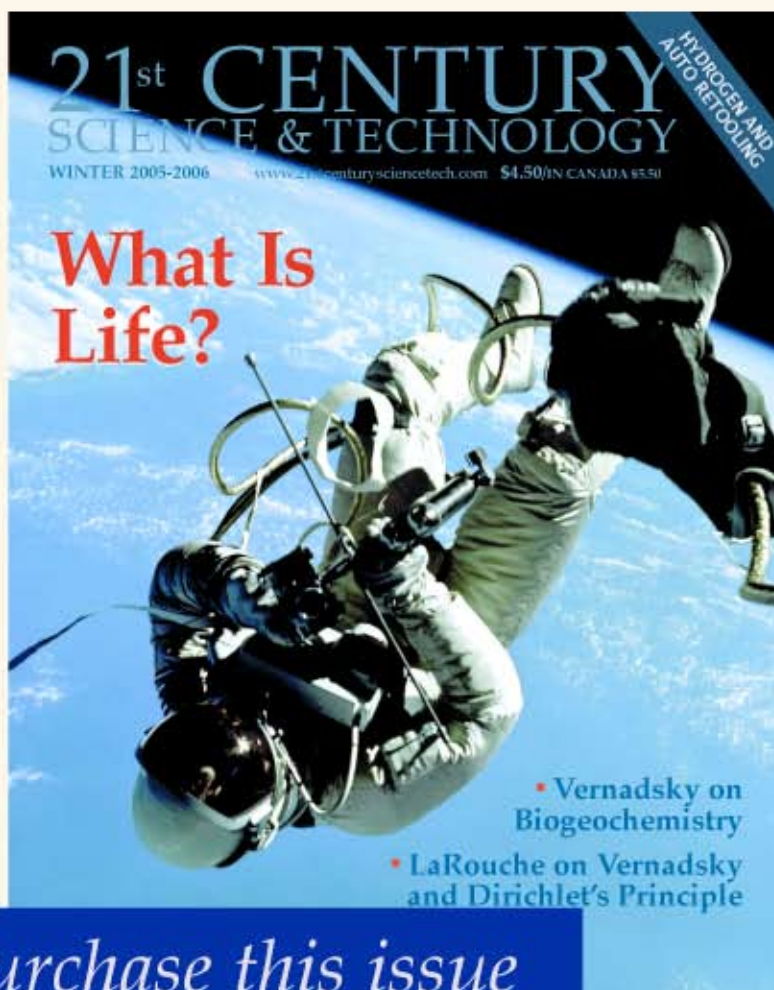


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A Keplerian Solution to The Quasicrystal Problem

by Laurence Hecht

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The discovery in 1984 of an aluminum-manganese alloy showing the “forbidden” pentagonal symmetry created a crisis in crystallography, and implicitly in all physical science, which has not been satisfactorily resolved. So far, attempts to explain how it is possible for a lattice to show quasi-periodic symmetry have required recourse either to a structure made up of several different unit cells, or to mathematical modelling of multidimensional space. Neither appears satisfactory to me.

By re-examining one of the fundamental assumptions of crystallography, returning to the method of Johannes Kepler in his *Six Cornered Snowflake*, I have found a simple means of constructing a three-dimensional lattice of pentagonal symmetry. By varying one of the traditional axioms of crystallography to per-

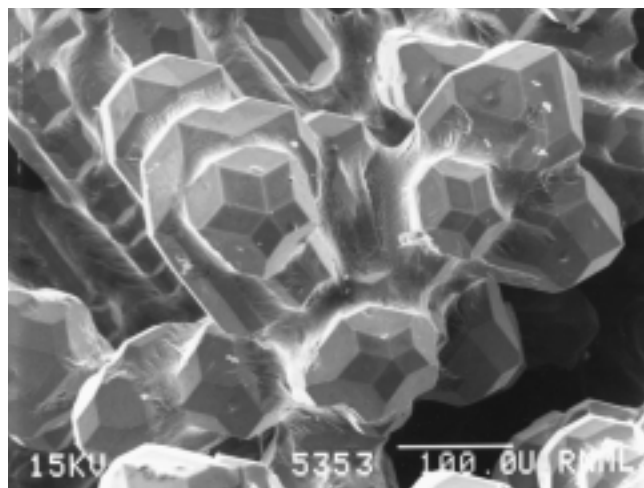
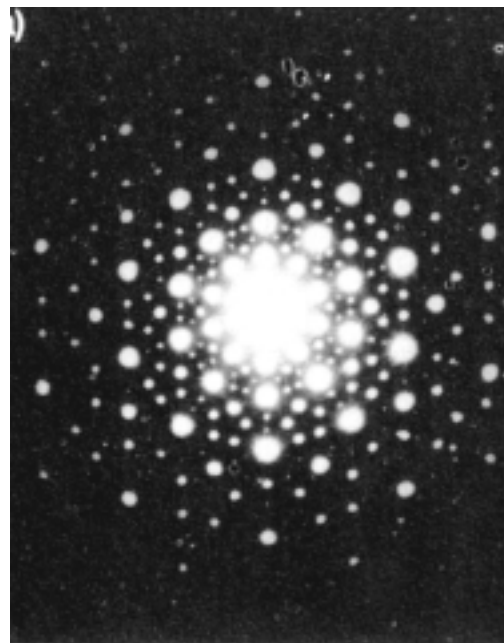
Evidence of five-fold symmetry first appeared in 1984 in samples of rapidly quenched aluminum-manganese alloys obtained by Dany Shechtman, et al. These produced diffraction patterns like the one at right, in which 10 points surround a central one in a decagonal pattern.

mit interpenetration of the cells, a regularly repeated dodecahedral or icosahedral unit cell may fill space, producing a self-similarly enlarging dodecahedron or icosahedron. From this it may be seen how a crystal of five-fold symmetry might grow. It is beyond my means presently to verify whether any of the variety of known quasicrystals corresponds to this

construction. I put forward this hypothesis as a contribution to the search for an explanation to this interesting new phenomenon, which will serve in any case as a construction of geometric interest.

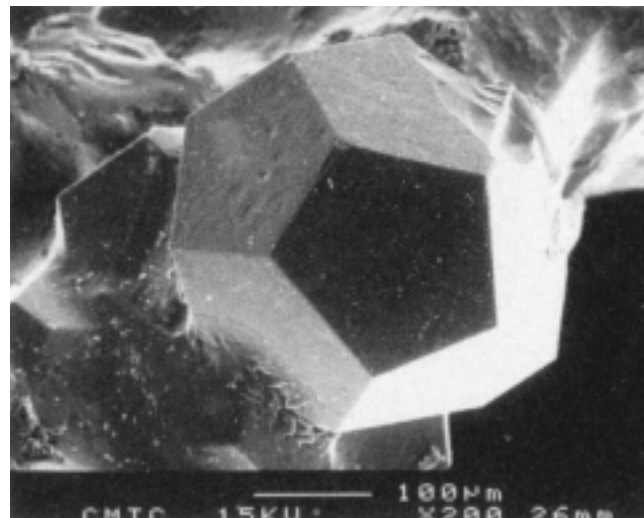
Pentagonal ‘Tiling’

My solution derives from a construction for creating self-similar plane pen-



Frank W. Gayle, Reynolds Metals

*Crystals of an aluminum-copper-lithium alloy (Al_6CuLi_3) obtained in 1986 showed the shape of the rhombic tricontahedron, with single grains approaching a size of 1 millimeter. The figure, discovered by Kepler and reported in his work *The Six-Cornered Snowflake*, consists of 30 rhombuses whose diagonals are in the golden ratio.*



From *Quasicrystals*, Janot (Oxford: Clarendon, 1992)

An almost millimeter-sized single grain of an AlCuFe alloy. Dodecahedral crystals of aluminum-iron-copper alloy were first obtained in 1988, followed by aluminum-palladium-manganese in 1990. They were formed by regular slow-casting methods and behaved stably.

tagons. I discovered this construction one day while contemplating the meaning of a fragment from Diophantus' lost work "On Polygonal Numbers," which describes a proposition by the classical Greek geometer Hypsicles:

"There has also been proved what was stated by Hypsicles in a definition, namely, that 'if there be as many numbers as we please beginning from 1 and increasing by the same common difference, then, when the common difference is 1, the sum of all the numbers is a triangular number; when 2, a square number; when 3, a pentagonal number [; and so on]. The number of angles is called after the number which exceeds the common difference by 2, and the sides after the number of terms including 1.'"¹

The problem of the quasicrystal is related to the so-called "tiling" problem (how to cover the plane by repetition of like shapes). However, the solution arose by considering the crystallographic problem from the standpoint implied in the Diophantus fragment: How to create self-similarly growing figures? Self-similar squares and triangles may be produced from square and triangular tiles in a manner that is fairly easy to see. The squares completely cover the area they enclose. The triangles leave holes, also of triangular shape, and thus the principle of tiling (that the plane be completely covered) is modified (Figure 1).

To construct self-similar pentagons, it is necessary to modify the principle of tiling in the opposite direction—that is, to allow the pentagons to overlap and thus to "overflow" the plane. By such means, a succession of self-similar regular pentagons consisting of 1,5,12,22,35, . . . pentagonal units may be constructed (Figure 2). The second-order difference of the series of pentagonal numbers so constructed, is, as Hypsicles noted, 3; that for the square numbers is 2; and for the triangular numbers, 1.

Hypsicles' expressed concern with the triangle, square, and pentagon suggested to me that he must have been investigating the five regular or Platonic solids, whose faces are restricted to these three polygons. From that consideration, I saw that there existed constructible mathematical functions, analogous to what we are familiar with as "squared and "cubed," for each of the Platonic solids.

Thus, on the base of the plane figure "2-triangled," one may construct the solid "2-tetrahedroned," which has the charming feature of concealing a regular octahedron in the unfilled space in its center. Like 2-cubed, 2-tetrahedroned is a larger tetrahedron of doubled edge length. However, its numerical value, that is the count of its unit cells, is 4, not 8. Also on 2-triangled as a base, may be constructed "2-octahedroned," and "2-icosahedroned." The latter solid, which consists of 12 icosahedral unit cells, "overfills" the three-dimensional space by causing each of its unit cells to interpenetrate (Figure 3).

Finally, on the base of "2-pentagoned," one may construct "2-dodecahedroned," a dodecahedron whose edges are twice the length of the original, and which consists of 20 interpenetrating unit cells (Figure 4). These solid figures may be continued indefinitely, always producing a larger solid self-similar to the original unit cell.

I believe that atoms arranged at the vertices of the figure of n-dodecahedroned would answer to the requirements of a quasicrystal lattice which exhibits a dodecahedral crystal form, such as the AlFeCu and AlPdMn alloys first produced in 1988 and 1990. The lattice points of this model arrange themselves in decagonal patterns around a given center, as I elaborate below, just as is seen in diffraction studies of quasicrystals. Also corresponding to the evidence of diffraction images, the spacing of the n-dodecahedroned lattice

in certain linear directions follows the golden section.

Hexagonal vs. Pentagonal

Modern crystallography originated with Johannes Kepler's studies of the "fitting together" (*congruentia* or *harmonia*) of figures in two and three dimensions. Of special importance to the development of crystallography was his study of the packing of spheres. In a single layer of spheres, pushed together in the most compact way, each sphere is touched by six others. This hexagonal theme is continued into the three-dimensional configurations of close-packed spheres.

As Kepler showed in his *Six Cornered Snowflake*, when 12 spheres are forced together around a central one (closely packed), the connection of the spherical centers forms a cuboctahedron, a solid



Figure 1
3-TRIANGLED

Note the triangular gaps in the tiling of the grey triangles which build 3-triangled.

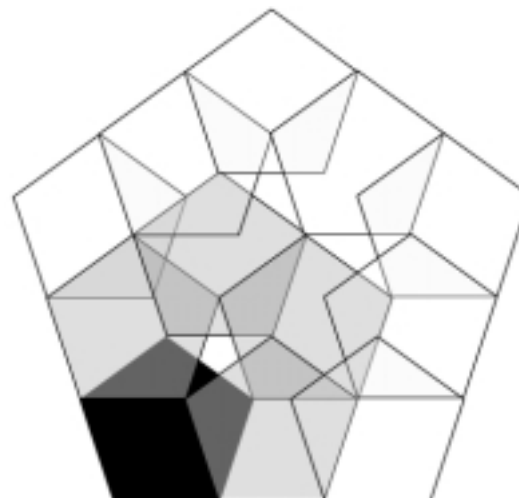


Figure 2
3-PENTAGONED

Five unit pentagons interpenetrate to form 2-pentagoned, and 12 to form 3-pentagoned.

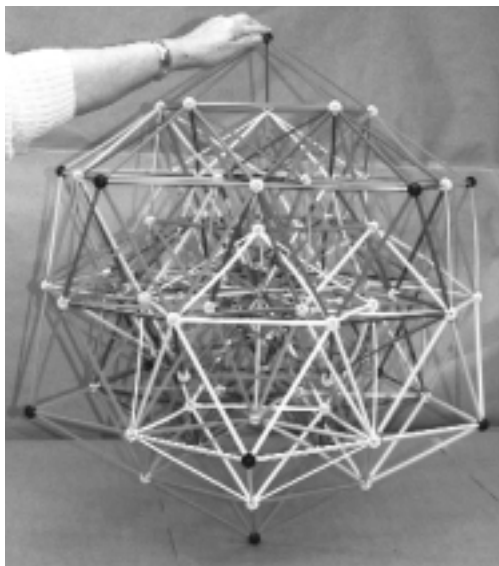


Figure 3
2-ICOSAHEDRONED

The large icosahedron envelops 12 interpenetrating unit icosahedra. Each face is 2-triangled.

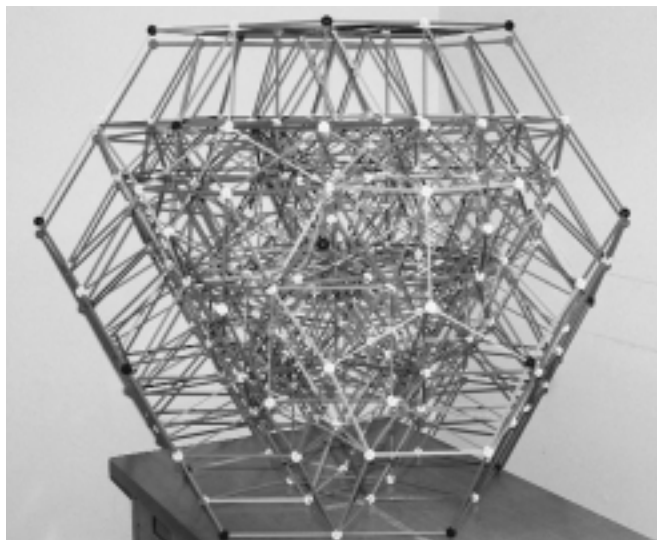


Figure 4
2-DODECAHEDRONED

2-dodecahedroned contains 20 interpenetrating unit dodecahedra. Each face is 2-pentagoned. (See color reproduction on back cover).

which may also be produced by the intersection of four circular hoops, each dividing the other into six parts (Figure 5). Hence the six-fold, or hexagonal symmetry. (The forms deriving from cube, octahedron, and tetrahedron are broadly considered as of hexagonal symmetry but of a lower class.)

Kepler wondered if an arrangement of that sort, at the microscopic level, might not be the reason for the ever-present hexagonal symmetry of snowflakes. He also noted that non-living things tended toward the hexagonal symmetry, while plants and animals often exhibited the pentagonal symmetry, and the associated golden ratio, or divine proportion, which is expressed in the ratio of edge length to diagonal on the face of a pentagonal dodecahedron.

His short work on the snowflake, written in a playful tone as a New Year's gift to his ducal sponsor, exposes his creative genius in a most compact way, and ranks among the most seminal pieces in modern science. Of special interest to crystallography, is his description of his discovery of a new solid, the rhombic triacontahedron, the shape exhibited by the first quasicrystals with clearly distinguishable grains grown in 1986.

What began as Kepler's musings on the

snowflake was later followed up by many others into the modern developments of crystallography. Notable was the work of the Abbé Haüy in the late 18th Century, explaining the regular shapes and angles of crystals as a result of repetition of an integrant form; Mitscherlich through his chemical investigations of crystal isomorphism; Pasteur with his groundbreaking discovery of hemihedral crystals of mirror symmetry; von Federov, who created a table of 10,000 different crystals, allowing the identification of an unknown substance by measurement of its facial angles; and Max von Laue who demonstrated in 1913, by means of X-ray diffraction, that there were indeed tiny points in the crystal lattice, corresponding to what had, by then, been assumed to be the locations of atoms.

A consistent feature of all these studies was that the crystals were considered to be made up of units which touched each other at their surface boundaries. With the n-dodecahedroned construction, I am suggesting that a new kind of "fitting together" be considered, in which a periodic form of interpenetration of the structural units takes place.

In Kepler's early concepts, the structural units were individual spheres. Haüy in 1784 proposed that crystals were built

up of little bricks, or parallelepipeds, of varying shape for each substance. That view reached a high stage of development in the early 19th Century when geometrical studies showed that only 32 types of crystal symmetry were possible. Then Frankenheim (1842) and Bravais (1848) established the concept of the unit cell, a way of representing the relationship of the lattice points to each other in the form of 14 different types of brick-like solids, a lattice point at each corner, which could be piled up to represent all possible crystal forms—or so it was thought.

It was at first supposed that the lattice points might correspond to the chemical molecules of the substance. But the development of X-ray crystallography tended to the view that the crystal was composed of individual atoms, and the lattice points of crystallographers became synonymous with atoms or ions. Crystals of compound substances came to be explained as interpenetrating combinations of the basic known space lattices. With the development of the electron theory, the glue that held the crystal together was thought to be the interaction of electrons, although metallic crystals posed a special problem. Thus, essentially forces emanating indi-

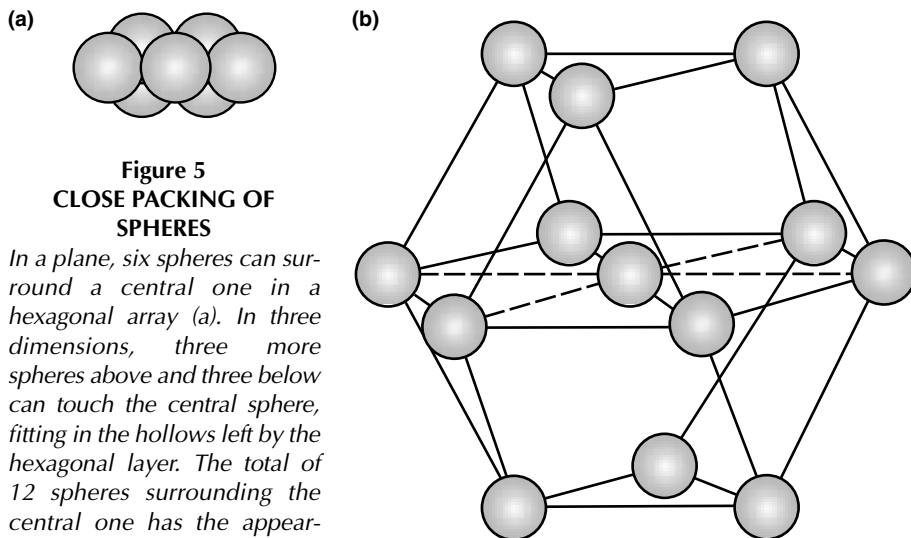


Figure 5
CLOSE PACKING OF SPHERES

In a plane, six spheres can surround a central one in a hexagonal array (a). In three dimensions, three more spheres above and three below can touch the central sphere, fitting in the hollows left by the hexagonal layer. The total of 12 spheres surrounding the central one has the appearance of the Archimedean solid, the cuboctahedron (b).

vidually from each point of the crystal seemed to hold the crystal together. If each atom acted according to its instincts, the job would be done.

But these views were challenged after 1984 with the discovery by Israeli metallurgist Dany Shechtman of metal alloys which showed the forbidden five-fold symmetry, and a quasiperiodic ordering of lattice points in their diffraction patterns. There seemed to be no way to imagine by the known rules of crystallography that such a structure could come together.

The Principle of Homogeneity

I believe I have shown in the n-dodecahedroned construction, a way of extending the so far accepted laws of crystallography to account for a crystal of five-fold symmetry. With one significant variation in the usually accepted axioms of crystallography, a regular unit cell, repeated in periodic fashion, can produce a dodecahedral or icosahedral crystal form. The required variation is, that instead of cells which fill space with no gaps, we must allow an interpenetration which produces an "overfilling" of the space.

I have spent some time trying to imagine how this variation might alter the relationship of one lattice point to another. Is it still possible to describe the structure as the result of the individual action of each constituent atom or ion, or is it necessary to suppose a sort of collective action or field determining the growth? If the quasicrystal is describable

as the result of forces emanating from each individual atom, then geometrically each lattice point must be indistinguishable from the next; that is, every atom must have the remaining atoms arranged about in the same manner. This is known in crystallography as the principle of homogeneity.

In the n-dodecahedroned lattice, 30 edges protrude from each vertex in the 30 directions of the vertices of an icosidodecahedron. (The pre-cut spheres of the Zome brand construction kits provide just enough positions for this arrangement.) In a model of 2-dodecahedroned, the central vertex at which 20 dodecahedral unit cells come together, will show these 30 directions. As the model is expanded, each vertex will show the same arrangement. As the icosidodecahedron may be produced by the intersection of 6 rings or hoops, each one dividing the other into 10 parts, one sees that there are 6 planes in which a decagon surrounds a central point.

However, as the n-dodecahedroned lattice grows, something new arises. Because of the overlap of cells, a vertex from an adjacent interpenetrating dodecahedral cell cuts the original edge in a golden section. Thus, around each vertex is a group of 30 nearer vertices coming from interpenetrating cells. However, closer inspection shows that each vertex is not the same. Because of the fact that the edges are cut in golden

section, there seem to be vertices which are distant by the smaller part of the section, and others which are distant by the larger part, from the nearest neighboring vertex.

Thus the principle of homogeneity, requiring that every atom have the remaining atoms arranged about it in the same manner, is violated.

This conclusion, apparently consistent with some of the results of X-ray diffraction studies, requires more thorough geometric investigation. If true, it would seem to require that the quasicrystal cannot be conceived as resulting from uniform forces emanating from each atomic center. We might instead suppose that the functional unit of formation is the

whole dodecahedron. We seem thus to return to the idea of the unit cell as a functional unit, rather than merely the descriptive unit it has become for modern crystallography.

However, it were then necessary to provide a reason why the dodecahedral cells assemble in the fashion that they do. The simplest explanation would seem to be that the whole crystal seeks a dodecahedral form, and finds it in the only way which geometry permits such a self-similar growth.

Such a hypothesis would be repugnant to the extreme mechanist or reductionist, who seeks to explain all events of nature from presumed elementary particles and the forces of attraction or repulsion between them. Yet, we have not found a clearer one. We hope to discuss this aspect of the matter further in future communications. We have also not addressed here the implications of the appearance of the dodecahedral form for our studies of the nuclear model of Prof. Robert J. Moon. The appearance of the elements aluminum ($Z = 13$), manganese or iron ($Z = 25, 26$) and palladium ($Z = 46$) is most suggestive in this respect.

Notes

1. Translation by Ivor Thomas, *Selections Illustrating the History of Greek Mathematics*, (Cambridge, Mass.: Harvard University Press, 1993) p. 515 (from Diophantus, *On Polygonal Numbers* [5], Dioph. ed. Tannery i. 470. 27-472. 4).