Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Received 1 October 2001
Accepted 17 October 2001

A simple isohedral tiling of three-dimensional space by infinite tiles and with symmetry $Ia\bar{3}d$

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A tiling of space by tiles that have all hexagonal faces and are infinite in one direction is described. The tiling is simple (four tiles meet at each vertex, three at each edge and two at each face) and carries a 4-connected net whose vertices are the lattice complex S^* with symmetry $Ia\bar{3}d$. The tiling is closely related to the densest cubic cylinder packing, Γ. It is shown that the other invariant cubic lattice complexes unique to $Ia\bar{3}d$ (Y^{**} and V^*) are also related to the same cylinder packing.

1. Definitions and terminology

Simple tilings of three-dimensional Euclidean space (hereafter just 'space') are those in which exactly four tiles meet at each vertex, three at each edge and two at each face. Normally the tiles are finite simple polyhedra (those in which exactly three edges meet in each vertex). Physical examples of such structures are provided by foams and related cellular materials such as plant cell tissue and the assembly of grains in polycrystalline materials. On the atomic level, the framework of tetrahedrally coordinated atoms in materials such as zeolites often corresponds to a simple tiling; the structure of faujasite provides a well known example. We say that the framework of edges and vertices is a net *carried* by the tiling. If the edges are all equal and correspond to the shortest distances between vertices, the positions of the vertices correspond to the centers of equal spheres in contact and we say that the structure is a *sphere packing*. Packings of spheres, and other objects such as cylinders, in which all the objects are related by symmetry are referred to as *homogeneous.* Structures of this sort are of particular interest to us as the underlying geometries of materials that are the targets of designed synthesis (O'Keeffe *et al.*, 2000)

Tilings are conveniently classified by their *transitivity* ⟨*pqrs*⟩ which signifies that the structure has p kinds of vertex, q kinds of edge, r kinds of face and s kinds of tile, Tilings with $s = 1$ are known as *isohedral* and with $p = 1$ as *vertex-transitive* or *uninodal*. The *dual* of a tiling is the structure in which a vertex is associated with each of the tiles, and edges connecting the vertices pass through faces of the tiles (note that dualization must be carried out in such a way that the dual of the dual is the original tiling, at least up to topology). The transitivity of the dual tiling is ⟨*srqp*⟩. A given net may be carried by more than one tiling, as we see below.

In a packing of objects such as spheres and cylinders, not all of space is filled. Positions of local maximum distance from the surface of the object are the location of *holes* on the packing. Holes equidistant from four neighbors are *tetrahedral holes.*

A detailed account of lattice complexes and their occurrences is given by Fischer & Koch (1983) and the invariant cubic ones mentioned here are illustrated by O'Keeffe & Hyde (1996).

2. Cubic sphere and cylinder packings with tetrahedral holes and their dual tilings

The body-centered cubic lattice is the only homogeneous cubic sphere packing in which all the holes are tetrahedral and related by symmetry. The holes are on the vertices of the dual structure which is known as the Kelvin structure (Thomson, 1887) or the sodalite structure and are at the positions of the invariant lattice complex W^*. The tiling is the familiar tiling of space with truncated octahedra (Fig. 1*a*). The structure has two kinds of face (transitivity ⟨1121⟩) so it is not regular.

The body-centered cubic cylinder packing labeled Γ (O'Keeffe *et al.*, 2001) has the same density as the body-centered cubic sphere packing (fraction of space filled = $3^{1/2}\pi/8 = 0.680\ldots$) and also has tetrahedral holes which fall at the positions [(3/8, 0, 1/4) *etc*.] of the invariant lattice complex S^* with symmetry $Ia\bar{3}d$. This set of points may be considered the dual of the cylinder packing in the sense that the points are in the holes of the original packing. They are the tetrahedral positions in the garnet structure, *i.e.* the Si positions in the prototypical garnet grossular, $Ca_3Al_2Si_3O_{12}$. The 4-connected net of the S^* structure can also be considered as carried by a simple tiling in which the tiles are infinite in one direction and the axes run in the cubic ⟨111⟩ directions, Fig. 1(*b*). All the vertices, edges, faces and tiles of this structure are related by symmetry so the transitivity is ⟨1111⟩.

We believe that the structure just described (Fig. 1*b*) is the only simple tiling with transitivity ⟨1111⟩. Certainly it is easy to show that any such tiling must have tiles that are infinite and have hexagonal faces. For a simple tiling in which the average number of edges per face is ⟨*n*⟩ and there are *F*/*P* faces per polyhedron (recall that each face is shared between two polyhedra), it follows (O'Keeffe & Hyde, 1996) from Euler's equation that $\langle n\rangle = 6 - 6P/F$. Tiling of space by simple polyhedra with all five-sided faces (*i.e.* regular dodecahedra) are well known to be impossible, and if $\langle n\rangle = 6$ then $P/F = 0$, *i.e.* there is an infinite number of faces per polyhedron.

3. Related structures with symmetry $Ia\bar{3}d$

A 4-connected structure related to S^* is obtained by replacing the vertices of that net by regular tetrahedra of vertices (O'Keeffe, 1991). The symmetry remains $Ia\bar{3}d$ and the vertices are in general positions

(0.065, 0.224, 0.424) *etc*. This net, labeled S^*4, is that of the sphere packing 4/3/*c*32 of Fischer (1974), and is carried by a simple tiling of space with infinite tiles with 3- and 12-sided faces and tetrahedra (Fig. 1*c*). The structure is still uninodal (transitivity ⟨1322⟩) so it provides a second new example of a uninodal simple tiling. Counting faces and polyhedra is performed as follows. Three 12-rings and three 3-rings meet at each vertex so there are 3/3 + 3/12 = 5/4 faces per vertex. The number of infinite polyhedra is vanishingly small compared to the tetrahedra of which there are 1/4 per vertex. Accordingly, $P/V = 1/5$ and $\langle n \rangle = 24/5$ as may be readily confirmed by direct counting.

The S^* structure is also carried by a tiling with the same symmetry that uses finite tiles (Fig. 1*d*). In fact, we consider this second tiling the *natural* tiling of the structure as there is a one-to-one correspondence between the strong rings of the structure and the faces of the tiles.[1] Each tile has five hexagonal faces so the dual of this structure is a 5-connected net. The dual tiling is shown in Fig. 1(*e*): each tile has eight vertices (it corresponds to the carbon framework of stellane, tricyclooctane) and a fragment of the net that it carries is shown in Fig. 1(*f*). This last structure is not a 5-coordinated sphere packing as there are two different edge lengths. The vertices of this structure correspond to the points of invariant lattice complex Y^{**} [positions (1/8, 1/8, 1/8) *etc*.]. As illustrated in the figure, these points lie on the axes of the cylinder packing. It is an example of a structure in which all rings are 5-membered. The structure of γ-Si is closely related (O'Keeffe & Hyde, 1996).

There is a third invariant cubic lattice complex unique to $Ia\bar{3}d$, namely V^* [positions (1/8, 0, 1/4) *etc*.]. It is also simply related to the cylinder packing Γ, as the points are the points of contact of the cylinders. These are the Ca positions in grossular garnet.

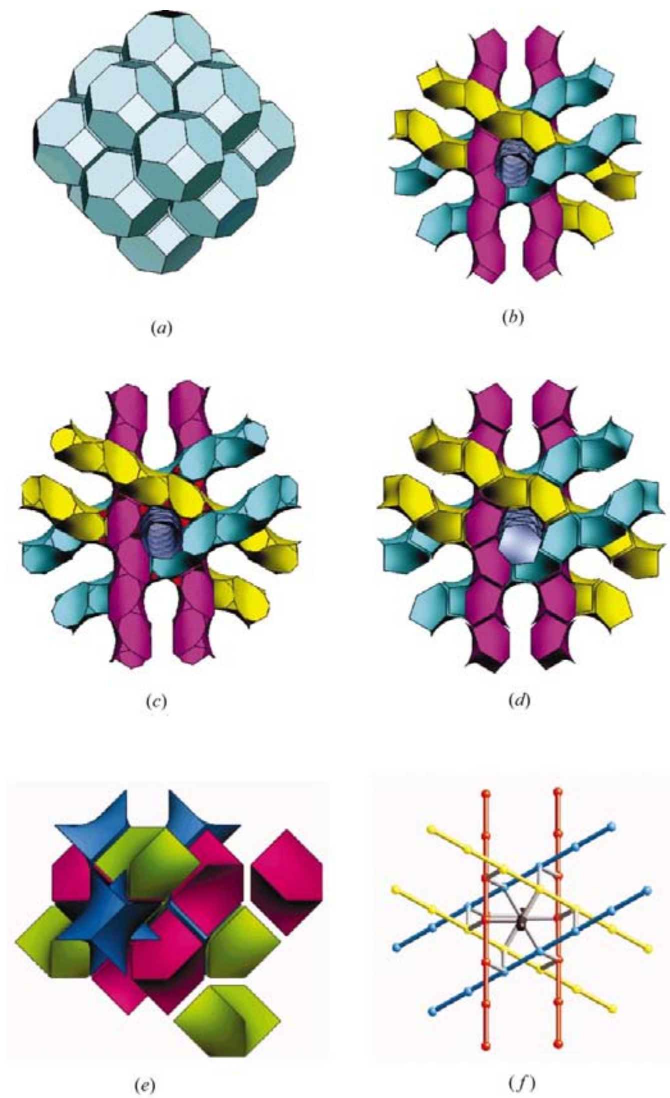

Figure 1
(*a*) Tiling by truncated octahedra (Kelvin structure). (*b*) The tiling by infinite polyhedra. (*c*) A tiling by a combination of infinite polyhedra and tetrahedra (red). (*d*) The structure in (*b*) broken up into congruent tiles with five faces. (*e*) The tiling dual to that in (*d*); the tiles are congruent and have four faces. (*f*) The structure dual to that in (*d*) shown as a ball and spoke model; each ball corresponds to the center of a tile in (*d*).

4. Other uninodal simple tilings

It is now well established (Delgado Friedrichs & Huson, 1999) that there are exactly nine simple tilings of space by finite polyhedra. They are of considerable interest (Delgado Friedrichs *et al*., 1999) as six of them, zeolite codes (Baerlocher *et al*., 2001) SOD, LTA, RHO, FAU, KFI and CHA, correspond to common zeolite structure types, including several of the most important with particularly open structures. Delgado Friedrichs & Huson (2000) showed that most of the other uninodal zeolite nets can be described with tilings in which some of the tiles have vertices at which only two edges meet (non-simple 'polyhedra'). It transpires that at least four of these, those with zeolite codes ATN, CAN, GME, MER, can be described by a combination of infinite and finite tiles, much as the structure S^*4 described above; however, now all the infinite tiles are parallel. Thus, if infinite tiles are allowed, there are at least six new uninodal simple tilings to be added to the nine with finite polyhedra. However, we note that these new tilings are not *natural* tilings in the sense indicated above.

This work was supported by the US National Science Foundation (grant DMR 98 04817) and by the Donors of the Petroleum Research Fund, administered by the American Chemical Society.

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[1] A strong ring is one that is not the sum of smaller rings (Goetzke & Klein, 1991). The S^* structure has only six-membered rings, so they are of necessity all strong.