SHORT COMMUNICATIONS

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Novel regular quinquehedral packing obtained by the local approach

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Abstract

A novel regular packing with a coordination number five and a square-pyramid coordination polyhedron for all the vertices and the same distances between closest neighbours is briefly presented within both the local and the global approaches.

1. Introduction

At the present time, there does not exist a universal method of deducing all possible regular packings in n-dimensional spaces (R^n) with $n \geq 3$. Partial solutions of a space-filling problem for R^3 were found by Fedorov (five polyhedra fill space when similarly oriented), by Andreini (combinations of regular and Archimedean semi-regular solids) and by Wells [mainly uniform (n, p)-nets, where n is the number of vertices in the shortest circuit and p is the number of links meeting at the vertex] (Wells, 1977). A general solution of this problem, an algorithm for the derivation of Voronoy–Dirichlet polyhedra for all points of a regular system proposed by Delone & Sandakova (1961), turned out to be very complicated even in R^3 and is apparently still not realized to date. Another approach, based on the construction of regular graphs using their automorphism groups, is restricted to those having only one fundamental domain (Konovalov & Galiulin, 1989).

The local approach proposed by the author for the description of amorphous solids (Manzhar, 1993) also provides the possibility of obtaining, in a certain way, various periodic packings depending on the number of vertices in a primitive cell and of classifying these packings on the basis of a fibre-bundle theory (Manzhar, 1991). An idea of the locality, *i.e.* of the construction of an assembly of atoms (points) proceeding from a finite number of local configurations, was reported by Delone, Dolbilin, Stogrin & Galiulin (1976), who proved a famous local theorem. Although being the same in nature, our local approach differs radically from the pure geometrical approach of Delone *et al.* in terms of the mathematics involved. It is by the local approach that a periodic packing with a coordination number (CN) five (5-connected net by Wells' terminology) and a coordination polyhedron (CP) in the form of a square pyramid has been obtained. Its structure is the subject of our short report.

2. Method and results

The local construction principle of the 5-connected net, herein referred to as the quinquehedral packing (QP), is the same as that of diamond or tetrahedral packing (TP) (Manzhar, 1990). As far as our local approach in general is concerned, we would like to stress that within the framework of this approach any structure is evolved from a certain convex polyhedron, *e.g.* from a cube in the case of the TP. Similarly, the QP is also evolved from a convex polyhedron consisting of ten vertices, which may be described as a 'cubic dipyramid' (CD) (two square pyramids with a deformed cube between them). Note that the cube and the CD are simply the CP's of vertices in body-centred cubic (b.c.c.) (CN = 8) and body-centred tetragonal (b.c.t.) (CN = 10) lattices, respectively. Hence, both the TP and the QP are derived by removing half of the vertices from corresponding lattices: the b.c.c. lattice in the case of the TP and the b.c.t. lattice for the QP. All the vertices of the CD split into two groups, with each of them defining a short-range-order configuration (coordination polyhedron) in the form of a square pyramid. Two such pyramids with opposite orientations are realized step by step in the QP by means of gauge fields (discrete complementary vectors in reciprocal space) (Manzhar, 1990). The QP obtained in such a way belongs to one of the eight topologically non-equivalent classes of three-dimensional so-called Z_2-structures (two vertices in the primitive cell) for which the preliminary

Table 1. *Radii and the corresponding coordination numbers of the first five coordination spheres in the quinquehedral packing*

	Coordination sphere radius	Coordination number
1	R	5
2	$(3/2)^{1/2}R$	4
3	$(5/2)^{1/2}R$	4
4	$3^{1/2}R$	12
5	$2R$	13

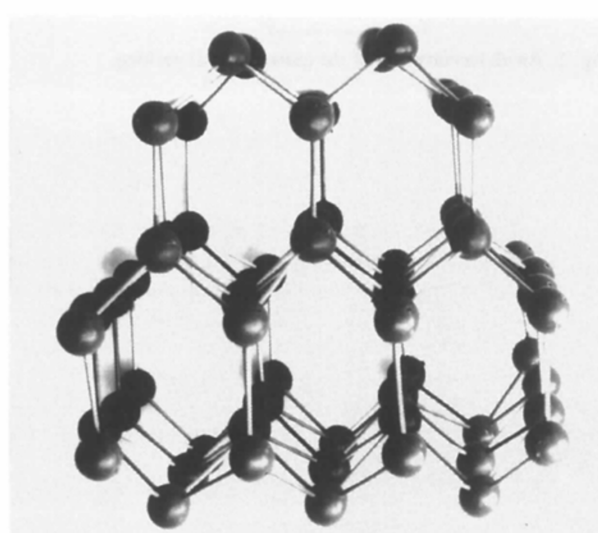

Fig. 1. A fragment of the quinquehedral packing (viewed along the x or y axis).

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topological classification in terms of fibre bundles and gauge fields have been made earlier (Manzhar, 1991). For a more visual picture of the QP, we describe it below by the usual (global) approach, *i.e.* in terms of space groups and space lattices.

The elementary cell of the QP containing four vertices and belonging to a tetragonal syngony [$a = (3/2)^{1/2}r$, $c = 3r$, where r is the shortest distance between vertices] with the space group $I4/mmm$ is shown in Fig. 2. A few of the CN's and corresponding radii of coordination spheres expressed by r are given in Table 1. The packing density, Δ, of the QP is given by $\Delta = 4\pi/27 \simeq 0.465$. It therefore lies between the density of the TP ($\Delta \simeq 0.3401$, CN = 4) and that of a simple cubic lattice ($\Delta \simeq 0.524$, CN = 6). All vertices belong to one symmetry side.

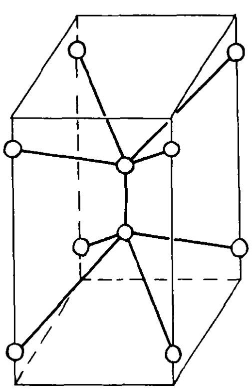

Fig. 2. An elementary cell of the quinquehedral packing.

3. Concluding remarks

It is well known that only two CP's with five vertices, namely the trigonal dipyramid and the square pyramid, occur in real structures (Wells, 1986). In R^3, there exists a regular points system in which five points in the trigonal-dipyramid configuration are placed around any point. This is a well known regular packing of hexagonal plane nets without shifting along the z axis with a period equal to the shortest distance between the vertices in the plane. It seems that the QP is the first (and possibly the last) example of a packing where each vertex is surrounded by five vertices in the square-pyramid configuration. The QP among nets with CN = 5, as well as the TP among nets with CN = 4, has the least basis (Z_2-structure). Some compounds, where single-type atoms have the square pyramid CP, have been found experimentally, *e.g.* Ge atoms are surrounded by five O atoms in $Ba_3Ge_9O_{20}(OH)_2$ (Malinovskii, Pobedimskaia & Belov, 1976) and $X_5GeO_5(OH)_3$, where X = Y, Sm, Gd, Dy (Genkina, Demyanets, Mamin & Maximov, 1989), which is not very typical for germanium. Some factors make the very existence of the QP as a monoatomic system almost inprobable. Unlike a tetrahedron (the coordination polyhedron in the TP), a weight centre of five identical atoms forming the square pyramid does not coincide with its geometrical centre, which makes such clusters unstable with respect to forces acting between the atoms. This unstability could be compensated for by replacing one or two neighbours in each square pyramid by atoms that are chemically different from the original ones. The QP might be obtained as a two- or three-component system with elements belonging to groups IV and VI or exclusively to group V of Mendeleev's table.

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