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A. L. Talis, **A. L. Rabinovich** (Moscow, INEOS RAS; Petrozavodsk, IB KarRC RAS). **Linear substructures as mappings from a four-dimensional diamond-like polytope: an approach for characterization of non-crystallographic symmetry.**

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Abstract: The Hopf fibration formalism for the polytope $\{240\}$ allows constructing a number of its linear substructures. An approach has been developed for their group-theoretical description. The symmetry groups of the complexes of such substructures are isomorphic to subgroups of the permutation group of the polytope's vertices.

Keywords: polytope $\{240\}$, linear diamond-like substructures, non-crystallographic symmetry.

A diamond-like polyhedron in 4-dimensional Euclidean space E^4 (the polytope $\{240\}$) [1, 2] has extreme structural characteristics for tetrahedrally coordinated systems, and the environment of each vertex is the densest in such systems [3]. The Hopf fibration [4, 5] allows to construct mappings of the polytope' $\{240\}$ linear substructures into the space E^3 that contain pendant vertices and six-fold rings [3]. These are "ideal prototypes" for the corresponding real linear structures. The possibility of combining such structures into complexes is determined by symmetries of the polytope $\{240\}$ or by the more highly symmetric structures into which they can be embedded.

The polytope $\{240\}$ is a union of two copies of a polytope $\{3,3,5\}$ [1, 2] (which is a 4-dimensional analogue of an icosahedron), so the vertices of the fibration base must be the vertices of a union of two icosahedrons with a common center, and the symmetry group of this union must be consistent with that of the polytope $\{240\}$ - this is the case for an octahedron symmetry group O_h [3]. The union of two ideal icosahedrons with a common center whose vertices are the vertices of a truncated octahedron is characterized by the group O_h [6]; each hexagon in the union has unequal edges and its symmetry group is a regular triangle group C_{3v}. Hexagons become regular, and the union preserves the group O_h only if both icosahedrons are *right* ones (a *right* icosahedron contains 8 regular and 12 isosceles triangles), and the bases of isosceles triangles are $(2/3)^{1/2}$ times shorter than the sides of regular triangles; the 24 vertices of this union are vertices of the Fedorov's parallelohedron [3] with 14 faces (8 faces are regular hexagons and 6 are squares).

The polytope $\{240\}$ symmetry group is represented in the Hopf fibration as the product of its subgroups for the "base" and "fibre". One of the fibration options is $\{240\} \to ([4^6,6^8])$ (fibre $\{10\}$), where $([4^6,6^8])$ is the base (Fedorov's parallelohedron). Each of its 24 vertices corresponds to a fibre $\{10\}$ that consists of 10 vertices joined by a screw axis 10_1. It is necessary to cover the 24 base vertices with the minimum number of triangles that do not have common vertices (in this formalism, a 30-vertex tetrahelix corresponds to each triangle [3–5]). To cover the 12 vertices of a *right* icosahedron with triangles, either 4 regular triangles, or 1 regular and 3 isosceles triangles are needed. It is necessary to construct the Fedorov's parallelohedron from two *right* icosahedrons, and various triangles will make it possible to distinguish symmetrically nonequivalent partitions of the base vertices into subsets.

To reveal the maximum possible symmetry of these substructures, e.g. groups of maximum order (which are, in general, subgroups of permutation groups), it is required that the elements of the systems are the same, contain only *regular* triangles, as in the union of two *regular* icosahedrons. The symmetry group of the 1^{st} regular icosahedron in such a union is Y_h of order 120; we decompose it into 20 cosets by its subgroup C_{3v} of order 6. The Y_h group of the 2^{nd} icosahedron of this union must be conjugated to the symmetry group of the 1^{st} icosahedron by an element σ of order 2 from the O_h group. We decompose it into 20 cosets by the subgroup C_{3v} as well. In the general case, the union of $2 \cdot 4 = 8$ regular triangles covering all 24 vertices has a common axis C_3 of order 3.

If we combine 4 unions of pairs of triangles from *different* icosahedrons, we get $(C_{3v} \bigcup \sigma C_{3v} \sigma^{-1}) \bigcup (C_3 (g_i C_{3v} \bigcup \sigma g_i C_{3v} \sigma^{-1}))$, where g_i are elements of the Y_h group that do not belong to C_{3v} ; $\bigcup$ is the union sign. The union of the two *nearest* triangles $g_i C_{3v}$ and $\sigma g_i C_{3v} \sigma^{-1}$ must have a (super)group of a symmetry group $\{1, \sigma\}$ of order 2 that can be only C_{3v} or rectangle group C_{2v} or C_2 or symmetry plane C_{1v}. This allows finding groups of automorphisms of the Hopf fibration base of each system, i. e. subgroups of the permutation group of 24 vertices consistent with the icosahedron geometry.

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