DOI 10.12851/EESJ201606C06ART03

Valeriy V. Ivanov,
ScD, associate professor,
South-Russian state polytechnic university n.a. Platov MI (NPI),
J-SC «SDTU «ORION», Novocherkassk

The Choice of the Structural Cells-Modules for Receiving of the Possible Modular and Corresponding Modulated Structures

Key words: *structure, polyhedron, structural module, modular cell, modular structure, modular design.*

Annotation: *Possible methods of choice of the structural cells-modules which may be used for receiving of some multitude of corresponding modular and modulated structures were discussed. The same variants of the splitting and structural cells-modules forming into space for following modular design were examined, too.*

It's known the cell of some modular structure can be used to receiving a multitude of new genetically related modular structures by a modular design method (1, 2). However, in order to implement a modular design it is necessary to solve at least two problems: the problem of 3D space splitting for spatial cell of a particular form and the problem of structuring 3D space by filling its structural modules with some geometry and topology (1, 2). The splitting problem of the 3D space is one of the most important and actual problems of modeling of modular and modulated crystals.

There are two options for solving the of the filling space problem.

1. The splitting of a structured space on modular cells and identification of basic structural module can be implemented by developed algorithm (3). However, in this case, the modular cell characterizes only one degenerated modular structure. Why carry out purposeful modification of the basic module until the appropriate modular cells with the necessary topological characteristics. Modification of the module is done by regular changes its configuration by changing the degree of non-isolating and the numbers of atoms accessories onto module borders. Obtained modular cells and their corresponding modules can be used for modular design (1, 3). Design of the possible modular structure is done by nesting modules in cell on different packaging laws (1-6).

2**.** Structuring of the space and its partitioning can be achieved by using of certain basic totality of atoms, for example, atoms at the vertices of the right or semi-right isogons (3, 4). However, only four of these combinations (12 {344}, 8 {444}, 6 {644} and 4 {466}) are leads to the formation of one-modular structures. It is necessary the procedure of the focused structural modification of the module for receiving of the multiple of non-degenerate modular structure (3).

Let's take a look at options for the modular cell not associated with partitioning 3D structured space.

Approach 1. If the crystal structure type is known, it is recommended that you use the following methods of forming module for modular design (3).

Method 1. Change packaging law of the basic module. Through targeted packaging law of the characteristic module a set of modular structures can be obtained. All these structures are polymorphic modifications of the original structural type.

Method 2. The purposive modification of crystal chemical topology of the characteristic basic module.

Method 3. Theoretical analysis of the packaging law of possible asymmetric modules and definition of their configurations. For each structural type the law of the packaging of the basic modules can be determined by the characteristic lattice complex. And asymmetrical non-isolated module for which the packaging on the same law corresponds to some modular structure can be determined, too.

Approach 2. In the absence of a structured space.

Method 1. Simulation of structural types of crystals and forming module for a modular design. One of the most effective methods of structuring space is based on the basic packages of atoms with identical topology environment of each atom. Geometry for base packages can serve as one of 28 well-know lattices, nodes which are formed by the vertices of the corresponding compact packaged in the space of combinations of certain isogons (3). From basic packages of atoms using Delaunay conversion you can go to the compact packaging to atomic polyhedral of Voronoi-Derichlet. The centers of these polyhedra are the topologically equivalent vertices of isogons, and the polyhedral vertexes are their geometric centers (4).

Method 2. Formation of cellular space with subsequent contingency investment the specific compatible structural fragments into equivalent cell. Formation of cellular 3D space can be based on one type of isogons, completely fill this space. The attachment of certain structural fragments in spatial cells is carried out on a specific program of forming near and far order of the future modular structure that describes with using of evolutionary models in the form of its genetic code (5, 6).

Another approach to obtain of the modular cells of 3D structures is the construction cells with using of projective representations of spatial cells of another dimension. As a prototype of modular cells, you can use the hyper-polygons or hyper-polygonal nets. If the prototype the probable fragment of modular cells considered a hyper-polyhedron – hyper-spatial polytop, then the projecting in 3D space can be obtained most symmetrical geometric its images. Certain topological transformation of these geometric images is generates a set of other vertex configurations, each of which formally can also be a fragment of probable modular cell.

Method 3. Finding of cells-modules from cells of structured 2D space. In this case, to obtain of the modular cells enough to use the ready crystal chemical solutions for cellular 2D space (1, 3). To solve the problem, you can use a set of 11-minute topologically distinguishable Kepler nets or some bi-colored Kepler-Shubnikov nets with topologically equivalent nodes (3). We will seek the necessary form of modular cells 3D structures, introducing them as hyper-cells as low dimensional prototype which are the cells of 2D structures. Using a intake doubling of the nods of modular cells 2D structures through their breeding in orthogonal 2D space direction in plane parallel is leads in the general case, to the formation of each {n}-gonal cell of the corresponding prismatic {n44}-cell of the likely 3D structure (3, 7).

Method 3. Finding of the cells-modules from hyper-cells of structured 4D space. In this case, can be effectively used the right poly-cells (or poly-tops) of 4D space, which are characterized by topologically identical nodes and identical cells-polyhedrons, as well as form in 4D space the compact packaging. To obtain the geometric images of these modular hyper-polyhedral structures in 3D space let's using their projective display, as well as the topological transformation of these images to obtain the modular structure (splitting-converting of the nods, stellation-design of the faces, the stretch open-design of the cell-polyhedron and Derichlet-conversion of the nods system).

Method 3. Finding of the cells-modules from hyper-cells of non structured 4D space. In this case, to obtain the modular cells 3D space can be used some of the semi-right polytopes of hyper-space (the cellular complexes and their projective geometric images into 3D space and modified variants) (8 -14).

Thus, the possible methods of choice of the structural cells-modules which may be used for receiving of some multitude of corresponding modular and modulated structures were discussed. The same variants of the splitting and the forming of structural cells-modules into 3D space for following modular design were examined.

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