SYMMETRY PRINCIPLES IN CONSTRUCTION OF MODULAR CRYSTAL STRUCTURES

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Modular crystal structures are natural buildings and their construction proceeds according to general laws governing the choice (formation) and stacking of their building modules (BM). The properties of crystals are the same in any part of them and this means that an atomic structure should be periodic and consist of sets of identical points forming a lattice. Homogeneity (or uniformity) is thus an inherent feature of crystal structures. The modules are energetically preferred and stable atomic or atomic coordination polyhedra assosciations and their stacking defined by their crystallochemical nature obeys the condition of equivalence for any adjacent modules. There is no need to know the exact module interaction field for evaluation equivalence because the symmetry of modules and module pairs reveals equivalent relative positions in the possible arrangements of modules. This consideration is the basic stone of the OD (order-disorder) theory created by K. Dornberger-Schiff (1964). It plays a leading role in understanding of construction of different ordered and disordered structures built of layers the adjacent pairs of which are symmetrically equivalent (OD layers) and it may be extended with some modifications to all modular structures (Zvyagin, 1995, 1997).

The BMs may adjust each other in modular structures if their lattices have common cells. These cells may be identical unit cells or supercells relative each of the unit cells in a superposition of lattices either of one kind modules in different orientations or of different kind modules in definite orientations.

The superposition of modules the unit cells of which are in rational relationships is characterized by several kinds of lattices defined by 1) the initial unit cells, 2) supercell formed by coinciding points of both lattices, and 3) subcell of a mesh to which the points of the superimposed primary lattices belong. The supercell in one space is reciprocal to the subcell in the reciprocal space and vice versa. Two kinds of modular sets forming modular structures are to be distinguished: alternation and stacking sets. The first ones form polysomatic systems, the second- provides hybride, polytype and OD structures. Possibilities were also revealed for formation of series intermediate between polytypes and pure polymorphs which may be both of the OD or not OD nature.

Module combinations and module selections in modular sets are represented by several kinds: single module, mixed module, combined module, and condenced module as examlified by spinelloids, sapphirines, ferrites and biopyriboles in the spinel-pyroxene modular system. Like OD structures both alternation and stacking series are subdivided into 4 categories depending on the polarity-nonpolarity of BMs and distribution of symmetry operations relating them in their sequences designed by K. Dornberger- Schiff (1964) with Greek letters ‚lambda', Isigmal, 'tau' and 'rho'. These operations play a guiding role in the spontaneous or conscious constructuion (simulation) of modular structures.

Each alternation series may contain different stacking series (single stacking and mixed stacking) of modular structures differing
in order-disorder, symmetry and periodicity. Variations of equivalent stockings leads to diversities of structures depending on the symmetry features of BMs and BM pairs, and on the symmetry differences of the BM structures and their lattices. The BMs are related by displacement, rotation and reflection operations which do not affect the BM lattices but provide different structural results.

Analythical means are elaborated involving symbols of BMs and of symmetry operations relating them for description, analysis, derivation, prediction and identification of modular structures.

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