MODELLING THE MULTIPLICATION OF HIERARCHICAL STRUCTURES USING THE ITERATED FUNCTION SYSTEM METHOD

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A method for modeling the formation of self-assembled structures of hierarchical crystals in high-temperature gas-transport synthesis environments by yielding an attractor of an iterated function system (IFS) was developed [1]. The parameters of affine reflections were chosen according to the most probable transformations configuration of polyhedral nanoscale nuclei spontaneously formed in the stochastic reaction medium [2]. The nuclei are considered singularity regions where the topological space of the crystal formation predictably breaks with the formation of a new multi-element symmetrical hierarchical structure.

The *rule of relation* of the IFS attractor dots to the reflection functions that yielded these dots was formulated. This rule allows to determine relations between the nanoscale topological space break-up regions constituting the attractor and the corresponding crystallisation regions of the modeled hierarchical crystal nanostructure.

Basing on *the rule of relation*, the *rule of separation* was formulated. The *rule of separation* allows to split the IFS attractor into hierarchical structuring subsets and define the *relation* between any generated dot and a defined topological base structure. The separation of the attractor into subsets happens according to the sequence of reflections that led to the generation of each dot of the yielded attractor. When modeling dendrite crystals this allows to define the crystallisation directions in any region of the attractor. These directions describe the hierarchical ordering of the modeled branching crystal substructure elements.

To restrict the infinite complication of the fractal IFS attractor's structure during its formation, the *rule of limitation* was formulated. It terminates the iteration process if the random choice of the next reflection requires to use reflections responsible for the hierarchical complication of the base structure *n* consecutive times. Implementing the *rule of limitation* in the IFS “chaos game” algorithm, defining the hierarchical branching reflections of the topological base structure as orthogonal and spatially separating them from the topological base structure yields an array of detached and structurally identical attractors. This models the multiplication phenomenon of hierarchical nanoforms, self-assembled in dynamic chaos conditions of the gas phase in accordance with the global crystal nuclei topological growth space break-up and restructuring rule characteristic of the studied thermodynamic conditions.

References

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