ISSN 1070-3632, Russian Journal of General Chemistry, 2013, Vol. 83, No. 12, pp. 2225–2236. © Pleiades Publishing, Ltd., 2013.
Original Russian Text © V.M. Talanov, V.V. Ivanov, 2013, published in Zhurnal Obshchei Khimii, 2013, Vol. 83, No. 12, pp. 1937–1948.

Dedicated to 100th anniversary of V.B. Aleskovskii,
Correspondent Member of the Russian Academy of Sciences

Structure as the Source of Information on the Chemical Organization of Substance

V. M. Talanov and V. V. Ivanov

Laboratory of Design of New Materials, South Russian State Technical University,
ul. Prosveshcheniya 132, Novocherkassk, 346400 Russia
e-mail: valtalavov@mail.ru

Received March 30, 2013

Abstract—General principles established by the authors on the structure formation in chemical substances which are based on series of ideas and concepts of V.B. Aleskovskii are presented in this review. Main pathways of the formation of the structure of a substance (iteration, dissymmetrization, modularization, hierarchization) are considered. It is shown that the structure of a substance is one of the sources of origin of information. New qualitative approach to the understanding of the information phenomenon is advanced. Information is considered as an inherent parameter of a system appearing in the course of the description of the "choice" by the system of one of its possible structural states.

DOI: 10.1134/S1070363213120013

In the works of V.B. Aleskovskii by an example of programmed synthesis of highly organized supramolecular structures the key problems of structural organization of substance were stated. Their solvation nowadays determines not only the level of development of nanotechnologies, but also some areas of chemistry, physics, biology, and material sciences [1–11]. In the nineteen sixties on the basis of the "skeleton hypothesis" [2, 3] V.B. Aleskovskii has developed a series of methods of synthesis of solid substances and materials, namely, the methods of "chemical assembly" [9, 10]. One of them is the method of molecular layering. Its main principles were formulated in [9, 10]. In the subsequent years on the basis of this method technologies were developed for obtaining monolayers, polylayers, multizonic heterostructures, etc. [12–17].

The ideas of V.B. Aleskovskii concerning structural units of solid substance (fragments, building blocks, modules) [1], about the information as the factor of organization and self organization of substance [7, 8], about quantum synthesis [11], and some others occurred to be actual.

In this work a brief review is presented of some ideas developed regarding our the scientific program of designing new materials [18]. This program is aimed at the investigation of general principles of structure formation in substances. It is connected with a series of ideas and conceptions of V.B. Aleskovskii.

"Metamorphity" – Amorphity – Structurality" of Substance

Let us give initial working definitions of main concepts. Structure is the assembly of relatively stable bonds between the elements of system providing its entirety. The notion of "structure" is opposite to the metamorphy[1] concept which means a complete absence of bonds between the elements of the set, the peculiar "ideal gas" of the components [19].

---

[1] Physicists use the "metamorphy" concept for describing infinite set of elements as well as the pair to the notion "structure" (see p. 24 in [19]). "Amorphous substance" means the intermediate structural state of substance where comparatively stable bonds between the atoms within the boundaries of several coordination spheres adjacent to the chosen atom are formed.

Intermediate between the structureless and structurized formations are amorphous substances (artificial and volcanic glasses, natural and artificial resins, glues, carbon, paraffin, wax, etc.) whose atomic structure possesses a near order and is deprived of remote order characteristic of crystalline structures.

The notion of "structurality of substance" has a broad scope. This "broadness" has two "coordinates" determining the variety of structural states of the substance. They include the type *of structure forming component* (spin, orbital, magnetic moment, ellipsoid of thermal vibrations of atom, atomic group, atomic associate or cluster, atomic layer, domain, crystallite, grain, and many others) forming the multilevel hierarchic structure and the *degree of structurality*. Last notion reflects the degree of bonding of components of the system in a single whole. Qualitatively it is described by such terms as "gas," 1D-, 2D-, 3D-"crystal" "distribution of composition and bonding of components along different directions in the space," etc.

In the course of several last decades new structural states of chemical substances were found and studied. They are as follows:

atomic (quasicrystals, fractal structures, unusual chiral suprastructures in $MgTi_2O_4$ [20–22], various multiple types of "common" and exotic nanostructures: keplerates [23–25], barrels, toroids, hakelites, diamondoids, supernanotubulenes, nanofoams, fulborenites, and so on [26], supramolecular systems like as clatrates, crown ethers, metal porphyrines, structures without bonds, etc. [27]);

orbital (various orbitally ordered states, the so-called orbitones, for example, orbital octamers in $CuIr_2S_4$ [28], orbital dimers in $MgTi_2O_4$ [20, 21]);

magnetic (unusual magnetic states of substance in strong magnetic fields [29–31]);

electronic (for example, the systems with heavy fermion behavior like in LiV_2O_4 [32], states of quantum spin liquid in a series of chalcogenides with the structure of spinel, like in $HgCr_2O_4$ [33]).

Polarized glasses, photon crystals, magnetized amorphous metals, the so-called Ridberg substance [34] were found and investigated. Extreme states of substance and many other ones are under study. Structural states of substance differing not in the symmetry, but in the topological order (structural states characterized by equal symmetry of location of particles in space, but having different picture of quantum bonds between them, another picture of entanglement of bonds[2] [35]).

But it is significant to note that in all the above-mentioned structural states of substance the order in the location of the structural units (spins, orbitals, magnetic moments, atoms and atomic groups, etc.) appears spontaneously. In the works of V.B. Aleskovskii, his disciples and followers the set of types of structural states of substance was fundamentally extended by including systems where the order was organized in chemical system artificially. That is why nowadays the problems of systematization and classification of structural states of matter with the spontaneously established and artificially organized order, the search for the common language of description, and establishing universal principles of structure formation in chemical, biochemical, and biogeochemical substances on nano-, micro-, macro-, and even megalevels[3] of the matter organization have risen in full length.

Main Pathways of Formation of Structurality of Chemical Substance

At least four main elementary pathways exist for transformation of infinite set of elements into a structure. They are as follows: hierarchization, dissymmetrization, modularization, and iteration. They are elementary because the real processes of structure formation may be the combination of several of the above-mentioned basic processes.

Iteration is the law (procedure) of multiplication of local structure in nD-space ($n = 1, 2, 3$) leading to the formation of nano-, mezo- (micro), and macroscopic structurized objects. The iteration assumes the multiplication of the object with its simultaneous alteration according to a definite rule. As a partial case, the iteration includes translation (transfer) of atoms, structure fragments, and other formations without their alteration. The generalization of iteration in our conception is the notion of the evolutional law of formation of the structure of substance.

---

[2] It is an official term which appeared in the 1930, but up to 1980 it has not been widespread.

[3] Different structural states of matter like exotic for chemical studies states of quark-gluon plasma or the neutron core on the surface of extinguished stars are known.

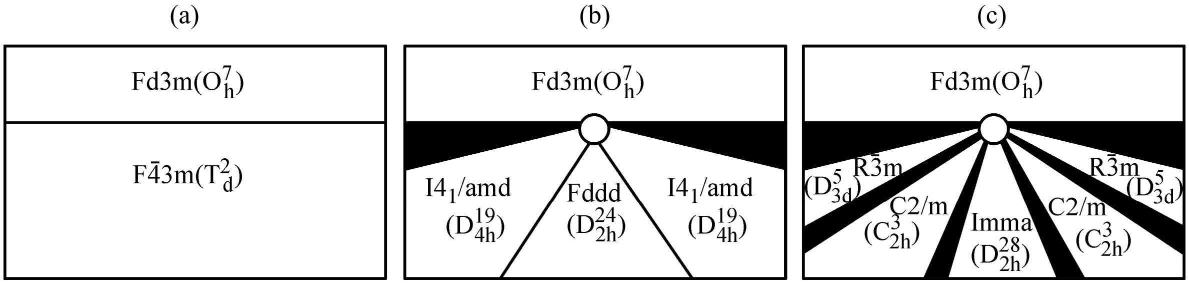

Fig. 1. Simplest examples of diagrams of possible symmetry states of crystals with the spinel structure. On these diagrams around the singular multicritical point cascades of possible low-symmetry phases are grouped. They may form as a result of structural transformations from the high symmetry structural state [36, 40, 41]. For (a)–(c) see the text.

Dissymmetrization, the decrease in symmetry, takes place during the formation of new bonds between the elements of the set. The formation of more complex structures from the simple ones is accompanied by the *decrease in symmetry* of the object [36]. This fundamental law is traced in all structural levels of development of matter [37].

The set of dissymmetric (low symmetric) states of substance may be ordered. We have offered a concept of diagrams of possible symmetry states of crystals [35]. These diagrams are the generalized maps of possible symmetry-structural and critical states of substance which appear from some starting state as a result of continuous and quasicontinuous changes in its symmetry and structure. Having such diagrams a chemist acquires the possibility to mark principle pathway of synthesis of a substance with the necessary combination of properties, and to establish the most probable phases in the course of the synthesis of the material. It is important to note that diagrams of possible symmetry states of crystals do not substitute classic phase diagrams. They reflect only possible symmetry-structure states of substance, while phase diagrams reflect real phase states (each of them is characterized by a definite symmetry and structure) at definite external parameters. Only in particular cases these two types of diagrams coincide. Various examples of diagrams of possible states and their use in designing new materials were discussed in [38–41].

In Fig.1 simplest examples of diagrams of possible states of crystals with the spinel structure (space group Fd3m) are presented. These diagrams reflect possible symmetry states and their mutual transformations in $CdIn_2S_4$ (Fig. 1a), $NiFe_{2(1–x)}Cr_{2x}O_4$, and $Cu_{1–x}Ni_xCr_2O_4$ (Fig. 1b), Li_2CoCl_4 (Fig. 1c). Coordinates of these diagrams are scalar intense parameters (temperature, pressure, concentration of components of solid solution). Diagrams are classified by the irreducible presentations of symmetry groups of the starting phase. Blackened parts of diagrams correspond to the first order structural transformations, and lines, to the second order ones. For each area diagram of possible symmetry states of crystal expected structures of substances can be calculated (for examples see [36, 40–42]).

Such diagrams may be plotted for any substance (crystals, quasicrystals, amorphous formations, molecular associates, supramolecular formations, nanostructures, etc.) if the symmetry group of the starting structure is known.

Ordered structures appear as a result of distortion of symmetry of the initial state. Such distortion is possible in strongly non-equilibrium media (hydrodynamic flows, autocatalytic reactions, etc.) as well as in systems existing in thermodynamic equilibrium. Though ordering is one of the mechanisms of dissymmetrization of structure of substance, this process must be marked specially because of its principal meaning in the systems of artificial order. Within the frames of Landau–Lifshitz theory of the second order phase transitions we have formulated the general principles of formation of low-symmetric (dissymmetric) ordered phases. They are the following.

Principle of finit number of low-symmetry phases (total number of low-symmetry phases induced by irreversible presentations of symmetry group of the space group G_0 is finit).

Principle of phase variety (decrease in symmetry of starting high-symmetry phase (G_0) leads to decrease in number of dissymmetric phases (G_D) which may appear from it as a result of monotonous and so-called quasimonotonous phase transitions).

Principle of finit number of types of structure of ordered phases [at the endless increase in number of components of thermodynamic system number of possible types of structures of ordered phases (chemical substances) which may form as a result of monotonous and quasimonotonous phase transitions remains finit].

Principle of structural complexity (if the substance undergoes monotonous and quasimonotonous structural transformations, modification with lower symmetry as a rule has more complex structure, and modification with a higher symmetry, simpler structure).

Compensational principle (low symmetry structure “tries” to compensate the decrease in symmetry. The structure is divided in several subsystems with opposite character of deformations and specific features of structure).

Generalyzed Fedorov-Grot law (substance with lower symmetry forming as a result of monotonous or quasimonotonous structural transformation order-disorder has more complex composition, and with a higher symmetry, the simpler one).

Examples, explanations, limits of application of the above-presented principles and references are compiled in [36].

Process of ordering may proceed as spontaneous natural process of self-organization of structural units of substance leading to its equilibrium state[4] [43–45].

Ordered structures may appear also in the compulsory process (in the process governed by an external action) of organization of artificial order (for more detailed discussion of these problems see reviews [15–17]). As a rule such structures are far from equilibrium state. The existence of a large number of such structures being in metastabile states including highly organized ones may be expected. In particular, the ordered distribution of one or several components of definite size in a matrix of another substance, the so-called “superordering” in solid body [16, 17] is possible. As a result of such template synthesis spatially separated artificially ordered chemical systems are formed. By the works of V.B. Aleskovskii, A.A. Malygin, V.M. Smirnov, and some other scientists, principally new field of chemistry including chemical systems of “artificial order” was created, and scientific principles of constructing solid nanostructurized substances and materials were developed. General symmetry principles of structural organization of artificial order are unknown up to now.

Modularization. Many structures of substances can be presented as compositions of several constructing modules (fragments, building units or structural blocks), differing by their combinations, distribution, and junction. Modules are the universal way of self organization of all known forms of solid bodies like crystals, amorphous bodies, quasicrystals, fractals, molecular biosystems, nanostructures, and so on. This notion really bounds various fields of science: physics, chemistry, biology, material sciences, etc.

As a unique example of module organization of substance double spirals in the structures of spinel (a, b, e) and quartz (c, d, e) is shown in the Fig. 2. In the spinel structure spirals are formed by tetrahedrons and hexahedrons (cubes), and in the quartz structure, by silicon-oxygen tetrahedrons. It is interesting that these spirals are topologically similar to the double spiral of deoxyribonucleic acid (DNA) [46–48]. Two chains of inorganic double spirals are complementary, namely, an unambiguous correspondence exists between the atoms of different spirals. But in contrast to the double spiral of DNA these double spirals are not “molecules.” They are characterized by complex endless hooking of one spiral by another one (Figs. 2e, 2f).

The description of structures by means of modules proved to be an effective way of systematization of structure of different classes of substances. Classic example is the combination of silicon tetrahedrons in construction of modules of different kinds (blocks, rings, chains, layers, etc.) which permitted to develop the basis of classification of silicates. V.B. Aleskovskii proved to be right: crystalline lattice has the conventional (nominal) meaning. Fundamental characteristic of crystals is the framework, the system of interatomic bonds within which the fragment can be chosen and the design of new structures of substances may be performed. For the case of crystals this possibility was proved in [49–54]. Let us consider this statement in more detail.

---

[4] The notion “ordered structure” in the first approximation may be defined as a state of structure which does not alter in time. This stability is not provided by proceeding of any process external to the structure and supporting its existence. In this case it turned out that the number of ordered phases permitted by theory is finit and relatively not large. All of them can be enumereted, and their structures calculated (methods of calculation and examples are described in [42–45]).

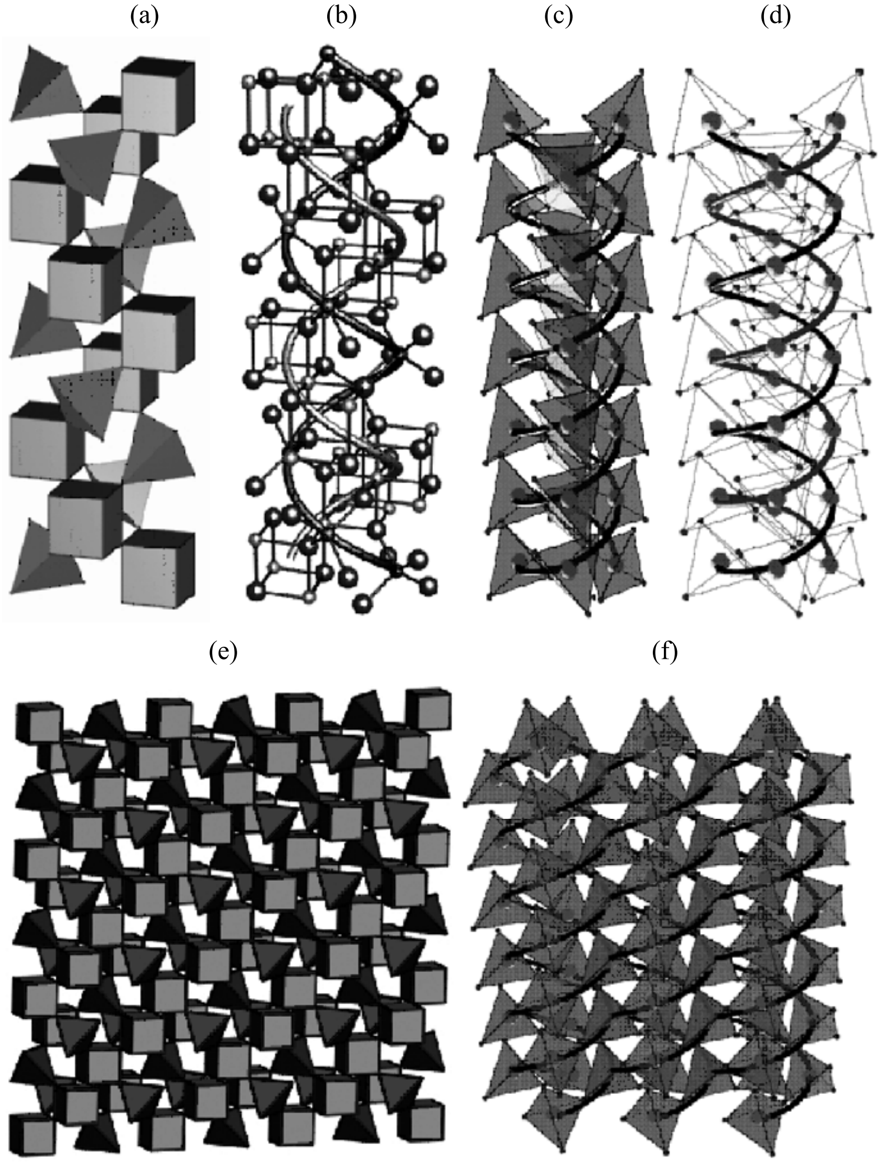

Fig. 2. Modular structure of double polyhedral spirals in the structures of spinel and quartz. (a, b) Double spiral in the structures of spinels; (c, d) double spiral in the structure of quartz, and (e, f) endless character of hooking of polyhedron spirals [46, 48].

The principle of modular constitution of crystals was formulated in [49]. The structure of any substance can be built up from modules with definite topological characteristics permitting to obtain some definite set of modular structures connected genetically with one another. They differ from initial structure by positional and orientational ordering of modules in the 3D space.

We have offered an algorithm of deducing a module of the given structural type for combinatorial molecular design of new substances [50]. The algorithm includes the procedures of evaluation of modular characteristics of the structural type by its crystallographic description, the identification of universal law of packing of modules in probable modular structures, the analysis of versions of purposeful changing the crystal chemical topology of basic modules, and the selection of the most probable kind of non-isolated and sufficiently compact asymmetric module. This algorithm of deducing the module may be used in the course of combinatorial modular design of any structural type of substance

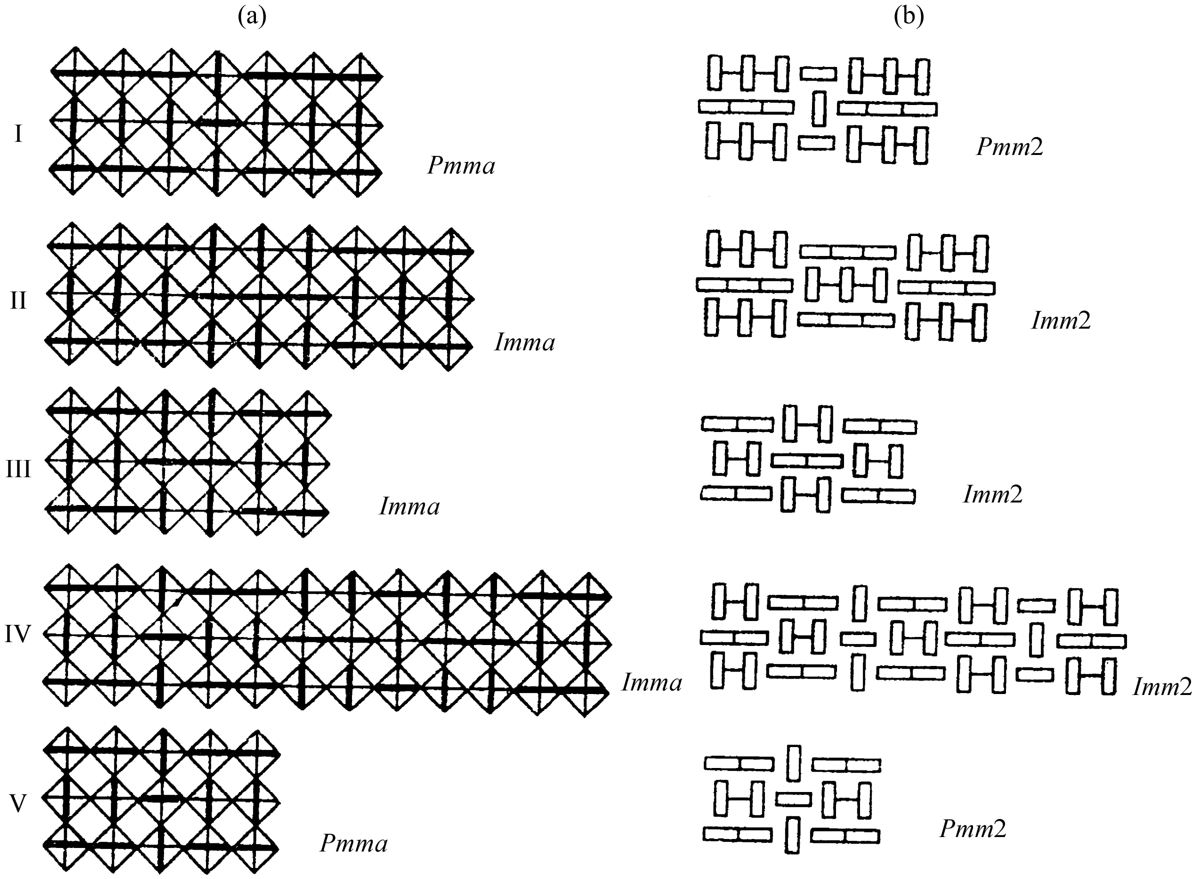

Fig. 3. Schematic image and symmetry of modular structures **I**–**V** of one-dimensional spineloids from (a) non-isolated and (b) isolated modules of spinel [55].

whose symmetry is described by Fedorov groups with the purpose of obtaining of variety of structures related to the given one with simpler physical and physicochemical properties. Using the library of modules (building blocks) from known compounds purposeful synthesis of polyfunctional material finally becomes probable. By an example of structural type of spinel the possibilities of modular design while obtaining new structures of substances were shown [55–60]. For the illustration of principle of modular structure of substance in Fig. 3 molecular structures of possible constructed one-dimensional spineloids are presented [55].

Hierarchization. Structural variety of chemical substances is hierarchized by many characteristic like spatial, time, energy, and some others. The principle of structural hierarchization means that structures of one type are modules, "building blocks," from which the structures of second level are formed. They have significantly larger spatial dimensions. The structures of second level in their turn join in the structures of third level, and so on. But this process cannot be endless. Main sense of structural hierarchy is the constituent nature of more complex formations as compared to the complexity of modules from which the above-located level is formed. It leads to the fact that modules while forming the structure provide it with some part of their functions, the degrees of freedom. Under these conditions many properties of complex structures cannot be reduced to the properties of modules. On the basis of analysis of structure of aerogels, dendrites, highly disperse dendrite particles (dendrimers) and many other fractal chemical objects the following principles can be formulated.

Principle of hierarchy of modules of molecular structures. The modular structure of substance may be presented as a set of definite modular structures whose modules belong to different levels of structural hierarchy. According to this principle the method of iterational modular design of 2D-nanostructures and

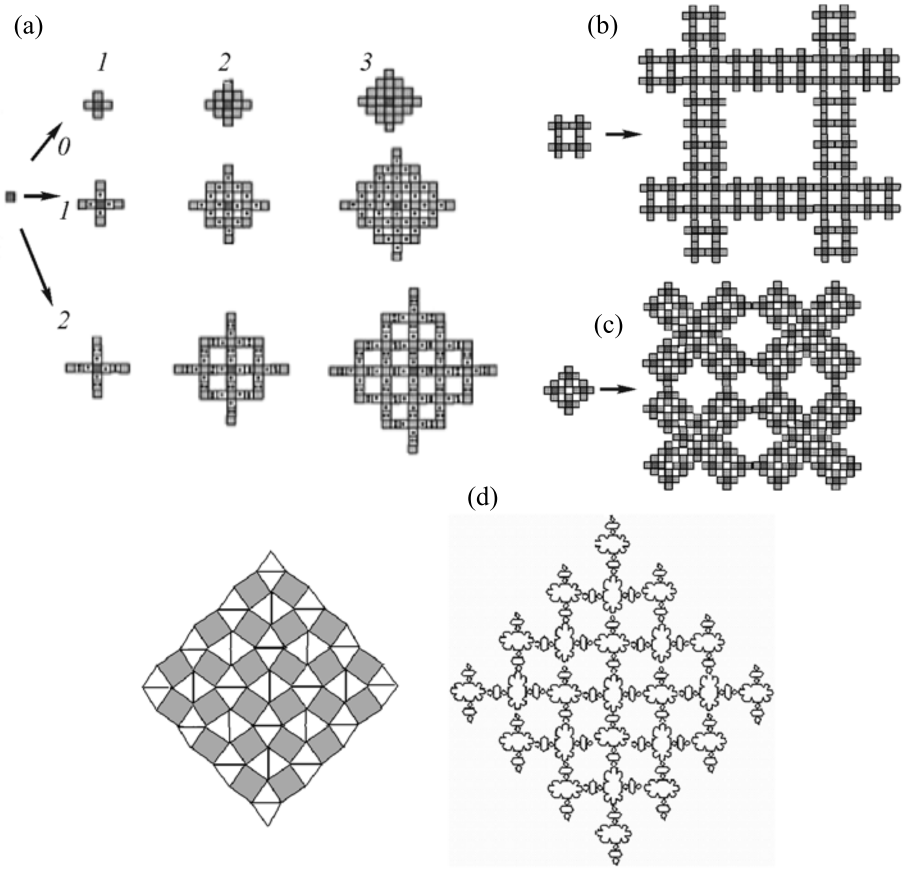

Fig. 4. Dynamics of growth of tetragonal $R_{\{4\}im}$-structures differing in number of tetragons-“links” (m = 0, 1, 2) and the way of branching of “nuclei” tetragons by means of the sides with $i_r = 4$ (a) [61]. Deterministic fractal lattices with 4mm symmetry obtained by means of one step of iterational building and from the corresponding generator: $L_{20\{4\},4®,1/6}$ (b), $L_{20\{4\},4®,1/6}$ (c) [64], 34334-[4(2)] net and corresponding ordered sets of tightly packed Koch snow flakes $F_{K(4/3)}\{4\}$(p4mm) and lacunar multifractals $MF_{K(4/3)}2\{3\}$(p2mm) adding them to 2D space (d) [65].

fractal structures in 2D-space was developed [61–64]. Examples of iterational design are presented in the Figs. 4a–4c.

Principle of modular structure of regular fractal structures. Any regular fractal structure may be presented from similar minimal modules whose structure and form contains structural information about this fractal structure as well as about any of its prefractals. Such modules carry out the function of generator $G \equiv F_1$ of modular fractal structure and in particular, of any prefractal of nth generation: $F_n(F_1)$, where n is the number of iterations.

Principle of hierarchy of modules of regular fractal structures. Self-similar (regular) fractal structure may be presented as modular from any of its prefractals. In particular, modular structure of each prefractal F_n of nth generation may be presented by modules-prefractals of preceding generations: $F_n(F_{n-1}\{F_{n-2}[F_{n-3}\ldots(F_1)\ldots]\})$. Modules by themselves are classified by complexity in hierarchic sequence $F_n \subset F_{n-1} \subset F_{n-2} \subset F_{n-3} \subset \ldots \subset F_1$.

The sets of fractal structures ordered in 2D-space may be simultaneously regarded as the packages of fractals in a shape of definite Koch snowflakes $F_{k(4/3)}\{Pg\}(G_2^2)$ as well as ordered sets of lacunar multifractals $MF_{K(4/3)}\{3\}$(p3ml) or $MF_{K(4/3)}2\{3\}$(p2mm) (Fig. 4d).

The above-formulated principles make a basis of evolutional model of formation of deterministic fractal structures with a fraction scale and ordered in 2D space multisets of locked fractal curves modeling the formation of real quasifractal structures on the surface of compositional materials [65–74].

Structure of Substance as One of Sources of the Origin of Information

A substance is characterized by three main groups of parameters, the composition (atomic and isotopic), structure, and properties. All these tree groups of parameters determine the information contained in the substance. One of the approaches to evaluation of the amount of information consists in presenting the structure of substance as the "text of the report."

Classical (Shannon's) theory of information defines it as a measure of uncertainty of situation in the state of "choice." The less is the probability of the formation of any structure, the larger information carries the report on its formation [75, 76]. For the direct use of Shannon's theory in quantitative calculations it is necessary to present any structure as a report (a word or a text).

Shannon put into operation the information entropy as a measure of uncertainty of the information. Let us consider the experiment having the results A_1, A_2,… A_k, and $p(A_1)$, $p(A_2)$,…$p(A_n)$, the possibilities of separate results of the experiments. According to Shannon to each result of the experiment A_i the uncertainty equal to $-\log_2 p(A_i)$ must be ascribed. For all the possible results value H as a measure of uncertainty is introduced.

$$H = -\sum_i P_i \lg_2 P_i$$

Let us use this formula for example to the calculation of uncertainty contained in the formula of any substance (formula of a substance is just the "text of the report"). Hence, the information entropy of formular unit of sulfuric acid consisting of seven atoms is equal to $H = -(2/7)\log_2 (2/7) - (1/7)\log_2 (1/7) - (4/7)\log_2 (4/7) = 1.379$. The same information entropy would have any substance of the composition A_2BX_4, for example K_2SeO_4. According to Shannon's formula the amount of information is determined irrespectively of its sense, in particular, of the peculiarity of the structure of the substance. As it was many times mentioned in literature, the sense of information and its value are ignored.

The absolute value of information containing in the substance is unknown, but for thermodynamic studies of chemical effects it is necessary to know the change in the information at the transition from one state to another. In chemistry the language recording the composition of the structure of substance is partially known. It includes the laws of D.I. Mendeleev, E.S. Fedorov, stereochemistry, and crystal chemistry. But substances by themselves in the course of interaction use more simple "configurational" language including the problems of their binding (complementarity programs) in larger aggregates. Complementarity of structural units of substance is coded by information contained in them (charge, polarity, size, nucleophilicity, etc.) Not all the processes of structure formation lead to creating new information. Simple translation of a unit cell leads to the formation of a crystal, but it does not lead to appearing of new information about the system. It is significant that the growth of crystals is a discrete process and proceeds practically according to one pathway (the possibility of strictly definite growth of structure in the configurational space of the system of interacting atoms is close to one).

Non-crystalline substances and nanostructures differ from the above-presented case. Here the aggregation of structural units proceeds according to programs [24, 77]. By an example of nanoobjects and ideal crystals the sources of origin of structural information are systematized and generalized.

Space geometry. In the case of nanoobjects the structure of different classes of substances is described by the Euclidean geometry and non-Euclidean geometries, and also fractal geometry, while in the case of crystals only by the Euclidean geometry. Some structures can be considered as bent Euclidean structures. Unusual non-Euclidean structures with spiral lattices have such minerals as halloysite, cylindrite, antigorite, clinochrysolite, asbestos. Structure of these inorganic compounds is based on the Archimedean spirals. Atoms are located analogously to the seeds in the head of a sunflower. Each spiral has a shape of a cylinder. Joint cylinders form the fibrous structure of total substance.

Geometry of fullerenes, nanotubes, schwazites, onions, and many other objects of nanoworld is non-Euclidean.

Aerogels, dendrites, fractal clusters, highly disperse dendrite species (dendrimers), friable particles formed while aggregation of colloids or gel formation, spherolite particles in polymers have fractal geometry.

Structurality of space. In the case of crystals there exist the equivalent spatial cells, and in the case of nanoobjects, the quasiequivalent spatial cells (among them the homologic and self-similar cells). In the crystals with OD-structures the structurality of Euclidean space may be caused by the existence of the "framework" of structure determining the set of substructures compatible with it. The structurality of space for fractal structures is determined by self-similarity of their structural elements on different hierarchic levels.

Symmetry of structure. Crystals are described by Fedorov symmetry. Structures of nanoobjects in general case are described by non-Fedorov symmetry. Accurate or approximated symmetry operations forbidden in 230 space groups are possible.

A. MacKay has offered a term “crystalloid” and determined it as follows: It is a configuration of a finit number of identical subunits, gathered in an unambiguous, regular, and reproducible way into a cluster which is not a crystallite, but corresponds to the real minimum point of free energy [77]. The structure of crystalloids may be described by operations of curvilinear and homologic symmetry, symmetry of similarity, and other generalizations of classic crystallographic symmetry.

The symmetry of nematic liquid crystals is described by the symmetry of rods, of smectic crystals, by layers and parquets, and of cholesteric ones, by the symmetry of a rotating cone.

Number and peculiarities of symmetry elements. Spatial symmetry of crystals is characterized by endless number of elements. Spatial symmetry of some nanoobjects is characterized by finit number of elements.

In crystals only the symmetry axes corresponding to rotations by 180°, 120°, 90°, and 60° are possible. In nanoobjects axes of fifth, seventh, eighth, tenth, twelfth, and other integer orders are possible which are forbidden in crystals, as well as the axes of fractional order. Nanostructures with non-integer symmetry axes are possible [78–83]. As an example of axis of non-integer order is the axis 30/11 which describes the Berdiyke-Cockseter spiral composed from ideal tetrahedrons [84].

Structural equivalence of atoms. In crystals atoms of the same chemical elements occupying definite regular system of points are equivalent. For nano-objects quasiequivalence is characteristic which includes the homology and similarity of structureal elements.

The structural equivalence of atoms is observed in 3D-structures, 1D-, and 2D-nanostrucrures whose symmetry is described by the groups G_3^3, G_1^1, and G_2^2 respectively. For them the absolute identity of the nearest surrounding of the chosen structural element is characteristic.

In some nanostructures (onions, fractal structures) the nearest surrounding of chosen structural element is characterized by quasi-identity, in particular, reflected in deformations of nearest surrounding.

Process of formation and uniformity of substance. The discrete growth by a single pathway in configurational space is characteristic for crystals and in the ideal crystal an absolute structural homogeneity is observed. In the case of nanoobjects the aggregation including other components and growth along the branching pathways are possible. For them structural heterogeneity and coherent conjugation boundaries between different parts of the whole are characteristic.

The structurally inhomogenic ZrO_2 nanoparticles have been for found the first time [78–80] consisting of interpenetrating fragments of phases of different symmetry. It is significant that the orientational relationships between the phases occurred to be “incompatible” from the point of view of classic crystallography: the boundary of separation is not necessary planar, the orientation relationships do not necessary correspond to Miller indexes, etc. These nanostructures with coherent boundaries were called centaurs.

Information in non-living systems arises when there is a choice among the multiple of possibilities of formation of structure of the substance. The structure registers information and plays the role of “memory of pathway” of the formation of the chemical substance.

This general statement corresponds also to living systems. Within the frames of statistical mechanics and thermodynamics it is impossible to distinguish living organisms from the non-living bodies. The appearance of a living substance is connected with mechanical, electric, thermal, and chemical processes, but neither one of these types of processes nor their assembly can describe the informational process. In particular, the organisms are informational systems. They obtain the hereditary information from their ancestors and live in order to transfer it to descendants. With such approach all the other mechanical, physical, and chemical processes may be considered auxiliary. They favor (provide the conditions) of fulfillment of the informational functions by the organism. The genetic code in the DNA molecule characterizes the sequence of "letters" meaning the type of location of nucleotide pairs against one another. The name "informers" was suggested for the compounds performing the function of information transfer [85].

Hence, informers in general are such chemical structures both of non-living and living matter whose formation corresponds to the choice of one among the versions for the formation from the initial state. That is why in the obtained structure the information is hidden and its "reading" means the establishing of evolutional pathway of the structure formation.

Let as clarify how this approach can be formalized. The equilibrium state of a uniform one-component structure is determined by two independent thermodynamic parameters, for example, its pressure p and temperature T (another versions like volume V and T, or V and entropy S also may be used).

But besides these parameters describing the state of a body under the given external conditions the internal parameter (parameters) ξ characterizing the structural peculiarities of the system can be introduced. By its sense ξ is a parameter of order characterizing the difference of symmetry-structural characteristics of various states of the substance. In general ξ is a multicomponent parameter, that is $\xi = \{\xi_1, \xi_2, \dots \xi_n\}$ having either scalar or vector or tensor nature. It is the extensive parameter of system analogous to the entropy, volume, or mass of components. The internal structural parameters of the system $\xi_1, \xi_2, \dots \xi_n$ may have quite different structural sources of origin, like the probabilities of occupation by atoms of different sublattices of crystals, the probability of appearance of a layer of a definite composition in heterostructure, the probability of orientation of a molecular group, or spin, or atomic orbital, the shift of atoms from the positions of equilibrium structure while the formation of its new modification, etc.

The internal parameter ξ is included in the expression of differentials of thermodynamic potentials, internal energy U, free energy F, Gibbs energy G as the additional member [86–92]. For example, differential of internal energy may be written as

$$dU = TdS - pdV + \psi_i d\xi_i.$$

Intense parameters ψ_i (i = 1,2…n) meaning the external effects ("forces") on the substance $\psi_i = (U/\xi_i)_{S,V}$ are conjugated with structural parameters ξ_i.

The information we regard as an internal parameter of system $\xi = \{\xi_1, \dots \xi_n\}$. Specific external actions conjugated with information ψ_i we define as the program governing action on the substance (program).

The multiplication of parameters $\xi\psi$ has the dimensionality of work (if the coefficient reflecting the specificity of introduction of ξ parameter in the thermodynamic potential would be considered). ξ-Parameter may be introduced as the dimensional as well as the dimensionless value. Its physical sense means the work of formation of structural organization of the substance. Specific external actions (sequence of definite operations with the substance) ψ_i provide the formation of structural organization of the substance. The sequence $\psi_1, \psi_2, \dots \psi_i$ is the program of the formation of the structure of substance. The program works when chemical system is in non-equilibrium conditions, because in the equilibrium state ψ_i (i = 1, 2, … n) = 0.

From the above approach it follows that the information cannot appear without energy expenditure, but it is insufficient for the appearance of the information. The ordered (described by ξ) spatial distribution of matter located according to definite rules (according to the programs given by the sequence of ψ_i) is also necessary. This ordered spatial distribution of matter is the new structure determined by internal parameters ξ_i. The comprehensive development of the described concept of information will be carried out in future.

Hence, in this work a brief review of our reports dealing with general principles of structure formation and the origin of information on chemical organization of substance is presented. The obtained results develop the ideas of V.B. Aleskovskii on the modular structure of substance, and on the interconnection of structure and information as a factor of organization and self organization of matter.

We express our gratitude to A.A. Malkov who acquainted us with some difficultly available works of V.B. Aleskovstii and to A.A. Malygin for valuable notes on the content of this article.

REFERENCES

1. Aleskovskii, V.B., *Stekhiometriya i sintez tverdykh soedinenii* (Stoichiochemistry and Synthesis of Solid Compounds), Leningrad: Nauka, 1976.
2. Aleskovskii, V.B., *Khimiya tverdykh veshchestv* (Chemistry of Solids), Moscow: Mir, 1978.
3. Aleskovskii, V.B., *Zh. Prikl. Khim.*, 1974, vol. 47, no. 10, p. 2145.

4. Aleskovskii, V.B., Artem'ev, Yu.M., and Smirnov, V.M., *Napravlennyi sintez tverdykh veshchestv* (Directed Synthesis of Solids), Aleskovskii, V.B., Ed., Leningrad: Leningrad. Gos. Univ., 1987, no. 2, p. 7.
5. Aleskovskii, V.B., *Kurs khimii nadmolekulyarnykh soedinenii* (Chemistry of Supermolecular Compounds), Leningrad: Leningrad. Gos. Univ., 1990.
6. Aleskovskii, V.B., *Zh. Obshch. Khim*., 1995, vol. 65, no. 11, p. 1928.
7. Aleskovskii, V.B., *Khimiko-iformatsionnyi sintez. Nachatki teorii. Metody* (Chemico-Informational Synthesis. Essentials of Theory. Methods), St. Petersburg: Sankt-Peterburg. Gos. Univ., 1997.
8. Aleskovskii, V.B., *Russ. J. Gen. Chem*., 2002, vol. 72, no. 4, p. 569.
9. Kol'tsov, S.I., and Aleskovskii, V.B., *Zh. Fiz. Khim*., 1968, vol. 42, p. 1210.
10. Aleskovskii, V.B., *Vestnik Akad. Nauk SSSR*, 1975, no. 6, p. 48.
11. Aleskovskii, V.B., *Kvantovyi sintez. Khimiya poverkhnosti i nanotekhnologiya vysokoorganizovannykh veshchestv* (Quantum Synthesis. Chemistry of Surface and Nanotechnology of Highly Organized Substances), Collection of Scientific Works, St. Petersburg: Sankt-Peterburg. Gos. Tekh. Univ., 2007, p. 8.
12. Malygin, A.A., *Rossiiskie Nanotekhnologii*, 2007, vol. 2, nos. 3–4, p. 87.
13. Malygin, A.A., *Izv. Sankt-Peterb. Gos. Tekh. Inst. (Tekh. Univ.),* 2007, no. 1(27), p. 14.
14. Malkov, A.A. and Malygin, A.A., *Izv. Herzen Ross. Ped. Univ*., 2007, no. 7(26), p. 127.
15. Smirnov, V.M., *Khimiya nanostruktur. Sintez, stroenie, svoistva* (Chemistry of Nanostructures. Synthesis, Structure, Properties), St. Petersburg: Sankt-Peterburg. Gos. Univ., 1996.
16. Smirnov, V.M., Zemtsova, E.G., and Morozov, P.E., *Khimiya poverkhosti i nanotekhnologiya vysokoorganizovannykh veshchestv* (Chemistry of Surface and Nanotechnology of Highly Organized Structures), Collection of Scientific Works, St. Petersburg: Sankt-Peterburg. Gos. Tekh. Univ., 2007, p. 81.
17. Smirnov, V.M., *Russ. J. Gen. Chem*., 2002, vol. 72, no. 4, p. 590.
18. Talanov, V.M., Collection of Scientific Works *"Periodicheskii zakon, D.I. Mendeleeva v sovremennykh trudakh uchenykh transportnykh vuzov"* ("D.I. Mendeleev Periodical Law in Modern Works of Scientists of Transport High School"), St. Petersburg: Peterburg. Gos. Univ. Putei Soobshch., 2009, p. 63.
19. Kulakov, Yu.I., *Teoriya fizicheskikh struktur* (Theory of Physical Structures), Moscow: Nauka, 2004.
20. Schmidt, M., Ratcliff, W., Radaelli, P.G., Refson, K., Harrison, N.M., and Cheong, S.W., *Phys. Chem. Lett.,* 2004, vol. 92, no. 5, p. 056402(1–4).
21. Talanov, V.M., Shirokov, V.B., Ivanov, V.V., and Talanov, M.V., *Crystallogr. Rep*., 2013, vol. 58, no. 1, p. 80.
22. Talanov, V.M., Shirokov, V.B., Ivanov, V.V., and Talanov, M.V., *Inorg. Mater.*, 2011, vol. 47, no. 9, p. 990.
23. Shevchenko, V.Ya., Madison, A.E., and Shudegov, V.E., *Glass Phys. Chem.*, 2003, vol. 29, no. 6, p. 577.
24. Talanov, V.M., Ereiskaya, G.P., and Yuzyul, Yu.I., *Vvedenie v fiziku i khimiyu nanostruktur i nanostrukturirovannykh materialov* (Introduction in Physics and Chemistry of Nanostructures and Nanostructurized Materials), Moscow: Akademiya Estestviznaniya, 2008.
25. Talanov, V.M. and Ereiskaya, G.P., *Metody sinteza nanostruktur i nanostrukturirovannykh materialov* (Methods of Synthesis of Nanostructures and Nanostructurized Materials), Novocherkassk: YuR-GUTU (NPI), 2011.
26. Pokropivnyi, V.V. and Ivanovskii, A.L., *Russ. Chem. Rev.*., 2008, vol. 77, no. 10. p. 837.
27. Len, J.-M., *Supramolekulyarnaya khimiya. Kontseptsii i predstavleniya* (Supramolecular Chemistry. Concepts and Notions), Novosibirsk: Nauka, 1998.
28. Radaeli, P.G., *New J. of Physics*, 2005, vol. 7, p. 1.
29. Menyuk, N., Dwight, K., and Wold, A., *J. Phys (Paris),* 1964, vol. 25, p. 528.
30. Hastings, J.M. and Corliss, L.M., *Phys. Rev*., 1962, vol. 126, p. 556.
31. Plumier, R.J., *Appl. Phys*., 1967, vol. 39, p. 635.
32. Singh, D.N., Blaha, P., Schwarz, K., and Mazin, I.I., *Phys. Rev., B*, 1999, vol. 60, no. 24, p. 16359.
33. Tomiyasu, K., Ueda, H., Matsuda, M., Yokoyama, M., Iwasa, K., Yamada, K., *Phys. Rev., B*, 2011, vol. 84, p. 035115 (1–5).
34. Shakhparonov, I.M., Kolotukhin, S.P., Chepenko, B.A., and Khandurov, Yu.N., Abstracts of Papers*, Congress-2004 "Fundamental'nye problemy estestvoznaniya i tekhniki"* (Congress-2004 "Fundamental Problems of Natural Sciences and Technique"), St. Petersburg, 2004, p. 490.
35. Chen, X., Gu, Z.-C., Liu, Z.-X., and Wen X-G*., Science*, 2012, vol. 338, p. 6114.
36. Talanov, V.M., *Glass Phys. Chem*., 2007, vol. 33, no. 6, p. 620.
37. Urusov, V.S., *Dokl. Akad. Nauk*, 2002, vol. 386, no. 3, p. 379.
38. Talanov, V.M., *Crystallogr. Rep*., 1996, vol. 41, no. 6, p. 929.
39. Talanov, V.M., *Litievye istochniki toka* (Lithium Current Sources), Transactions of VI Int. Conf., Novocherkassk, September 19–21 2000, Novocherkassk, Nabla 2000, p. 26.
40. Ivanov, V.V. and Talanov, V.M., *Neorgan. Materialy*, 1995, vol. 31, no. 2, p. 258.
41. Talanov, V.M., *Izv. Akad. Nauk, Neorg. Materialy*, 1989, vol. 25, no. 6, p. 1001.
42. Talanov, V.M. and Shirokov, V.B., *Crystallogr. Rep.*, 2010, vol. 58, no. 2, p. 296.
43. Lifshits, E.M., *Zh. Teor. Exp. Fiz*., 1941, vol. 11, p. 255.

44. Talanov, V.M. and Chechin, G.M., *Crystallogr. Rep.*, 1990, vol. 35, no. 4, p. 1008.
45. Talanov, V.M., *Phys. Stat. Sol. A*, 1989, vol. 115, p. K1.
46. Talanov, V.M., *Izv. Vysshikh Uchebnykh Zavedenii Sev.-Kavk. Regiona, Est. Nauki*, 1994, no. 3, p. 16.
47. Talanov, V.M., *Acta Cryst., A*, 1996, vol. 52, p. 341.
48. Talanov, V.M., Kiroy, R.I., and Ivanov, V.V., in *Evolutsiya zhizni na zemle* (Life Evolution on Earth), Transactions of IV Int. Symp., November 10-12, 2010, Tomsk: TML-Press, 2010, p. 150.
49. Ivanov, V.V. and Talanov, V.M., *Crystallogr. Rep.*, 2010, vol. 55, no. 3, p. 362.
50. Ivanov, V.V. and Talanov, V.M., *Russ. J. Inorg. Chem.*, 2010, vol. 55, no. 6, p. 915.
51. Ivanov, V.V. and Talanov, V.M., *Glass Phys. Chem.*, 2008, vol. 34, no. 4, p. 401.
52. Ivanov, V.V. and Talanov, V.M., *Usp. Sovr. Estestvoznan.*, 2012, no. 8, p. 75.
53. Ivanov, V.V. and Talanov, V.M., *Usp. Sovr. Estestvoznan.*, 2012, no. 9, p. 74.
54. Ivanov, V.V. and Talanov, V.M., *Usp. Sovr. Estestvoznan.*, 2012, no. 10, p. 78.
55. Ivanov, V.V. and Talanov, V.M., *Izv. Akad. Nauk SSSR, Ser. Neorg. Mater.*, 1991, vol. 27, no. 11, p. 2356.
56. Ivanov, V.V. and Talanov, V.M., *Izv. Akad. Nauk SSSR, Ser. Neorg. Mater.*, 1991, vol. 27, no. 11, p. 2386.
57. Ivanov, V.V. and Talanov, V.M., *Neorg. Mater.*, 1992, vol. 28, no. 9, p. 2022.
58. Ivanov, V.V. and Talanov, V.M., *Zh. Strukt. Khim.*, 1992, vol. 33, no. 3, p. 137.
59. Ivanov, V.V. and Talanov, V.M., *Neorg. Mater.*, 1992, vol. 28, no. 8, p. 1720.
60. Ivanov, V.V. and Talanov, V.M., *Phys. Status Solidi, A.*, 1990, vol. 122, no. 2,, P.K. 109.
61. Ivanov, V.V., Shabel'skaya, N.P., and Talanov, V.M., *Sovrem. Naukoemkie Tekhnologii*, 2010, no. 10, p. 176.
62. Ivanov, V.V., Dem'yan, V.V., and Talanov, V.M., *Mezhdunar. Zh. Eksperim. Obrazovaniya*, 2010, no. 11, p. 153.
63. Ivanov, V.V. and Talanov, V.M., *Nanosistemy: Fizika, Khimiya, Matematika*, 2010, vol. 1, no. 1, p. 72.
64. Ivanov, V.V., Talanov, V.M., and Gusarov, V.V., *Nanosistemy: Fizika, Khimiya, Matematika*, 2011, vol. 2, no. 3, p. 121.
65. Ivanov, V.M., Shcherbakov, I.N., and Talanov, V.M., *Sovrem. Naukoemkie Tekhnologii*, 2012, no. 1, p. 54.
66. Ivanov, V.V. and Talanov, V.M., *Usp. Sovr. Estestvoznan.*, 2012, no. 3, p. 56.
67. Ivanov, V.V. and Talanov, V.M., *Sovrem. Naukoemkie Tekhnologii*, 2012, no. 2, p. 76.
68. Ivanov, V.V. and Talanov, V.M., *Sovrem. Naukoemkie Tekhnologii*, 2012, no. 11, p. 22.
69. Ivanov, V.V. and Talanov, V.M., *Sovrem. Naukoemkie Tekhnologii*, 2012, no. 11, p. 24.
70. Ivanov, V.V. and Talanov, V.M., *Sovrem. Naukoemkie Tekhnologii*, 2012, no. 12, p. 16.
71. Ivanov, V.V. and Talanov, V.M., *Usp. Sovr. Estestvoznan.*, 2012, no. 11, p. 61.
72. Ivanov, V.V. and Talanov, V.M., *Usp. Sovr. Estestvoznan.*, 2012, no. 11, p. 63.
73. Ivanov, V.V. and Talanov, V.M., *Crystallogr. Rep.*, 2013, vol. 58, no. 3, p. 370.
74. Ivanov, V.V. and Talanov, V.M., Gusarov, V.V., *Nanosistemy: Fizika, Khimiya, Matematika*, 2013, vol. 3, no. 4, p. 82.
75. Shennon, K., *Raboty po teorii informatsii i kibernetike* (Works in the Field of Theory of Information and Kibernetics), Moscow: Inostrannaya Literatura, 1963.
76. Heartly, P.V.L., *Peredacha Informatsii. Teoriya informatsii i ee prilozheniya* (Transfer of Information. Theory of Information and Its Applications), Moscow: Fizmatgiz, 1959, p. 5.
77. Mackkay, A.L., *Crystallogr. Rep.*, 1981, vol. 26, no. 5, p. 910.
78. Shevchenko, V.Ya., Khasanov, O.L., Yur'ev, G.S., and Ivanov, Yu.F., *Neorg. Mater.*, 2001, vol. 37, no. 9, p. 1117.
79. Shevchenko, V.Ya., Madison, A.E., and Glushkova, V.B., *Glass Phys. Chem.*, 2001, vol. 27, no. 3, p. 419.
80. Shevchenko, V.Ya., Khasanov, O.L., Madison, A.E., and Li, J.Y., *Glass Phys. Chem.*, 2002, bol 28, no. 5, p. 459.
81. Alok Singh and A.P., *Scripta Mater.*, 2003, vol. 49, no. 2, p. 143.
82. Mitsuhashi, T., Ichihara, M., and Tatsuke, U., *J. Am. Ceram. Soc.*, 1974, vol. 57, no. 2, p. 97.
83. Shevchenko, V.Ya., Samoilovich, M.I., Talis, A.L., and Madison, A.E., *Glass Phys. Chem.*, 2004, vol. 30, no. 6, p. 732.
84. Lord, E.E., Mackkey, A.L., and Ranganatan, S., *Novaya geometriya dlya novykh materialov* (New Geometry for New Materials), Moscow: Fizmatlit, 2010.
85. Zhdanov, Yu.A., *Entropiya informatsii v organicheskoi khimii* (Entropy of Information in Organic Chemistry), Rostov-on-Don: Rostov. Univ., 1979.
86. Talanov, V.M., *Izv. Vysshikh Uchebnykh Zavedenii, Ser. Khim., Khim. Technol.*, 1997, vol. 40, no. 5, p. 65.
87. Talanov, V.M. and Fedii, V.S., *Izv. Vysshikh Uchebnykh Zavedenii, Ser. Khim., Khim. Technol.*, 1997, vol. 40, no. 6, p. 38.
88. Talanov, V.M. and Fedii, V.S., *Izv. Vysshikh Uchebnykh Zavedenii, Ser. Khim., Khim. Technol.*, 1998, vol. 41, no. 1, p. 34.
89. Talanov, V.M., *Izv. Vysshikh Uchebnykh Zavedenii, Ser. Khim., Khim. Technol.*, 1998, vol. 41, no. 4, p. 23.
90. Talanov, V.M., *Izv. Vysshikh Uchebnykh Zavedenii, Ser. Khim., Khim. Technol.*, 1998, vol. 41, no. 5, p. 16.
91. Talanov, V.M., *Izv. Vysshikh Uchebnykh Zavedenii, Ser. Khim., Khim. Technol.*, 1998, vol. 41, no. 6, p. 87.
92. Talanov, V.M. and Fedii, V.S., *Izv. Vysshikh Uchebnykh Zavedenii, Ser. Khim., Khim. Technol.*, 1998, vol. 41, no. 6, p. 91.