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TOPOLOGICAL CHARACTERISTICS OF THE STRUCTURE OF COMPOSITE MATERIALS

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Abstract. The article discusses methods for modeling composite materials using graph theory. For this purpose, the method of structure-oriented and structure-invariant modeling of composite materials was analyzed. As a basis for such modeling, it is supposed to use structural descriptors – quantities that describe the structure of the material at different scale levels, including the molecular one. Structure-oriented modeling of hierarchical systems, which, in particular, are composite materials, can be carried out on the basis of regression statistical modeling, which takes into account the possibility of implementing the previous structural level at the next one, and, in particular, the molecular level at the microscopic or mesoscopic level. A form of experimental-statistical models, which includes descriptors of several structural levels was proposed. A simplified approach, which takes into account the regularities of two levels: molecular and subsequent (micro- and mesoscopic) was considered. Examples and algorithms for constructing a representative graph for cross-linked and branched polymers, as well as silicate materials, were considered. It is shown that the representing graph of cross-linked polymers is infinite stochastic. An experimental procedure for constructing a discrete model based on microphotographs of a hardening binder was considered and implemented. For a quantitative description of this graph, an incremental scheme was used, as well as topological indices obtained as a result of the transformation of topological indices of graphs of low molecular weight compounds. For the purpose of transformation, there is a transition to probabilistic characteristics – shares and average (normalized) values. The transformed topological indices are supposed to be applied in the statistical model of the composite material.

Keywords: discrete models of composites, hierarchical organization, crystallization structure, topological indices.

Introduction. In modern materials science, there are several approaches to the problem of obtaining materials with the required properties. A necessary stage of each of them is the study and modeling of the "recipe-technology-properties" relationship. The modeling method traditionally used in building materials science relies on a direct approach, in which the physical or direct performance characteristics of composite materials are compared with recipe-technological factors. With the help of a set of mathematical statistics algorithms, and, in particular, nonlinear regression, performance characteristics are compared with recipe-technological factors. This approach is the main scheme of experimental-statistical (ES) modeling in materials science [1] (Fig. 1).

In this article, the considered scheme was phenomenological, it is characterized by a number of advantages, but has some disadvantages. During the study, in accordance with the above scheme, a sufficient level of correlation of operational properties with recipe-technological factors was found, so there was no need to use time-consuming and technically sophisticated methods for studying the structure and properties of the material. At the same time, different-scale structural characteristics of the

material partially or completely fall out of the scheme, and there is a difficulty in bringing the models to each other ("to the canonical form"), their classification. In addition, for the traditional method it is impossible to directly track cause and effect relationships in the "composition-technology-properties" chain. The main reason for the given shortcomings is the incompleteness of the given chain. The complete chain of modeling, which allows to investigate cause-and-effect relationships, looks like this: "composition-technology-structure-properties". The modeling procedure based on the full sequence is characterized as structure-oriented modeling [2]. It necessarily includes multi-scale structures of composite materials as the main "carrier" of cause-and-effect relationships in the above sequence.

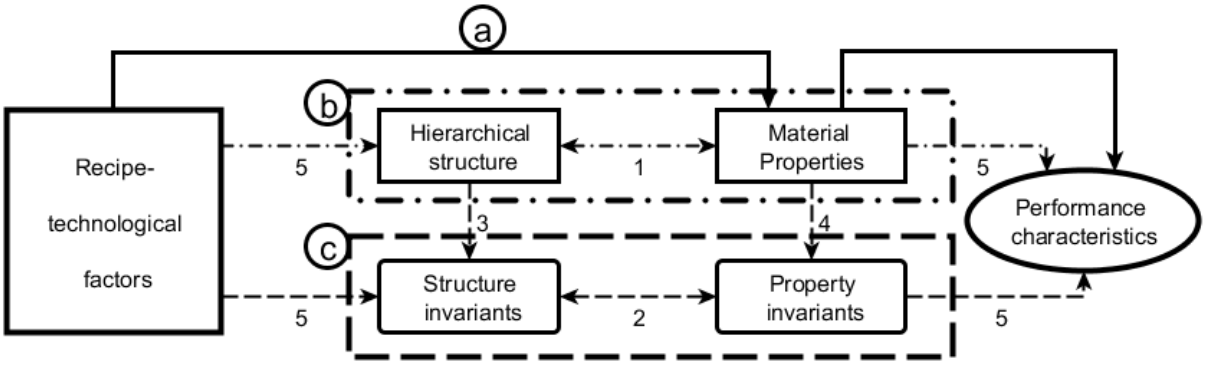

Fig. 1. The main directions of modeling methods in materials science:
a – traditional approach; b – structure-oriented research; c – the structurally invariant method;
1 – low level of correlation; 2 – high level of correlation; 3 – determination of the invariant characteristics of the structure (structure invariants); 4 – determination of invariant characteristics of a set of properties from experimental data (obtaining property invariants); 5 – ambiguous mappings

One of the difficulties of structure-based modeling is the need to somehow numerically identify the structure of the material. In addition, visual analysis, which is often used in the description of microphotographs, does not allow one to objectively distinguish some structures from the background of others. Thus, it is necessary to switch to the use of invariant characteristics of the structure, which may be similar for visually different structures or structural invariants, and to structurally invariant modeling methods. Part of the structural characteristics of the material at different scale levels can be described typologically. For this purpose, in the considered structure, the first category of elements of a similar nature (composition, size, geometry, etc.) and those elements that can be compared to the connections between them (the second category) were distinguished. Such a process can be implemented in many ways, some of which are discussed below. The first elements are assigned to the vertices, and the second – to the edges of the graph [3]. Thus, for modeling, the considered material is replaced by a graph or network as a mathematical model. In contrast, for example, to chemical graphs, the material graph is an infinite stochastic one, with some invariant properties that can be described numerically. It should be noted that when moving to graph models, the geometric aspect of the system is partially or completely neglected, since the graph is a topological object, that is, for the corresponding description, it is important, for example, not the length of the connection, but its presence. However, the transition to graph models reflects an important aspect of material structure that is relatively easy to quantify. For this, topological indices can be used, which are widely used in theoretical chemistry when solving the QSPR problem (Quantitative Structure-Property Relationship) [4]. Options for reflecting the structure of the material by graph models and methods for adapting existing topological indices to application in the case of obtained infinite stochastic graphs are reflected in this article.

Analysis of recent research. Discrete models of the hierarchical structure of complex systems are quite common [5]. The range of coverage of modeling using graphs is extremely large: sociology [6], biology [7], chemistry [8, 9], electronics and electrical engineering [10], etc. The reference in this work is the use of graph theory in chemistry. There are several areas of application of graphs in chemistry, one of them is related to the topological description of relatively small molecules of a certain structure [11]. To date, topological indices are widely used for predicting the biological activity

and other properties of such molecules [12], for virtual screening of chemical compounds in order to obtain formulas of compounds with a high level of activity and other properties. The procedures for calculating topological indices for small molecules are integrated into modern software systems [13]. Topological indices or, in general terms, molecular descriptors of polymer molecules have been periodically developed [14], but sufficient systematicity has not been achieved. Meanwhile, many topological indices for low molecular weight compounds can be easily transformed and applied in a new form to graphs representing the structure of polymers [15], as well as to graphs of meso-, macro-, and microstructures. The present work is devoted to the construction of discrete models of composite materials and the development of indices describing such structures.

Targets and goals. The main goal of the study is to develop methods for quantitative description of the multilevel structure of composite materials using graph-theoretic models and topological indices. Relevant tasks: analysis of the features of experimental-statistical modeling of the hierarchical structural organization of materials using structural descriptors, construction of graph-theoretic models of the structural organization of composites at the molecular and mesoscopic levels, development of a technique for obtaining discrete models of the emerging structure of a material based on the results of microscopic examination, as well as development of a scheme transformation of existing topological indices to describe stochastic infinite graphs representing a discrete material model both at the molecular and mesoscopic levels of organization.

Objects and methods of research. The object of the study was microscopic preparations of hardening gypsum binder dough as models of composite compositions, during hardening of which crystallization processes predominate.

A gypsum binder (gypsum G-5-B-II (DSTU B V. 2.7-82:2010) produced by Ivano-Frankivskcement) was used for microscopic study of the hardening processes. The water-gypsum ratio was taken equal to 1 (taking into account the observation under the conditions of a microscopic specimen). The drug was the original binder, brought into contact with the aqueous phase, placed on a glass slide. Observation and taking pictures were carried out on a setup based on a MIN-8 microscope with a total magnification of 70 times. The observation was carried out for 80 minutes, the images were recorded with a period of 3 minutes, after 60 minutes – with a period of 10 minutes. In a series of images, those were identified that reflect the main features of the hardening process. Two of them were used to build discrete grip models.

Research results. Structure-oriented modeling of composite materials is impossible without taking into account its hierarchical structure, from the atomic-molecular level to the microscopic (10^{-9}-10^{-3} mm), further – to mesoscopic (10^{-3}-1 mm) and macroscopic (10-10^{2} mm) (Fig. 2). Moreover, the properties are affected by all structural levels that can be changed under operational conditions [16]. In a conditional state of rest, the interaction between the levels weakens in favor of the intralevel ones, and under operating conditions, the interlevel interaction increases. The key point of interlevel interaction is the intermediate mesoscopic level.

The presence of several large-scale levels of material organization creates prerequisites for the use of certain forms of ES-modeling. Structure-oriented ES-modeling should be based on a set of quantitative characteristics of the material structure – structural descriptors of several hierarchical levels (1):

$$\left(X^1, X^2, \ldots, X^i, \ldots, X^n\right) \equiv \left(\left(x_1^1, x_2^1, \ldots, x_{m_1}^1\right), \ldots, \left(x_1^i, x_2^i, \ldots, x_{m_i}^i\right), \ldots \left(x_1^n, x_2^n, \ldots, x_{mn}^n\right)\right), \quad (1)$$

where $i = 1, \ldots, n, i$ – hierarchical level number. One of the forms of ES-models that have an advantage for hierarchical systems with two adjacent structural levels of organization (simplifying assumption) is a quadratic polynomial in various products of structural descriptors of these two levels (2):

$$\hat{Y}(X) = b_0 + \sum_i \sum_j b_{ij} x_i^1 x_j^2 + \sum_i \sum_j \sum_k \sum_l b_{ijkl} x_i^1 x_j^2 x_k^1 x_l^2 . \quad (2)$$

Arbitrary physical and operational characteristics of the composite, such as strength, adhesion, thermal conductivity, and vapor permeability, can serve as responses $\hat{Y}(X)$ in such modeling. Form (2) meaningfully reflects the implementation of the primary structural level X^1 in the structures of the secondary X^2.

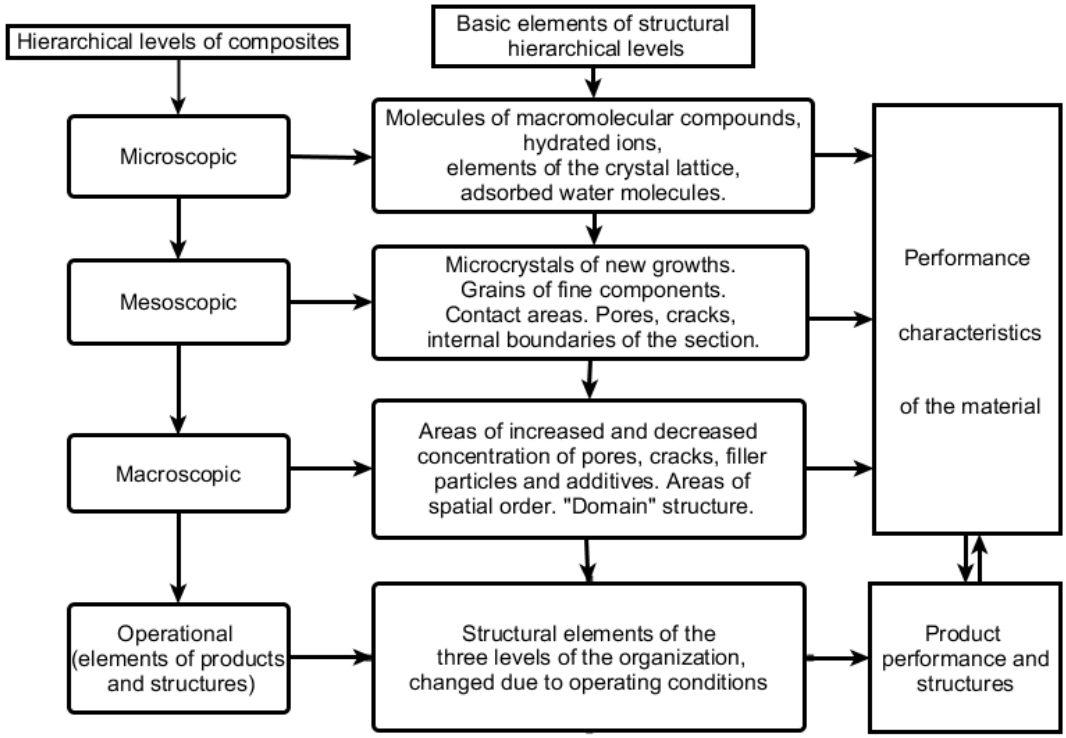

Fig. 2. Simplified diagram of the hierarchical structural organization of a building composite material

The molecular level can be considered as the primary structural level, and the micro- and mesoscopic levels can be considered as the secondary one.

The topological description of the structure of different scale levels can be based on different content, the vertices and edges of the graph can correspond to different objects.

At the primary structural level, graphs of organic and inorganic polymers, especially cross-linked and highly branched ones, are of most interest for materials science (Fig. 3). In them, the vertices correspond to repeating fragments of high molecular weight, for phenol-formaldehyde resin [17] they correspond to phenyl fragments connected to each other by repeating low-molecular fragments that play the role of bridges, in the case under consideration, to methylene fragments. In copolymers and composites, the vertices can belong to different classes.

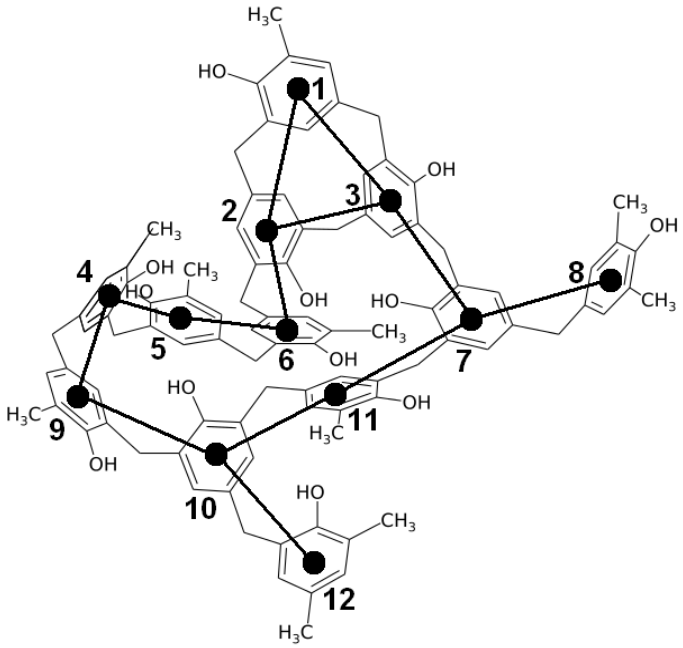

Fig. 3. Phenol-formaldehyde resin (bakelite) molecule fragment and its representation using graph

The oxygen bridge acts as a structural equivalent of a graph edge, which is typical for both organic and inorganic polymers, for example, silicates and aluminosilicates (Fig. 4). On figure 4, the oxygen bridging atom corresponds to an edge of the representing graph, silicon-oxygen tetrahedra (aluminate octahedrons and similar structures) correspond to the vertices of the graph.

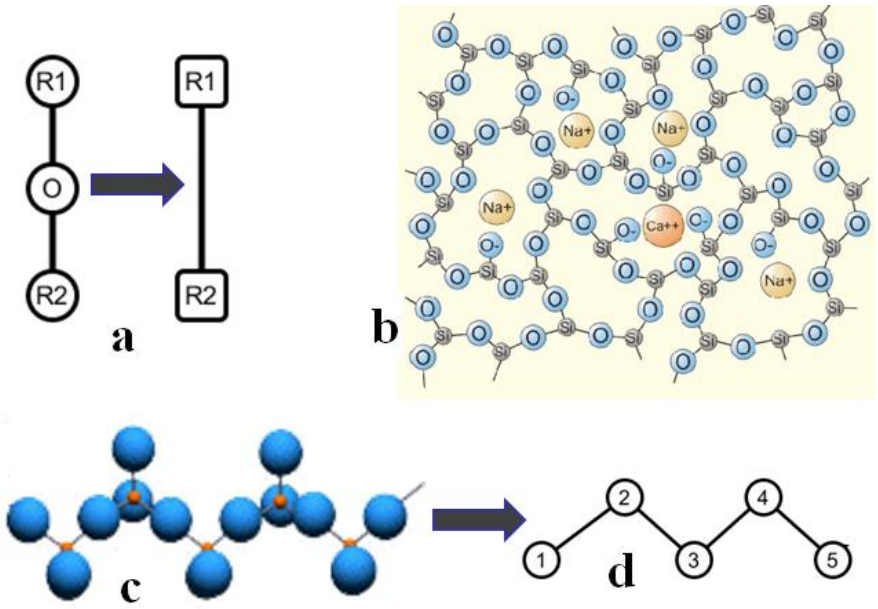

Fig. 4. Basic principles of discrete modeling of silicate structures:
a – replacement of the oxygen bridging atom by a graph edge; b – stochastic organization of silicate structures (glass); c – a chain of linked silicon-oxygen tetrahedra in a pyroxene chain; d – the graph representing this chain

Examples of interpreting the structures of fragments of macromolecular compounds using graph theory show the relative simplicity and ease of transition to graphs. An important problem in materials science is the correct application of such a transition scheme for other, larger-scale structural levels of material organization. Here, as in the first case, many transition schemes can be implemented that differ in meaningful interpretation. The development of examples of such an interpretation, especially in connection with experimental data, is of significant interest.

One of the discrete material models for structural levels is quite obvious. Let it be a matter of composite materials with coarse filler, the particles of which are suspended in the matrix material. The vertices of the representing graph can be associated with coarse filler particles, and the edges with transitions through two interfaces (particle 1 – matrix material – particle 2). Moreover, the transitions can be realized only along the segments connecting the centers of mass of the filler particles. An example of transition to a discrete model is shown in Fig. 5. It should be noted that discrete models of the porous structure of materials can be built in a similar way.

One of the discrete models of structural organization can be built on the basis of experimental data from a microscopic study of the hardening processes of gypsum and cement binders. In the process of hardening, the binder particles undergo physical and chemical transformation, in the initial period affecting its surface layers, as a result of which fine-crystalline neoplasms are formed on their surface. At the moments of completion of the setting between the particles (more precisely, between their central parts, nuclei), a network of contacts is formed, evolving from coagulation to phase [18]. Thus, the formed crystallization structure has the features of a discrete system, the characteristics of which change during the setting period. The vertices of the graph in it correspond to the centroids of the cores of the binder particles, corresponding to the maximum intensity of the planar model system (Fig. 6). The connecting particles of neoplasms correspond to the edges of the representing graph. It should be noted that some particles undergo complete dissolution and the number of vertices of the corresponding graph changes, as well as the number of edges.

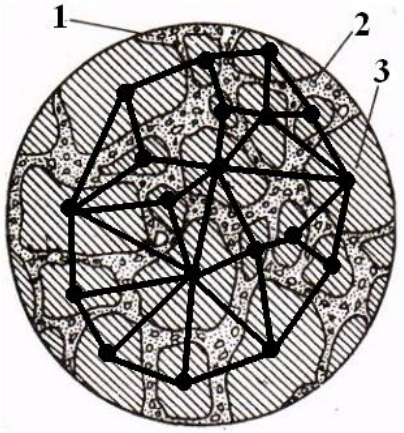

Fig. 5. Discrete models of the macrostructure of a composite material:
1 – matrix material; 2 – particles of small fillers and additives; 3 – coarse filler particles

In the structure of a hardening cement stone, the vertices can be compared to unreacted cement grains surrounded by layers of a silicate structure, and to the edges – large crystals of the aluminate phase.

The most characteristic features of discrete graph models of the first, molecular and second, mesoscopic (microscopic) levels is the fact that they are infinite stochastic, reflecting the probabilistic-statistical organization of the material structure at the considered scale levels. The analysis of such graphs should be built taking into account the fact that the structural descriptors of the levels under consideration are given in a probabilistic way, using distribution functions and their characteristics – moments and cumulants.

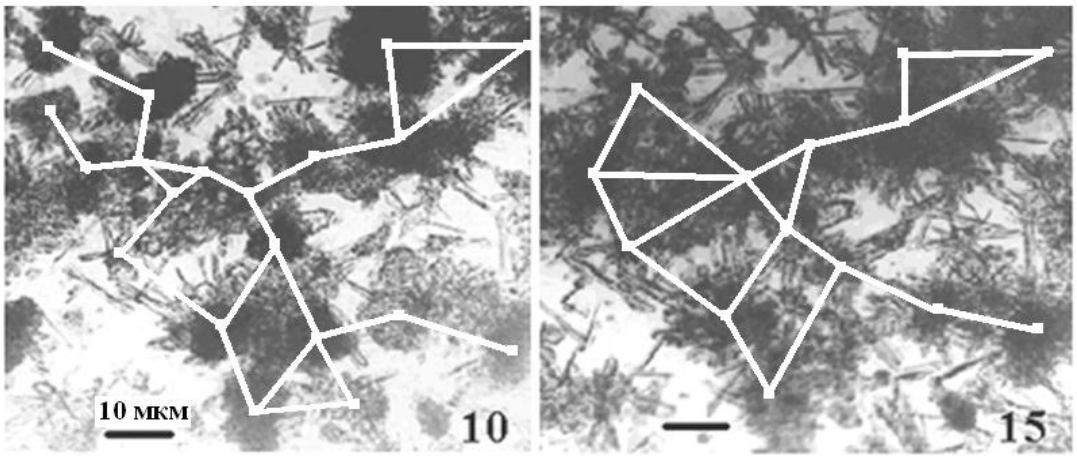

Fig. 6. Discrete models of processes of structure formation of a model system. The given numbers of images correspond to the following periods from shuttering:
10 – 30 min; 15 – 45min

The simplest and closest to the experimental results is the model of structurally additive properties at different scale levels. Thus, an incremental scheme is used to build a statistical model of a polymer. For its implementation, the number of vertices, the number of bonds of various types and other simple fragments are taken into account, each of which is characterized by a certain contribution to the property. The incremental contribution makes it possible to calculate the molecular refraction, the enthalpy of formation, and other similar characteristics (Fig. 7). The number of vertices can be determined from the recipe, the number of bonds and other various types allow you to determine the chemical and physico-chemical methods of analysis. In practical applications, not the number of vertices and bonds is used, but the mole fractions of monomers in the mixture and the fraction of diatomic fragments in the polymer.

The incremental scheme, with appropriate modifications, turns out to be useful for determining a number of characteristics of polymer-based composites. These include, for example, thermal conductivity, heat capacity, and vapor permeability [19]. However, the main performance properties of composite materials, such as strength and adhesion characteristics, are not structurally additive. To model and predict structurally additive and structurally nonadditive properties, other structural descriptors, the so-called topological (topochemical) indices [11], used in theoretical chemistry when solving the QSPR (Quantitative Structure-Property Relationship) problem, can be used.

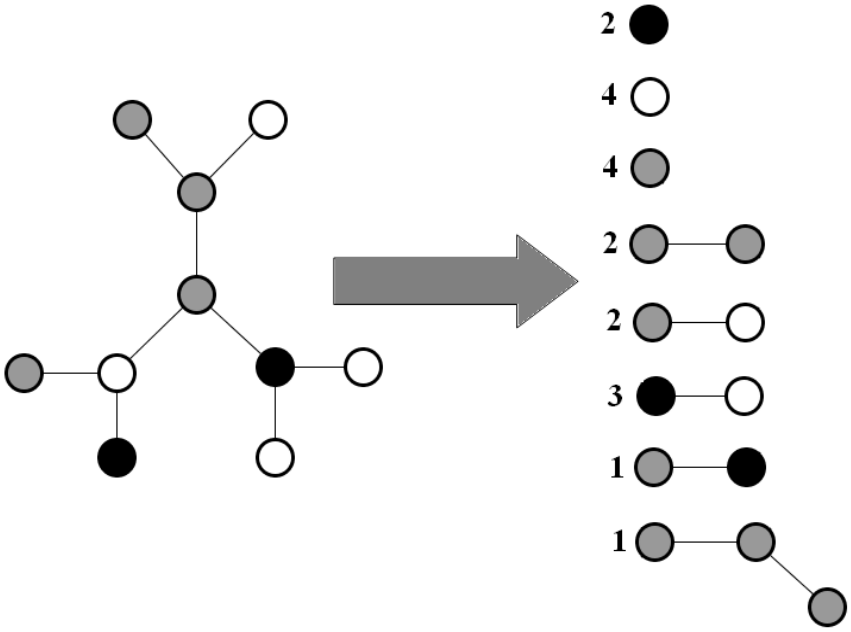

Fig. 7. Determination of properties according to the incremental scheme. The values on the right indicate the numbers of the respective fragments and the factors of the respective contributions

Topological indices are determined for chemical graphs – discrete models of molecules with a relatively small number of atoms and low molecular weight. The corresponding graphs are finite deterministic. The initial information is matrices of several types representing the corresponding graphs. Let us consider examples of such matrices. The graph shown in Fig. 3 G(V,E), where V is the set of vertices and E is the set of edges of the graph G, the adjacency matrix A (3) corresponds, the unit element corresponds to the presence of the graph edge and connection in the modeled structure, 0 to its absence. Such a matrix and the distance matrix D, whose elements are equal to the length of the shortest path connecting any two vertices, are the main source of information for constructing topological indices – structural invariants of the system being modeled.

$$A = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \quad (3)$$

Of interest is the problem of transforming these and other topological indices for application to random infinite graphs representing the (network) structure of organic or inorganic polymers. The same transformed indices can also be used to display the structure of some intermediate level – macroscopic or mesoscopic.

The method of calculating information indices based on information theory and, in particular, on the Shannon entropy formula [20] (4) is transferred to the graphs of the considered types most simply (with the least changes):

$$H = -\sum_{i=1}^{n} p_i \log_2 p_i . \quad (4)$$

Based on (4), the information content of the graph IC_k is calculated (5):

$$IC_k = -\sum_{i=1}^{n} p_i \log_2 p_i , \quad (5)$$

here $p_i = \frac{n_i}{n}$ – the probability that the selected fragment (vertex, edge) corresponds to the i-th set, taking into account the k-th environment (neighboring fragments up to the k-th order). In this case, the vertex under consideration is taken alternately without environment (k=0), with its first environment (immediate neighbors, IC1 k=1), second environment (IC2), and so on. The proportion of vertices of each of the i-th class p_i is determined. The considered approach can be significantly extended and, in particular, applied to both polymer graphs and structural graphs. With this approach, statistical information about nodes and their environment in the case of polymers can be obtained, for example, as a result of physicochemical studies, for material microstructures – using microscopic methods. Along with the information content IC_k they can calculate the derived quantities − SIC_k (structural information content) and the binding information content BIC_k, which characterizes the relation IC_k to it's maximum value $IC_{k\max} = \log_2 n$, where n – the number of graph vertices, a similar ratio is for the number of edges m (6):

$$SIC_k = \frac{IC_k}{\log_2 n} , \quad (6)$$

$$BIC_k = \frac{IC_k}{\log_2 m} , \quad (7)$$

Similarly, complementary information content is defined CIC_k as deviation IC_k from $IC_{k\max}$ (8):

$$CIC_k = \log_2 n - IC_k . \quad (8)$$

If information-theoretic indices, including those given here, actually do not need adaptation when passing to stochastic infinite graphs, then in other cases such adaptation (to varying degrees) is necessary.

A slight transformation is required for the procedure for calculating the index by Narukami and Katayama [21], which is equal to the product of the degrees of the vertices of the corresponding graphs (9):

$$p(G) = \prod_{k=1}^{n} d_k . \quad (9)$$

In another notation, this index has the form (10):

$$P(G) = 1^{n_1} 2^{n_2} 3^{n_3} \ldots i^{n_i} , \quad (10)$$

where n_i − number of vertices of degree i.

When using infinite stochastic graphs n_i for research, it is necessary to use not the number of vertices, but their share from 1: $n_i = \frac{N_i}{N}$, where N – is the total number of vertices, N_i – is the number of vertices of degree i.

To transform a series of topological indices, it is necessary to introduce a valuation that allows one to pass to values that obey the limit theorems of probability theory, while such indices go over to converge to constant values when passing to infinite graphs.

Thus, the Plat topological index [22] is equal to the sum of the degrees of each edge of the molecular graph (i.e., the number of edges associated with the vertex under consideration), and accounting can be carried out not only for the first neighbors F^1, but also for subsequent ones, up to the k-order (11):

$$F^k = \sum_{i=1}^{m} \deg^k(e_i). \tag{11}$$

During passing to stochastic infinite graphs, it is necessary to introduce a normalization on the number of edges and pass to the average degree of edges m (12):

$$F_p = \frac{1}{m} \sum_{i=1}^{m} \deg^k(e_i). \tag{12}$$

The properties of probabilistic graphs are described by the distribution function of structural descriptors or by a set of its characterizing values – moments and cumulants. The values of the classical Plath index can be considered as a mathematical expectation; for this and other indices, higher moments can be defined, for example, variances (13):

$$s(F_p) = \frac{1}{m} \sum_{i=1}^{m} (\deg^1(e_i) - F_p)^2 \ . \tag{13}$$

Another topological index, the Wiener polarity number, is equal to the number of pairs of atoms in the graph separated by three bonds along the shortest path (14):

$$P = \frac{1}{2} \sum_{i,j} f(d_{ij}), \tag{14}$$

where d_{ij} – elements of the distance matrix, the function f is given as (15):

$$f(g) = \begin{cases} 1 & g = 3 \\ 0 & g \neq 3 \end{cases}. \tag{15}$$

During passing to infinite graphs, it is necessary to normalize to the number of pairs of vertices $\frac{1}{2} n(n-1)$. The modified Wiener polarity number [8] looks like (14):

$$P = \frac{1}{n(n-1)} \sum_{i,j} f(d_{ij}). \tag{16}$$

The developed methods for modifying topological indices for infinite stochastic graphs are largely universal and applicable to many other topological indices. It should be noted that a similar conclusion can be drawn for other molecular descriptors that take into account not only the topological, but also the geometric structure of both the molecular graphs of polymers and the macrostructure of composite materials. In the latter case, rich information about the topological structure of the meso (macro-) level can be obtained from the study of microscopic preparations. Such a study can be carried out, for example, in the manner shown here in the processing of microphotos.

The above and many other topological indices, adequately transformed for random infinite graphs, can be used for experimental and statistical modeling of composite materials under operational conditions.

Conclusions. The work shows that structure-oriented modeling of hierarchical systems, which, in particular, are composite materials, can be carried out on the basis of regression statistical modeling (a variant of experimental statistical modeling), which takes into account the possibility of implementing the previous structural level at the next one, and, in in particular, molecular at the microscopic or mesoscopic level.

Methods for discrete (graph-theoretic) modeling of the structural organization of composite materials at several structural levels, including the molecular one, are considered.

A method for restoring representing graphs for hardening binders is proposed.

The vertices are associated with the binder particles, and the edges of the graph are associated with the system of crystallization contacts. An example of an experimental study of a model system of a hardening composite with subsequent restoration of the representing graph is given.

For the numerical description of infinite stochastic graphs obtained for polymer composite materials and composite mesostructure graphs, a scheme is proposed for transforming the topological indices of small graphs (representing a compound molecule in chemical applications) into the required ones. One of the approaches to such a transformation is the transition to normalized values.

The obtained indices, along with the incremental scheme, are proposed to be used to model the properties of composites under operating conditions.

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ТОПОЛОГІЧНІ ХАРАКТЕРИСТИКИ СТРУКТУРИ КОМПОЗИЦІЙНИХ МАТЕРІАЛІВ

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Анотація. У статті розглянуто методи моделювання композиційних матеріалів за допомогою теорії графів. З цією метою аналізується метод структурно-орієнтованого та структурно-інваріантного моделювання композиційних матеріалів. За основу такого моделювання передбачається використання структурних дескрипторів – величин, що описують структуру матеріалу на різних масштабних рівнях, у тому числі і на молекулярному. Структурно-орієнтоване моделювання ієрархічних систем, якими є композиційні матеріали, може проводитися на основі регресійного статистичного моделювання, в якому враховується можливість реалізації попереднього структурного рівня на наступному, і, зокрема, молекулярного на мікроскопічному або мезоскопічному. Пропонується форма експериментально-статистичних моделей, що включає дескриптори кількох структурних рівнів. Розглядається спрощений підхід, у якому враховуються закономірності двох рівнів: молекулярного і наступного (мікро- і мезоскопічного). Розглядаються приклади та алгоритми складання представляючого графа для зшитих та розгалужених полімерів та силікатних матеріалів. Показано, що граф, який представляє зшиті полімери – нескінченний стохастичний. Розглядається і реалізується експериментальна процедура побудови дискретної моделі по мікрофотографіям твердіючого в'яжучого. Для кількісного опису цього графа застосовується інкрементна схема, і навіть топологічні індекси, що отримані внаслідок трансформації топологічних індексів графів низькомолекулярних сполук. З метою трансформації відбувається перехід до імовірнісних характеристик – часток та середніх (нормованих) значень. Трансформовані топологічні індекси передбачається застосувати до статистичної моделі композиційного матеріалу.

Ключові слова: дискретні моделі композитів, ієрархічна організація, кристалізаційна структура, топологічні індекси.

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