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ANALYTICAL DESIGN OF COMPOSITES IN TERMS OF SYSTEMS ANALYSIS

Irina Garkina*, Alexander Danilov

Penza State University of Architecture and Civil Engineering, Penza, Russia

*Corresponding author's e-mail: fmatem@pguas.ru

Abstract

Introduction. The development of composite materials is considered with account for the shifts of paradigms based on the basic models of the continuous self-developing environment towards paradigms based on the models of the structured self-developing environment using the ideas and methods of the system approach and synergetics. The system approach can: reduce or even eliminate the uncertainty inherent to the problem to be solved; reconstruct it in models meeting the objectives of the study; identify objects, properties, and relationships in the system under consideration, taking into account the mutual influence of the external environment. **Methods.** It is shown that the structural organization of the material determines the design of the product or structure and largely determines the functional properties of the entire system. Composite materials are considered as large, complex systems formed based on a modular principle; material properties are determined on the basis of autonomous studies of individual subsystems. **Results**. It is assumed that individual subsystems have a certain degree of autonomy; it is possible to introduce customizable reference models with the simultaneous decentralization of modules by inputs; the conditions for transferring the results of autonomous studies to the system as a whole are determined by the completeness of understanding the processes of the formation of the structure and properties of the system. In the development of composites, the relative importance, the mutual utility of the quality criteria, a reasonable balance between the internal logic of science and its practical significance are taken into account. Partial criteria are analyzed, and a generalized quality criterion for the building material is formalized. The following is considered: the complexity of the object of study (multi-dimensionality, multi-connectedness, incompleteness of diagnostic information), diagnostic interpretation of the analyzed factors, the probabilistic nature of diagnostic information (using methods of both concrete and abstract-logical cognition; each new logical stage continues the previous one and serves as a prerequisite for the previous one).

Keywords: composite materials, complex systems, system approach, systems analysis, mathematical modeling, quality assessment, functionals.

Introduction

There are several dozen definitions of the “system” concept. L. von Bertalanffy (Bertalanffy L. Von., 1973) defined a system as “a complex of interacting elements” or “a set of elements standing in interrelation among themselves and with the environment”. In a philosophical dictionary, a system is defined as a set of elements standing in interrelation and interconnection among themselves and forming some coherent unity. V. N. Volkova (Volkova V. N., Denisov A. A., 1997) suggests considering a technical system as “a set of enlarged components, essentially necessary for the existence and functioning of each other”:

$$S = \{A, B, C, D\},$$

where A — the set or structure of the goals; B — the set of structures implementing the goals (formulation, technological, production, organizational, etc.); C — the set of technologies implementing the system; D — the conditions for the existence of the system or the factors affecting its creation and functioning. As can be seen, the definitions of complex technical systems available in the systems theory are applicable to the description of composite building materials. Therefore, it is fair to consider the construction composite as a complex technical system (Korolev E. V., 2020) and apply the optimal control theory and methods of systems analysis to the synthesis of such composites.

Mathematical modeling of the structure and properties of new-generation materials

Materials are presented as systems, which makes it possible to apply the system approach to the full extent in solving problems of their synthesis, identification, management, the use of an information-computing environment, including the conceptual aspects of modeling. When the problems of identification are solved, based on the application of a particular mathematical apparatus and the degree of its development, a preliminary analysis of a priori information is performed. The main efforts are directed at structuring and absolute formalization. It is assumed that the human has an unconditional priority over the results of the analysis: the construction of fully automatic quality management systems is not considered.

When building materials with controllable structure and properties are developed and their quality is managed, methods of vector optimization are used (lexicographic problem; method of successive concessions; scalarization of quality criteria based on linear convolution and introduction of benchmarks; construction of Pareto sets, etc.). The target function is determined by the required types of the kinetic processes for the formation of the main physical and mechanical characteristics of composites (Figure) based on solving at first the general and then the partial problem of identification (Budylina et al., 2021; Garkina et al., 2017).

Curve 1 (a particular case of curve 2; $x_0 = 0$) represents a solution to the Cauchy problem:

$$\ddot{z} + 2n\dot{z} + \omega_0^2 z = 0;\ z = x - x_m;\ z(0) = -x_m;\dot{z}(0) = x(0)$$

and has the following form:

$$x = c_1 e^{-\lambda_1 t} + c_2 e^{-\lambda_2 t} + x_m \quad (\lambda_1 > \lambda_2).$$

The parametric identification of kinetic processes of this type can be easily carried out by sequentially determining l2, d, l1, $\left(-\frac{c_1}{c_2}\right)$, $\dot{x}_0$ (e.g., for epoxy composite, the $\dot{x}_0$ value determines the initial polymerization rate). The identification of a process of parametric type 2 (e.g., heating of epoxy composites during initial structure formation) is carried out in a similar manner:

$$\ddot{z} + 2n\dot{z} + \omega_0^2 = 0,\ (z = x - x_m;\ x = z + x_m);$$

$$z(0) = x_0 - x_m;\ \dot{z}(0) = \dot{x}_0;\ (x(0) = x_0).$$

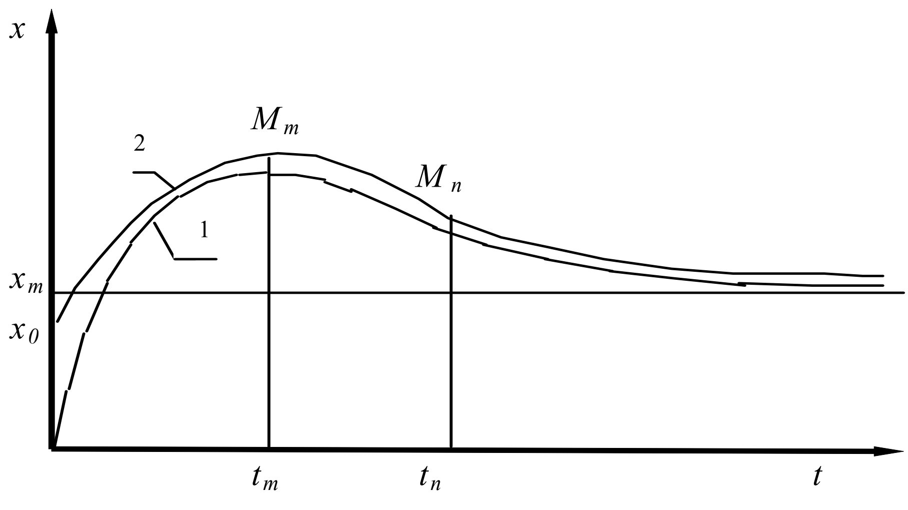
The determination is based on the known values of λ_1, λ_2, x_m, $\left(-\frac{c_1}{c_2}\right)$, x_0.

The possibility of establishing a connection between the composite structure and changes in macroscopic characteristics is taken into account. Considering the complexity of establishing the influence of formulation and technological parameters on the characteristics of materials, a special methodology for controlling the output characteristics of the material is developed, cross-links (synergy) between the material properties are determined, mathematical models of subsystems are specified with the subsequent identification of parameters (for individual systems — based on the conditions for obtaining extrema of target functions).

The use of the Pareto principle and diagrams (where the initial 20% determine the subsequent 80% of the time for the controlled parameter to reach its operating value) proved effective in the quality management of composites: it facilitates formulation development with the allocation of elements that determine the performance characteristics of the material. For instance, for epoxy composites used for radiation protection, strength and density were mainly determined by the degree of filling and type of modifier. An iterative method of improving the quality of the material was also used, based on the sequential construction of corresponding Pareto diagrams at each stage.

Cognitive modeling

Cognitive modeling is one of the ways to study complex weakly structured systems with many contradictory goals and criteria ((Tolman E. C.,1948); structuring, involves formulating and clarifying a hypothesis about the object functioning). At the preliminary stage of studies, most complex systems can be considered as weakly structured. Cognitive modeling is based on a cognitive map (an oriented graph; incomplete, fuzzy and even contradictory information can be used). The vertices of the oriented



Standard types of kinetic dependences for changes in material stability (“overshoot” phenomenon (Bobryshev A.N. et al., 1994) graph are the factors (concepts), while its arcs indicate the causal connections between the factors (the weights determine the degrees of influence). Various modifications of models (corresponding to various interpretations of vertices, arcs, and weights) are studied using the formal apparatus. Substantial human participation in the formalization of the primary representations by subject-formal methods does not make it possible to guarantee the reliability of the obtained solutions (e.g., the risk of inadequate application of a formalized model to a specific problem situation due to misunderstanding of the mathematical meaning of structures by specialists in the problem area). It is reasonable to represent the factor in a normal form (a variable on a particular rating scale). In terms of linguistics, the normality of the factor makes it possible to use such verbal contexts as: “more – less”, “growth – decline” (it is often difficult even to choose contexts “worse – better” similar in meaning), etc. Cognitive clarity of the “factor” concept as a variable of the required type is necessary. In modeling, the same causal relationships can be represented in a cognitive map with the use of different concepts. The validity of the principle of transitivity of causal concepts (from the fact that A causes B, and B causes C, it follows that A causes C), which is usually assumed, is not true in many cases (false transitivity is possible). As can be seen, a cognitive map reflects subjective ideas about the system functioning and development (the strategic step $S^i \to S^{i+1}$ means taking the system from the state S^i to the state S^{i+1}). When building a hierarchical structure of quality criteria, as well as a hierarchical structure of the system itself (if possible) with its help, we can further consider the system as a structured one. The target state of the system is considered to be achieved if the assessment of the targeted development of the system, specified in the form of a goal achievement functional, almost does not change.

The system complexity requires: interdisciplinary studies and involvement of specialists competent in various narrow subject areas in the construction of a cognitive map; formalization of the primary representations of a weakly structured problem in the form of a collective cognitive map (to generalize and coordinate different representations). It is possible to solve this problem to some extent with the use of the methods of conceptual structuring, criteria and special technologies for the formation and coordination of collective concepts.

The above approach has been successfully used in the synthesis of radiation protective composite as a complex system, its identification, formation and formalization of goals, a set of alternatives for their achievement, and, finally, multi-criteria optimization (Garkina and Danilov, 2019; Smirnov and Korolev, 2019).

Principal component analysis in quality management of materials used for protection against ionizing radiation

The chemometric approach is based on the use of projective mathematical methods, which make it possible to isolate latent variables in big data and analyze the relationships in a system under consideration. Unfortunately, despite the simplicity and efficiency of such an approach (which is often visual) to the analysis of experimental data, it is almost not used in construction materials science. By using the principal component analysis (PCA), we ranked the quality criteria $q_i, i=\overline{1,p}$ according to the obtained values for n experimental prototypes. The first principal component was defined as the direction of the largest change (scattering along some central axis — a new variable) in the data $\mathbf{q}=\left\|q_{ij}\right\|, i=\overline{1,p}, j=\overline{1,n}$ in the Cartesian coordinate system $Oq_1q_2...q_p$ (approximated — purely geometrically; clarified — based on the best linear approximation of all the initial points q_{ij} by the least squares method). The second principal component was assumed (by definition) to be orthogonal to the direction of the first component (along it, the next largest change in the values q_{ij} occurs), and the third component was assumed to be perpendicular to both the first and second components (lying in the direction in which the third largest change in the data occurs). The subsequent principal directions were determined in a similar manner. The resulting system of the principal components provides a set of orthogonal axes, each of which lies in the direction of the maximum change in the data in descending order of these values. Due to the orthogonality of the principal components in the new resulting set, the variables (linear combinations of the initial variables) no longer correlate with each other. The transition from the initial Cartesian coordinate system to the new set of orthogonal axes makes it possible to get rid of the dependence between the criteria. The upper limit of the number of the principal components does not exceed $\max\{n-1,p\}$. The effective dimension of the principal component space is determined by the $\mathbf{q}=\left\|q_{ij}\right\|$ matrix rank. The last principal component lies in the direction in which the difference between the prototypes will be minimal (in fact, it is impossible to distinguish the prototypes here, since all these differences are just random noise). The principal components with large numbers were considered as directions in which the principal component is noise. Thus, the PCA made it possible to decompose the initial data matrix into a structural part (several first principal components lying in the directions of maximum changes) and noise (directions in which the difference between the positions of the points is small and can be neglected)

(Danilov et al., 2009). Each of the properties (quality criteria) is an integral characteristic of the material, depending on the properties of the components, composition, preparation conditions, curing, etc. The assessment of the composite quality is made by the set of both dependent and contradictory criteria (chemical resistance, frost and heat resistance, impact and abrasion resistance, radiation heating, adhesion properties, protective properties in relation to the steel reinforcement, etc.). With the help of the PCA, a set of linear combinations of the initial criteria (practically independent) was distinguished, which subsequently, using methods of experimental design and multi-criteria optimization, made it possible to develop radiation protection and corrosion-resistant materials. Dimensionality reduction (separation of the initial data into the substantial part and noise) within the principal component analysis is achieved by neglecting the directions corresponding to small eigenvalues. There are no common rules for choosing the number of significant principal components (determined by the eigenvalues of the covariance matrix, the research tasks (visualization on the plane or in space), the intuition of the researcher, etc.).

Among the priority criteria were the following: strength, density, and porosity of the material. The dependences of porosity $q_1(x_1, x_2)$, %, compressive strength $q_2(x_1, x_2)$, MPa, and density $q_3(x_1, x_2)$, kg/m3, obtained by methods of mathematical experimental design, on the encoded volume fractions of the aggregate (lead pellets with a diameter of 4–5 mm) $x_1 \in [0,5;0,6]$ and filler (barite, $S_{sp} = 250$ m^2/kg) $x_2 \in [0,35;0,4]$ were used:

$$q_1(x_1, x_2) = 5.18 + 3.44x_1 + 0.96x_2 - 1.33x_1x_2 + 3.83x_1^2;$$

$$q_2(x_1, x_2) = 22.5 - 3.72x_1 + 1.43x_2 - 2.87x_1^2;$$

$$q_3(x_1, x_2) = 7143 - 147x_1 - 181.7x_1^2.$$

The covariance matrix obtained based on the experimental values ξ_{ui} of the listed indicators has the following form:

$$C = \frac{1}{N-1}(\xi_{ui})^T(\xi_{ui}) = \begin{pmatrix} 0.169 & 0.023 & -1.35 \\ 0.023 & 0.220 & 0.149 \\ -1.35 & 0.149 & 21.5 \end{pmatrix}.$$

The eigenvalues λi and eigenvectors $\mathbf{v}i$ of the covariance matrix:

$$\lambda_1 = 0.226,\ \mathbf{v}_1 = (0.221; 0.975; 0);$$

$$\lambda_2 = 0.077,\ \mathbf{v}_2 = (0.973; -0.221; 0.063);$$

$$\lambda_3 = 21.6,\ \mathbf{v}_3 = (-0.063; 0; 0.998).$$

The matrix of transition to the principal components G_1, G_2, G_3 has the following form:

$$L = \begin{pmatrix} -0.063 & 0 & 0.998 \\ 0.221 & 0.975 & 0 \\ 0.973 & -0.021 & 0.063 \end{pmatrix}.$$

The principal components are linearly related to the initial indicators q_1, q_2, q_3:

$$G_1 = -0.063q_1 + 0.990q_3;$$

$$G_2 = 0.221q_1 - 0.975q_2;$$

$$G_3 = 0.973q_1 - 0.021q_2 + 0.063q_3.$$

By virtue of $\lambda_3 >> \lambda_1$ and $\lambda_3 >> \lambda_2$, the significant principal component is unique and corresponds to the principal direction $\mathbf{v}_3$; the vector of the first principal direction forms a small angle with the axis of the third principal variable. The dominant indicator is the average density (the third indicator).

Industrial applications of system methodologies, system identification and control theory

The relevance of the studies is conditioned by the need to ensure the environmental safety of nuclear power facilities, extremely hazardous chemical production facilities, bases, and arsenals; bunkers, burial sites, and storage facilities for low-level radioactive waste, etc. The prerequisites in the synthesis include the principle of 100 % mathematics efficiency, the hierarchy of quality criteria, and the hierarchical structure of the radiation protection composite material, developed with account for the following:

- the paradox of integrity (a holistic description of a system is possible only when it is “holistically” broken down into parts; when a given system is described as some unity; cognition of a system as a unity is impossible without analysis of its parts);

- the paradox of hierarchy (description of a system is possible only if it is described as an element of a supersystem (a broader system) and vice versa, description of a system as an element of a supersystem is possible only if there is a description of this system (subsystems are systems for their subsystems; each system is part of some supersystem)); in the synthesis of building material (system), the supersystem is represented by building materials suitable for use in the given operating conditions;

- system-forming properties (integrative; formed with the coordinated interaction of the elements combined in a structure, which the elements did not possess before) (Chernyshov and Makeev, 2022; Selyaev et al. 2016).

Based on the classification of the main kinetic processes for the formation of the structure and properties of special-purpose composite materials (radiation resistance coefficient, linear coefficient of gamma-radiation attenuation, strength gain, change in the elastic modulus, contraction and shrinkage, increase in internal stresses, heat emission, chemical resistance, water absorption, water resistance, etc.), their generalized model is built in a class of ordinary differential equations with constant coefficients up to the fourth order inclusive.

Each of the kinetic processes is a special case of the generalized model and can be represented as a solution to the Cauchy problem:

$$z^{(4)} + a_1 z^{(3)} + a_2 z^{(2)} + a_3 z^{(1)} + a_4 z = 0;$$

$$z = x - x_m;\ x(0) = x_0,\ \dot{x}(0) = \dot{x}_0,\ \ddot{x}(0) = \ddot{x}_0,\ \dddot{x}(0) = \dddot{x}_0;$$

$x_0,\ \dot{x}_0, \ddot{x}_0, \dddot{x}_0$ are determined by the required type of kinetic process and given operating value x_m of the material characteristic under study (aperiodicity of the processes is assumed; sufficient conditions are specified). The parametric identification, formalized quality assessment, and one-dimensional optimization of each of the kinetic processes are carried out (functionals of the form $\Phi(S) = f\lambda_m + a\frac{1}{\lambda_m} + br + c\frac{1}{r}$ are used, which allow for considering the formation of the composite structure and properties in time; $\lambda_m = \min_i\{\lambda_i\}$, $r = \max_i\left\{\frac{\lambda_i}{\lambda_m}\right\}$; $k_i = -\lambda_i$ — the roots of the characteristic polynomial, $\lambda_i > 0,\ i = \overline{1,\ n}$). The multi-criteria synthesis of radiation protection composite is carried out using vector optimization methods (solution of the lexicographic problem, narrowing of the search area by the method of successive concessions, scalarization by introduction of metrics in the space of target functions (strength, porosity, density), construction of Pareto sets) (Smirnov and Korolev, 2019).

Portable implementation of an image processing language

Tools and methods of digital image processing are currently used in various fields. In construction materials science, these applications are used in the study of the material structure: when determining the distribution of the structural objects under study (air cavities, particles of dispersed aggregates, etc.), determining the fractal dimensionality of cracks, hardness, etc. Each of these methods involves several stages, where the discretization of the continuous color-brightness field and the transformation of the resulting image are mandatory. Discretization is carried out by the hardware of a receiving device. The resulting two-dimensional array of chromatic coordinates serves as the input data, and it is also a result of most operations. There are software environments available that make it possible to perform matrix calculations. Many of them are driven by high-level languages (being in fact *interpreters* from those languages). The standard is the MATLAB package with its features available through tool chains including one intended for image processing. In particular, the tools make it possible to perform the two-dimensional Fourier transform and calculate convolution. However, no functions of image processing in different color spaces are implemented. The image processing tools are also contained in software packages for working with raster graphics. For example, GIMP has advanced tools for switching between color spaces, performing statistical analysis, calculating convolution in the spatial domain, and working in batch mode (the input language is a superset of LISP). However, most packages use single-byte integer values for internal data representation, which leads to loss of information.

To describe image processing tasks, we suggest a specialized image processing language — the IPL language. In the IPL-interpreter implementation, the following requirements are taken into account: support for batch mode, use of floating point values for internal representation, support for tools of convolution in the inverse length domain. The emphasis is on openness (understood as the capability to maintain and extend features) as well as portability between heterogeneous computing platforms (WinAPI and POSIX).

The fundamental language types are vector, matrix and binary decomposition. In the structure of the interpreter, two levels are distinguished: application and service ones (implemented in ANSIC). The first one encapsulates parsing and basic processing algorithms. The second one involves the implementation of abstract types of data and objects that isolate system calls to the target platform.

The functionality of the proposed language and the operation of the interpreter were tested when solving a number of applied problems: assessment (calculation of scalar criteria) of the quality of protective-decorative coatings, recognition of features in the spatial domain and inverse length domain, comparison of digital filtering means (Gusev et al., 2018).

Analytical methods for the synthesis of materials: experience in application

Based on the experience of developing and managing the quality of special-purpose materials, we determined the approach and methodological principles of creating materials using the methods of systems analysis and modeling of kinetic processes. First, the material is considered as a weakly structured multi-purpose system. As a result of interdisciplinary studies (incomplete, fuzzy and even contradictory information is used), the interaction of the basic relationships existing in the system that determine its functioning is formalized. Hierarchical structures of quality criteria and the system itself are built using a cognitive map (including a collective map), which makes it possible to view the system as already structured. During the qualitative assessment of material properties and determination of relationships between them, methods of rank correlation were used (in particular, stress-strain properties (14 indicators were taken into account) and the relationships between them were studied for 10 types of epoxy composites)

(Garkina and Danilov, 2018). It was shown that some properties (e.g., compressive strength or hardness) do not need to be determined due to the availability of significant relationships between them. Based on the statistical significance of the sample value of the concordance coefficient, the lack of consistency within the entire set of indicators was shown in the presence of pairwise consistency between some of the indicators. Considering the compressive strength as a resultant variable, the problem of regression on ordinal variables was solved.

The kinetic processes (in particular, the residual strength by years of operation) were considered as time series, and autoregressive models with a moving average were developed:

$$x_t = a_1\, x_{t-1} + \ldots + a_p\, x_{t-p} + b_0 e_t + b_1\, e_{t-1} + \ldots + b_q\, e_{t-q}.$$

The Markov, Yule, and Yule–Walker processes were considered. The Levinson–Durbin algorithm was used to determine the model coefficients. The formalization of processes for the formation of physical and mechanical characteristics of the material was carried out as a solution of the general identification problem in the class of ordinary differential equations (for radiation protective composites — not higher than the fourth order); the parametric identification of kinetic processes was performed. In the optimization of formulation and technological parameters and material quality management, the problem of multi-criteria optimization with the preliminary minimization of the dimensionality of the criteria space was solved. The Pareto principle, diagram and sets were used (the analytical dependences of properties on the points of the factor space were determined in advance by methods of experimental design; nonlinear programming methods were used). The multi-criteria optimization under contradictory criteria was performed using the method of sequential concessions; methods of criteria scalarization based on the results of solving single-criterion problems (as benchmarks) were considered.

The effectiveness and prospectivity of using the proposed methods are confirmed by the results of the multi-criteria synthesis of radiation protective materials (Budylina et al., 2021; Garkina et al., 2017; Korolev and Smirnov, 2013).

Conclusions

1. The methods for mathematical modeling of the structure and properties of new-generation materials were developed based on cognitive modeling.

2. The partial criteria and the formation of a generalized criterion for the quality of the material with a hierarchical structure were proposed.

3. The effectiveness of using the principal component analysis to minimize the dimensionality of the criteria space and manage quality was shown by the example of materials with special properties.

4. The specialized image processing language was proposed (IPL) for solving a number of applied problems (calculation of scalar criteria; assessment of the quality of protective-decorative coatings).

The common approach to industrial applications of system methodologies, system identification and control theory was presented.

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АНАЛИТИЧЕСКОЕ КОНСТРУИРОВАНИЕ КОМПОЗИТОВ С ПОЗИЦИЙ СИСТЕМНОГО АНАЛИЗА

Гарькина Ирина Александровна*, Данилов Александр Максимович

[1]Пензенский государственный университет архитектуры и строительства,
г. Пенза, Россия

*E-mail: fmatem@pguas.ru

Аннотация
Введение. Разработка композиционных материалов рассматривается с учетом смены парадигм, основанных на базовых моделях непрерывной саморазвивающейся среды, в сторону парадигм, основанных на моделях структурированной саморазвивающейся среды на идеях и методах системного подхода и синергетики. Системный подход может уменьшить или даже устранить неопределенность, присущую решаемой задаче; реконструировать ее в моделях, отвечающих задачам исследования; выявлять объекты, свойства и отношения исследуемой системы с учетом взаимного влияния внешней среды. **Методы.** Показано, что структурная организация материала определяет исполнение изделия или конструкции и во многом определяет функциональные свойства всей системы. Композитные материалы рассматриваются как большие сложные системы, образованные по модульному принципу; свойства материалов определяются на основе автономных исследований отдельных подсистем. **Результаты.** Предполагается, что отдельные подсистемы обладают определенной степенью автономии; возможно внедрение пользовательских эталонных моделей с одновременной децентрализацией модулей по входам; условия переноса результатов автономных исследований на систему в целом определяются полнотой понимания процессов формирования структуры и свойств системы. При разработке композитов учитываются относительная важность, взаимная полезность критериев качества, разумный баланс между внутренней логикой науки и ее практическая значимость. Анализируются частные критерии, и формализуется обобщенный критерий качества строительного материала. Учитывается сложность объекта исследования (многомерность, многосвязность, неполнота диагностической информации), диагностическая интерпретация анализируемых факторов, вероятностный характер диагностической информации (использование методов как конкретного, так и абстрактно-логического познания; каждый новый логический этап продолжает предыдущий и служит исходной предпосылкой для предыдущего).

Ключевые слова: композиционные материалы, сложные системы, системный подход, системный анализ, математическое моделирование, оценка качества, функционалы.