The Experience of Designing Building Materials

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Abstract. The evolution of views on the development of composite materials is analyzed from the point of view of paradigm shift based on basic models of a continuous self-developing environment towards paradigms based on models of a structured self-developing environment based on ideas and methods of a systematic approach and synergetics. A system approach can reduce or even eliminate the uncertainty inherent in the problem being solved; to reconstruct it in models that meet the objectives of the study; identify objects, properties and relationships of the investigated system, taking into account the mutual influence of the external environment. It is shown that the structural organization of the material determines the structural 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 on a modular principle: integrative properties are approximately determined on the basis of autonomous studies of separate subsystems. Separate subsystems are supposed to have a certain degree of autonomy; the introduction of custom reference models with the simultaneous decentralization of modules by inputs is possible. It is shown that 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 formation of the structure and properties of the system. When developing composites, the PATTERN method and the SATURN technology are used to determine the criteria for assessing the relative importance, mutual utility, state and timing of research and development, maintaining a reasonable balance between the internal logic of science and its practical significance. Partial criteria and formalization of the generalized quality criterion of building material are analyzed. As an illustration, the definition of flocculation conditions in a disperse system is given on the basis of its representation as a system of particles moving under the action of gravitational and pair interaction forces, interaction with boundaries and a dispersion medium. It is shown that the uniformity of the steady-state configuration and the sedimentation stability of the polydisperse system are mainly determined by the volumetric degree of filling. Given the complexity of the composite as an object of study (multidimensionality, multiconnectedness, incompleteness of diagnostic information), diagnostic interpretation of the analyzed factors, the probabilistic nature of diagnostic information the necessity of using methods of both specific and abstract logical cognition is shown (each new logical stage continues the previous one and serves as the initial prerequisite for the previous one).

1. Introduction

The main unifying principle in materials science is the unified style of thinking inherent in materials scientists and their recognition of certain fundamental theories and methods. Increasingly widespread methods of system analysis in the design of composite materials. Naturally, the usefulness of the
systematic approach depends on how successfully the backbone factor is identified and how fully its significance is established for the formation of the composite as a complex system. Only those mathematical calculations that are formulated taking into account important system-forming factors will be useful. Moreover, the most important criterion for the isomorphism of two systems, of course, is the isomorphism of a system-forming factor.

The design of a composite as a complex system actually comes down to the construction of its generalizing model: the system project is implemented taking into account particular, interconnected, interdependent models. A project is a series of dependencies between design goals, possible goals for their achievement, environment and resources. It can be considered as a complex model, reflecting all the interesting properties of the future real system.

2. Paradigm shift in material design
At present, a new paradigm is being formed to solve the problems associated with the architectural and construction complex: increasing the multifunctionality and service life of building materials and structures, reducing the cost of creating comfortable living conditions while reducing the negative impact on the environment, etc.; widespread use of BIM technologies and 3D construction is expected.

In the evolution of ideas about a number of materials, three stages are distinguished, differing in the research methodology and the level of practical development [1]. The first stage is the emergence of new technology (the initial accumulation of data, experience and skills in the production of new material). The technology is dominated by the prescription approach; in research, trial and error; process control is intuitive, based only on the experience of the technologist. The second is the formation of a new technology (the development of technology is based on a generalization of the accumulated data, identifying the patterns of the influence of various factors on the properties of the material; research is carried out with the involvement of fundamental sciences). Here, ideas about the influence of control factors on the structure of the material and its relationship with properties are formed. The classification of control factors is carried out, the dominant, combined into a system of prescription and technological factors are distinguished. The third stage is the development of effective technology for the scientific ownership of production (obtaining building material with a given level of quality). The concept of “quality” is expanding and includes not only the requirements for the manufacture of the material (technological process), but also its compliance with the operating conditions of the product (operational properties and durability). The technology includes two interconnected cycles: technological and operational. At each of the cycles, the impact of control actions on the quality of the material is evaluated; when they deviate from the specified parameters, a decision is made to change the formulation and conditions for the manufacture of the material (conditions of structure formation).

The principle of adjusting the recipe and the manufacturing mode of products should be implemented not only according to the results of the initial state of the product (quality after the completion of the technological cycle), but mainly taking into account transformations of the structural parameters of products under the influence of operational factors. It is supposed to identify the technological process and build an adequate model of “recipe-technological factors - structure - material quality”. In a crisis of the old paradigm (revolution in science; the search and design of a new paradigm), competing theories are tested and eliminated. Accepted rules are abolished, except for those suitable for the new paradigm (reconstruction of prescriptions: not just denial of the rules, but the preservation of positive experience suitable for the new paradigm). It is important to note that the new paradigm does not include the old. With a paradigm shift, there is no continuity of theories. It involves the formation of a different frame of reference based on fundamentally new basic models and a change in the principle of controlling the initial structure formation: not the formation of a material structure with parameters that provide “initial” quality (after manufacturing), but the formation of a structure (organization) that ensures quality over time (in operation period); acceptable decline in quality indicators. In particular, nanotechnology is just
a tool for controlling structure parameters and / or imparting additional properties. In the models of structural material science, it is assumed the existence of a certain hierarchical structure of objects, considered as systems [2], which are the basis for the formation of new ideological scientific installations. The choice of model is determined by the objectives of the structural description of the object, the boundaries of the scale level, the selected priority number of structural elements, based on the purpose of the object of analysis; processes at each level obey the laws of this particular level. The design of the system as a whole is based on the hierarchical structure of its quality criteria (each individual property can be obtained with different sets of structural components) [3].

3. Methodological principles for constructing mathematical models

With a systematic approach, the methodological basis for constructing mathematical models of complex systems is the modularity of structural properties. Composite materials as complex systems are represented as a set of interacting elements. It is possible to decompose composites into separate subsystems with a certain degree of autonomy (integrative properties can be approximately determined on the basis of autonomous studies of separate subsystems). Integrative properties are determined by the relationships between modules, levels, and at each level. The use of the results of autonomous studies of separate subsystems in the design of the composite as a whole is associated with the need to eliminate intersystem connections (the introduction of custom reference models with the simultaneous decentralization of modules by inputs). When determining some properties of the material depending on the particle size distribution, you can use ingredients from other materials, but with the same particle size distribution as in the synthesized material. However, it is necessary to provide similar, as accurate as possible, intersystemic bonds (for example, wettability). When transferring the results of autonomous wettability studies to the formation of the structure and properties of the material, it is necessary to know the wettability parameters of the incoming components in cramped conditions. In principle, this can be achieved using a customizable reference model that provides for pressure regulation between the components. Tuning can be achieved using experimental data on samples.

Traditionally used in building materials science data on kinetic processes of structure formation and physical and mechanical characteristics of the material are essentially autonomous studies of individual separate modules. Here, the required parameters of kinetic processes are determined taking into account intersystem connections. Implicitly present are reference models involving simultaneous decentralization of inputs.

The presentation of a complex composite model is possible in the form of interacting subsystems, modules, elements and the relationships between them; complexity is considered at the model level; First of all, the composite nature of the mathematical model is taken into account. The selection of functional subsystems is based on a clear statement of goals by levels. The number of goals is not limited, but they are expected to be detailed with an indication of the relationships (the principle of dividing a complex problem into smaller ones using the results of quantitative expert evaluation of each of the subproblems, based on various criteria). In particular, the formation of the basic physical and mechanical characteristics of composite materials can also be studied on the basis of retrospective identification methods for dynamic systems [4].

4. PATTERN method and SATURN technology

Complex hierarchical structures in accordance with the PATTERN methodology can also be considered as a set of typologically typed elements and the relationships between them in a certain way (multi-level representation of structures). Here, composite materials are presented as complex systems, the design of which is carried out in compliance with the basic principles of a systematic approach:

- hierarchy; each system or element is considered as a separate system;
- structural; the ability to describe the system through a description of the relationships between its elements;

- interdependence; the manifestation of the properties of the system only when interacting with the external environment;

- plurality of description; system description by a set of interacting mathematical models;

- designing the whole part.

The transition from one level to another is carried out by selecting substructures, which, in turn, can be considered as macroscopic elements; lower-level elements can be considered microscopic. Then the system during its design is configured using patterns as successful standard solutions to the problem. In the general case, pattern design is a formalized description of a frequently encountered design problem. A correctly formulated design pattern makes it possible to use the solution once successfully found repeatedly.

At each step of the study, when searching for acceptable solutions, the structure and values of the model parameters vary; the results are evaluated and a decision is made on the future direction of the study. From a theoretical point of view, automated intelligent technology and a system environment for the machine study of materials as systems are needed. The fundamental role is played by algorithmic knowledge and evidence-based programming methods based on the regular use of logical equations as the main formalism for representing the problem domain model - SATURN technology [5] (can be considered as a modification of the PATTERN method).

We have effectively used these methods to control the structure and properties of radiation-protective and chemically-resistant composite materials. Design began on the basis of technical specifications indicating the organization and properties of the material as a system. The ability to create a composite and the implementation of technical specifications was initially determined at the stage of cognitive modeling with the establishment of intensive and extensive properties with the allocation of control parameters. Based on the cognitive map, hierarchical structures of quality criteria were determined, and in accordance with the selected quality criteria, the corresponding structural schemes of the system (for each selected scale level) were determined. Further, formalization of the system quality criteria was carried out and mathematical models were developed in accordance with each of the criteria. Finally, based on the solution of single-criterion optimization problems using the found optimal values, the multicriteria problem was formalized and solved (the optimal structure and properties of the composite system were determined).

5. Particular criteria for the quality of composites as systems
As an illustration, we consider the definition of flocculation conditions in a disperse system based on its representation as a system of particles moving under the action of gravitational and pair interaction forces, interaction with boundaries and a dispersion medium [6,7]. The flocculation mechanism is determined by the interaction between structure-forming elements. To purposefully change the properties of composites, we performed mathematical modeling of flocculation and sedimentation in dispersed systems; evolution was described by a system of equations:

\[ m_i \ddot{r}_i - k_i (\dot{r}_i - v_i) = -\nabla U_i, \quad i = 1, N, \tag{1} \]

where \( m_i \) is the mass of the \( i \)-th particle; \( x_i, y_i, z_i \) - its coordinates; \( \vec{r}_i = (x_i; y_i; z_i) \); \( k_i \) - is the coefficient characterizing the dissipative properties of the dispersion medium; \( v_i, U_i \) - speed and potential of the
dispersion medium at point \((x_i; y_i; z_i)\). The potential is determined by the nature of the interfacial interaction.

On the basis of a numerical experiment using the developed program package, the flocculation and sedimentation stability of a composition with a polydisperse filler was determined \([\)\]. To increase the computational efficiency during modeling, specially developed stand-alone software was used, which allowed visualization of configurations and particle dynamics (Fig. 1).

\[ h_{\text{c,max}} = \frac{\sigma_m \cos \theta}{RT} \frac{M}{\rho_m} \]

\( \sigma_m \) - surface tension of the matrix material, \( \theta \) - contact angle, \( \rho_m \), \( M \) - density and molecular weight of the binder, \( RT \) - thermal energy of one mole of binder.

6. Some models of diagnostics of the properties of composites

Consider a simple diagnostic model. The set of properties of material \( S_1, S_2, \ldots, S_m \) determines the final list of the resulting characteristics of material \( D_1, D_2, \ldots, D_n \): properties are assumed to be binary. Let for definiteness there are only two characteristics \( D_1 \) and \( D_2 \) (for example, hydrophobicity and the appearance of fungi) and only three observed properties \( S_1, S_2 \) and \( S_3 \). Let there be knowledge: \( D_1 \rightarrow S_1, D_2 \rightarrow S_2, S_3 \rightarrow D_1 \lor D_2 \). The conjunction of these statements is equivalent

\[ \overline{D}_1 \& \overline{D}_2 \& \overline{S}_3 \lor \overline{D}_1 \& \overline{S}_2 \& \overline{S}_3 \lor \overline{D}_2 \& S_1 \& \overline{S}_3 \lor S_1 \& S_2 \& \overline{S}_3 \lor \] (2)

\[ \lor D_1 \& \overline{D}_2 \& S_1 \lor D_1 \& S_1 \& S_2 \lor D_2 \& D_2 \& S_2 \lor D_2 \& S_1 \& S_2 \lor \] (3)

If the material has \( S_1 \& \overline{S}_2 \& \overline{S}_3 \), then these data, together with the disjunctive normal form of the knowledge system formulated above, give \( D_1 \& \overline{D}_2 \& S_1 \& \overline{S}_2 \& \overline{S}_3 \) (any formula of the propositional logic can be reduced to a disjunctive normal form, i.e. abstract model for diagnosis). And from here we get the desired result \( D_1 \& \overline{D}_2 \), i.e. the material in question has a characteristic of \( D_1 \), not \( D_2 \). The procedure for using normal forms gives a procedure for searching for a diagnosis, while in case of withdrawal you must know in advance what we want to display.
You should not think that when carrying out the procedure formulated above, you can always get a definite answer. With the same knowledge that was formulated above, but with other data on the material, you can get an indefinite answer.

Let the material is characterized by data $S_1$&$S_2$&$S_3$. Then we get

$$D_1&D_2\lor D_2\lor D_1\lor D_2\lor D_1\lor D_2.$$

That is, we conclude with certainty that the material does not have characteristic $D_2$, but the question of whether it has characteristic $D_1$ remains open. It is required to attract additional knowledge or to measure other characteristics.

A case is possible when knowledge and data about the material will give zero information about its type. Let the third material exhibit properties $S_1$ and $S_2$ and no property $S_3$:

$$S_1$&$S_2$&$\overline{S}_3.$

With the same knowledge about dependencies that were formulated above, we have

$$D_1\lor D_2\lor D_1\lor D_2\lor D_1\lor D_2.$$

That is, all cases are possible, and thus the diagnosis is not established. There was not enough information to rule anything out. The above abstract diagnosis model is deductive. Let us briefly consider another model of diagnosis, based on plausible reasoning and, above all, on an analogy.

Let them accumulate information about a finite set of materials. For example, suppose that materials $a_1,a_2,\ldots,a_n$ were observed for which properties $S_1,S_2,\ldots,S_m$ were detected, on the basis of which characteristic $D$ was diagnosed. Materials $b_1,b_2,\ldots,b_k$ showed some properties from group $S_1,S_2,\ldots,S_m$, but some of these properties were absent, and it was concluded that there was no characteristic $D$. Suppose further that the presence of all the properties of $S_1,S_2,\ldots,S_m$ was observed in the material. Since material $C$ is similar to materials 1 in these properties, it can be concluded that the material has the characteristic $D$. This is a typical example of reasoning by analogy.

The conclusion that $c$ has characteristic $D$ does not logically follow from the accepted premises. This conclusion is only plausible conjectural in nature. As experience accumulates, more and more information about various materials and various manifestations of their characteristics $D$ is stored in memory. It may turn out that two materials possess the same characteristics from this set, but one has $D$ and the other does not. In this case, it is necessary to introduce additional characteristics into consideration by adding them to the initial set of properties. On the other hand, some characteristics may not be informative. In this case, they should be discarded (excluded from the list of properties).

It was assumed above that general knowledge is reliable; the relationship between the resulting characteristic and the property is deterministic. However, in reality, this relationship is in most cases only probabilistic. More often, knowledge is not of the form «if there is characteristic $D$, then there is $S_i$», but rather of the form «if there is characteristic $D_i$, then in
97% there is \( S \). The use of this kind of knowledge allows deductively deriving the consequences from this knowledge and data about the material only with a certain degree of probability.

It is known, the conditional probability:

\[
P(S|D_i) = \frac{P(S \& D_i)}{P(D_i)}; \quad (7)
\]

the last two probabilities are easily calculated based on the analysis of statistical data.

Now it is already possible to use not only deterministic relationships between characteristics \( D \) and properties \( S \), but also probabilistic relationships. The problem of probabilistic diagnostics is formulated as follows: how to determine the probability \( D \) with respect to the probability of properties relative to the resulting characteristic \( S \). This can easily be done using the well-known Bayes formula.

The proposed models were effectively used in the preparation of cognitive maps (digraphs) to build models of a number of special-purpose composite materials (radiation-protective, chemically resistant) [8…12].

7. Conclusions

It is shown that the design of composites actually comes down to the construction of a generalizing model: it is carried out taking into account particular, interconnected, interdependent models; represents a series of dependencies between design goals, possible goals for their achievement, environment and resources.

An analysis is given of the evolution of views on the development of composites in terms of paradigm changes; the modern paradigm is based on the ideas and methods of a systems approach and synergetics.

The methodological principles of constructing mathematical models of composites under the hypothesis of modularity of structural properties are given.

The methodology for determining the integrative properties of composite materials based on autonomous studies of separate subsystems is indicated.

A technique is given for determining assessment criteria based on the use of the PATTERN method and SATURN technology.

An illustration is given of an analytical study of the properties of materials as particular quality criteria using the example of flocculation and sedimentation processes.

Probabilistic models for diagnosing the properties of composites are proposed.

The results of the studies were positively evaluated in the design of radiation-protective and chemically resistant composites.

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