

Methodological Principles Design of Composite Materials

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Abstract: The algorithm of the synthesis of composite materials is derived on the base of representation of composites as complex systems with modular structure. The adjustment of the PATTERN method for the algorithm is performed during design (which is based on system approach) of the radiation-protective composites. The concept development of materials with special properties based on the study of kinetic processes of structure formation and basic physical and mechanical characteristics of the material is proposed. The conditions of formation of floccula and sedimentation stability in disperse systems (visualization of configuration and dynamics of particle).

Key words: Composite materials, structure and properties, radiation-protective and chemical-resistant composites, modeling of complex systems, modification of the method PATTERN

INTRODUCTION

Importance of system research in the design of composite materials has now become apparent. In complex systems parts (subsystems) is strongly interconnected by a plurality of forward and backward linkages; changing one of them often leads to significant changes in other parts. Becomes difficult decomposition of the entire system as well study of selected parts of it (with the possibility of the synthesis of these parts of the system). We need methods for assessing and analyzing the whole system.

MATERIALS AND METHODS

Formulation of the problem methods of solution: The most well-known approach to the design of complex systems is a method PATTERN (Planning Assistance Through Technical Relevance Number); it was intended to solve the problems of planning research and development activities in the face of uncertainty (Garkina *et al.*, 2011). It provides for the allocation in complex conflicting system functional subsystems on the basis of a clear statement of objectives of the hierarchical levels. The number of objectives is not limited to (taken into account their relationship); complex problem is divided into smaller. Determined list of final objectives, indicators of scientific and technological significance of (the sum of the relative importance of factors for each level of the hierarchy is taken equal to unity). Efficient

allocation of resources is made in accordance with the obtained coefficients. The method allows to determine a reasonable balance between the internal logic of science and its practical significance: its violation leads to indifference of society towards science or loss of perspectives in basic research.

Here systems with complex hierarchical structure can be viewed as a set of typical elements and connections between them (multi-level structures). Here, the transition from one level to another is carried out through the allocation of sub-structures which can be regarded as a macroscopic elements interconnected by a simple and understandable way. Elements of the lower level are considered as microscopic. The system is configured using a pattern (not to be confused with the procedure PATTERN!). The pattern can be seen as a kind of model good solution to the problem or how to systematically recurring fragment or sequence of elements of the system (widely used in the creation of software). Pattern design is actually a formalized description of frequent design problem. Working with patterns is actually adequate modeling of the subject area. The lowest level of representation of the system is its description in terms of classes (with their attributes and operations), their corresponding objects (microscopic elements) and relations between them. Description of the structure of the system in terms of microscopic elements (additional typology) is given in the simulation system at the class level. Macroscopic element next level there is a system architecture (basic substructure system). The highest

level is the integration of individual systems which are regarded as macroscopic elements. When the system model is based on design patterns are easily determined the structural elements and their relationships that are important to solve the problem. Properly formulated pattern makes it possible to reuse once successfully found solutions.

When searching for suitable solutions at every step of the study are set the structure and values of model parameters is evaluated the results; the direction of future research is determined. The methodological basis of mathematical models of complex systems is the modularity of the structural properties (complex system is represented as a set of interacting elements).

Modification pattern method for the development of composites: Consider the possibility of using the pattern method for designing composite materials, based on their representation in the form of complex systems. In this case, the complexity is seen as the complexity of the composite model (interacting subsystems, modules, components and connections between them). There is the possibility of composite design based on the basic principles of a systematic approach:

- Hierarchy; each system or component is considered as a separate system
- Structuring; the ability to describe the system through the description of relationships between its elements
- Interdependence; expression system properties only in the interaction with the external environment
- Multiple description: description of a variety of mathematical models of interacting systems
- The design of the whole subject

In the case of large complex systems formed by a modular principle (including composite materials), often fails to produce the decomposition of the system into separate subsystems that have a certain degree of autonomy (approximately integrative properties can be determined on the basis of independent studies of separate subsystems). Here, each element of the hierarchical structure of the system determines the quality of a stand-alone (without taking into account all the interconnections), the quality of a separate system. The results of independent research modules can be used to determine the integrative properties (defined connections

between the modules, levels and at each level, mainly on a qualitative level only). The ability to use the results of independent studies of separate subsystems when designing the system is determined by the possibility of eliminating interconnections. For example, the introduction of customizable reference models with a simultaneous decentralization of modules for inputs. Conditions for the transfer of the results of independent research on the system as a whole are determined by the fullness of understanding of the processes of formation of structure and properties of the system. In particular, in defining some of the properties of the material depending on the particle size distribution of ingredients can be used in other materials but with the same particle size distribution as in the synthesized material. However, it should provide similar as accurately as possible, interconnections (e.g., wettability). When you transfer the results of independent studies on the wettability on the formation of structure and properties of the material is necessary to know the parameters of the wettability of the components in cramped conditions. In principle this can be achieved using reference model which provides pressure control between the components. When you set up, you can use experimental data on samples.

RESULTS AND DISCUSSION

Evaluation of the quality of materials in the parameters of kinetic processes: Used in building materials science on the kinetic processes of formation of structure and physico-mechanical characteristics of the material are the results of independent testing of individual subsystems. Here, the required parameters of the kinetic processes are determined by the interconnections. Implicit reference models are providing simultaneous decentralization of the inputs. A generalized model is easily constructed based on the classification of the most common types of kinetic processes (ordinary differential equation of n -th order with constant coefficients). Each of the processes under consideration kinetic (set strength, elastic modulus, shrinkage, internal stress, heat resistance, chemical resistance, water absorption and water resistance and others) can be considered as a special case of the generalized model. Parametric identification may be performed in accordance with algorithms that are based on characteristic points kinetic processes (e.g., the characteristic polynomial roots, points of extremum, an inflection points, etc.) (Garkina, 2015; Danilov and Garkina, 2015).

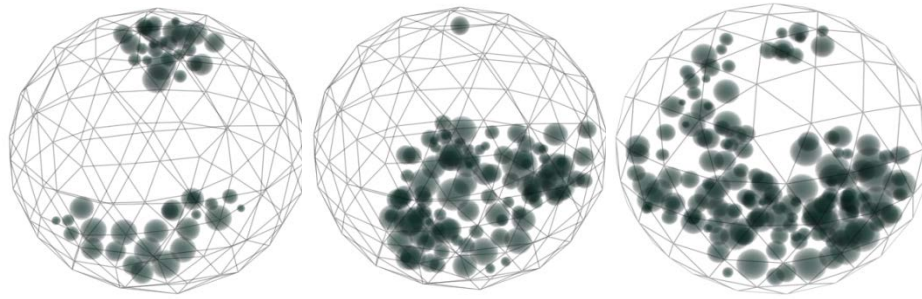


Fig. 1: Some established types of configurations of systems

To assess the quality of materials (structure and properties) are encouraged to use the kinetic parameters of the processes of formation of physical and mechanical characteristics (radiation resistance, curing, evolution of heat, shrinkage and others). Quality functional it is taken as:

$$\Phi(S) = f\lambda_m + a \frac{1}{\lambda_m} + br + c \frac{1}{r}, \lambda_m = \min_i \{\lambda_i\}, r = \max_i \left\{ \frac{\lambda_i}{\lambda_m} \right\}$$

where, $(-\lambda_i)$, the roots of the characteristic polynomial, $\lambda_i > 0, i = \overline{1, k}$; f, a, b, c weightiness; the higher the quality of the material, the less $\Phi(S)$ (for systems with a quality indicator, equal, fair: $\Phi(S) = \text{Dequal level line}$). For models of the second order is valid:

$$\Phi(S) = \left(\xi - \sqrt{\xi^2 - 1} \right) \cdot \omega_0 + \frac{a}{\left(\xi - \sqrt{\xi^2 - 1} \right) \cdot \omega_0} + b \cdot \frac{\xi + \sqrt{\xi^2 - 1}}{\xi - \sqrt{\xi^2 - 1}} + c \cdot \frac{\xi - \sqrt{\xi^2 - 1}}{\xi + \sqrt{\xi^2 - 1}}$$

$$\lambda_1 = n + \sqrt{n^2 - \omega_0^2} < 2n, \lambda_2 = n - \sqrt{n^2 - \omega_0^2} < n, \xi = \frac{n}{\omega_0}, n \geq \omega_0$$

In area $d_{k-1} \leq \Phi(S) = k$ the quality of the material is considered to be the same (k class system; $k = \overline{1, N}; \leq \Phi(S) = \text{const}$ -border of area with the same assessment d). Identification of areas of equal ranking is based on the choice of numerical values d for the boundaries of each class based on the comparison of the calculated and experimental boundaries. Communication of characteristics of the material is determined from the model parameters on experimental data. When choosing the ingredients and the characteristics of the material as a whole can use gradient methods.

Flocculation and sedimentation formation in dispersed systems: Flocculation is defined as the result of the interaction between the structure-forming elements. For

purposeful change the properties of composites can use the results of mathematical modeling of flocculation and sedimentation formation in dispersed systems. Models of the pair interaction described by the system of equations:

$$m_i \ddot{r}_i - k_i (\dot{r}_i - v_i) = -\nabla U_i, i = \overline{1, N}$$

Where:

- m_i = Particle mass
- x_i, y_i, z_i = Its coordinates
- $r_i = x_i, y_i, z_i$ k = Coefficient characterizing the dissipative properties of the dispersion medium
- v_i, U_i = Speed and potential (determined by the nature of interfacial interaction) the dispersion medium at the point (x_i, y_i, z_i)

On the basis of the numerical experiment are determined the conditions of flocculation and sedimentation stability (Garkina *et al.*, 2008) with polydisperse filler composition (stand-alone software was developed for the visualization of complex configurations and particle dynamics (Fig. 1).

It turned out that the homogeneity and sedimentation stability of the configuration of a polydispersed system, mainly determined by the volume filling degree. When you reach the limit of the volume fraction of the dispersed phase ($v_f = 0.16$) split the system into isolated subarea does not occur. The formation of floccules only possible for particles whose linear dimensions and interparticle distance comparable:

$$h_{cmax} = \frac{\sigma_m \cos \theta}{RT} \times \frac{M}{\rho_m}$$

Where:

- σ_m = Surface tension of the matrix material
- θ = Contact angle ρ_m
- M = The density and molecular weight of the binder
- RT = The thermal energy of one mole of a binder

CONCLUSION

It is proposed the algorithm for the design of composite materials as complex systems:

- Development of technical specifications; indication of structure and properties of material as a system
- Cognitive modeling composite (definition of intensive and extensive properties, the identification of the control parameters)
- Construction of cognitive maps
- The definition of quality criteria hierarchical structure
- Definition of a hierarchical structure of subsystems for each selected scale level
- Formalization of a system of criteria of quality development of mathematical models according to each of the criteria
- One-criterion optimization of systems and subsystems for each of the criteria
- Multi-criteria formalization
- Multi-criteria optimization (determining the optimal structure and properties of the composite) using a variety of methods to overcome the uncertainties purposes (Budylna *et al.*, 2015)

- Is given an application of modification of the method PATTERN for control of structure and properties of composite materials for special purposes
- The conditions of formation of floccula and sedimentation stability in disperse systems (visualization of configuration and dynamics of particle)

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