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Systems Approach to the Modeling and Synthesis of Building Materials

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Abstract

The methodological principles of building materials synthesis with the usage of the classic theory of control, methods of systems analysis in combination with experimental, heuristic methods of materials technology are suggested. The unified concept of elaboration of building materials with special properties is adduced (on the basis of analysis of kinetic processes of structure formation and main physical-mechanical characteristics of a material) with an estimation of their mathematical modelling accuracy with simultaneous experimental and theoretical ascertainment of connections between parameters of structure and kinetic processes. At the selected hierarchy of criteria the optimization of parameters of a considered technical system enables the usage of an iterative method. As an example, elaboration of radiation-shielding materials with an adjustable structure and properties is given.

Keywords: special-purpose materials, hierarchical structures, cognitive and mathematical modeling, structure and properties, quality criteria, optimization

Introduction

The core part of the new approach is the hierarchical structure of efficiency criteria for radiation-protective composite (Fig. 1). There are most general criteria on the top level of hierarchy: utility of system (target characteristics of a material, importance, area of application). On the second level of hierarchy there are quality of functioning (insensibility to noise, accuracy, reliability, sensitivity to control, quality of control); organization of system (quality of structure, complexity etc.); evolutionary efficiency and characteristic of development (practicability, resources, ability to renovation); an economic efficiency.

The decomposition of system within the framework of this hierarchy proceeds as long as elements belonging to developed types will not be received at the bottom level or the technical tasks of creation [1…3] are formulated.

For use of the each criterion in particular tasks arising on a considered development cycle of a material, the quantitative parameters for description, together with units and ways of measurement (rated, experimental or expert estimates) should be defined. Without such quantitative parameters the only alternative will be unfounded judgments about quality of the system.

The dependencies between criteria can be explored by methods of cluster analysis and statistics. Such dependencies represent empirical laws and usually can be derived on the basis of hypotheses estimation and weighing of the factors.
The basis for the long-term development planning for the whole system and for individual subsystems is a hierarchical structure of quality criteria is considered. In accordance with it developed a hierarchical structure own material.

The first level of structure of a radiation-protective material is macrostructure (characterized by grain size distribution, ratio of diameters of coarse fillers, character of surface of grains, porosity, size and concentration of capillaries, cracks and emptiness). The second level is microstructure (characterized by specific surface of disperse phases, thickness of binding layer, size and concentration of microcracks, size of micro- and macropores, thickness of contact zone); microstructure (size of typical structural element, type and concentration of inter-phase contacts and defects). Synthesis of the specified systems involves determination of necessary components and directions of quality management, including various ways of system optimization.

Uncertainty of purposes. Approaches to optimization

The most important problem arising in development process due to multiple optimization objectives is the *uncertainty of goals*. Thus, it is impossible to achieve best values for all criteria simultaneously [4, 5].

During materials' synthesis the uncertainty of goals can be eliminated by:

– linear convolution of form: $F(\mathbf{x}) = \sum_{i=1}^{n} c_i f_i(\mathbf{x}),$

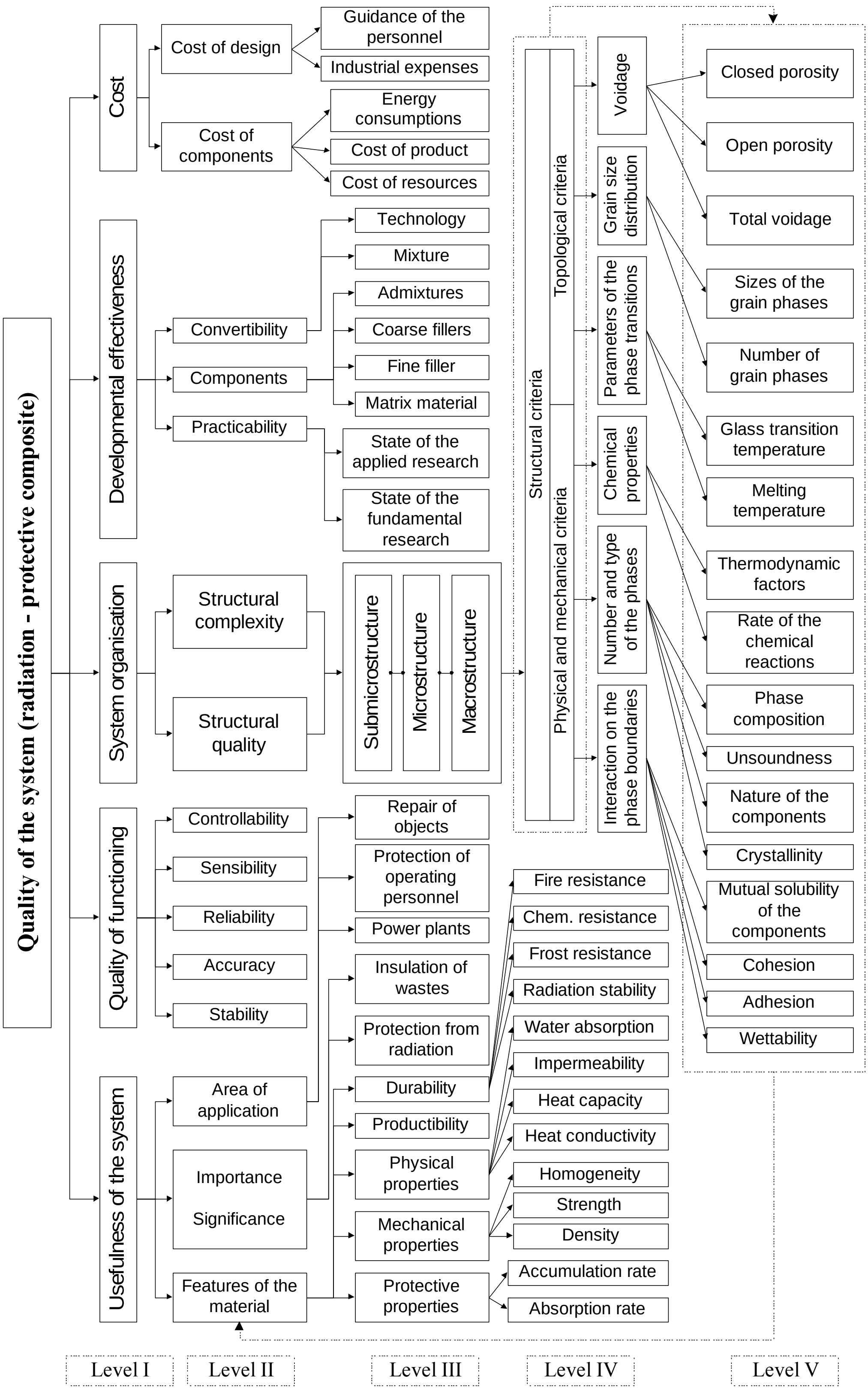

Fig. 1. Hierarchical structure of efficiency criteria

where f_i are the individual criteria (for example, kinetic characteristic of processes, presence of local resources, cost etc.); c_i are the weight constants (which can be determined as a result of expert examination or other methods; for example, on the basis of correlation estimation between generalized and individual criteria);

– introducing control parameters (for example, restriction of cost, durability, radiation resistance, energy consumption of the technology, safety of the technology, etc.);

– construction of Pareto sets.

The formation processes of primary physical and mechanical properties of composite materials (radiation stability, durability, modulus of elasticity, chemical stability, water resistance, etc.) can be characterized by kinetic parameters, which, in turn, can be viewed as the basis for objective function construction.

In particular, such choice for objective function offers opportunity to establish dependence between macro-structural changes of properties (shown under the appropriate conditions) and structure of a composite material [6].

An idealized model for the most widespread types of kinetic processes can be constructed as the result of classification. In particular, each process $x(t)$ can be represented as the solution of Cauchy problem:

$$\ddot{z} + 2n\dot{z} + \omega_0^2 z = 0, z = x - x_m, x(0) = x_0, \dot{x}(0) = \dot{x}_0; n^2 - \omega_0^2 \geq 0,$$

- where $x_0, \dot{x}_0, x_m$ can be determined by the type of kinetic process being investigated.

Each kinetic process can be viewed as a special case of the idealized model. The algorithms for parametric identification were constructed on the basis of characteristic points positions.

The developed model can be easily generalized both for systems with different grain size distributions and for some other systems characterized by kinetic processes of higher orders.

Parametric identification of kinetic process consists of definition of parameters of the idealized model (for example, roots of characteristic polynomial).

Solution of individual tasks were performed by the means of using objective function. The objective function for such tasks was formed either on the basis of reaction analysis while exposing the system to trial influences, or synchronous measurements of the system characteristics and managing influences during operation.

The dependencies between different properties of material were established. On the given basis the structural and mathematical models of systems and subsystems with the subsequent identification of parameters were specified. For isolated systems such task can be performed during maximization of objective function.

During the process of double-criteria synthesis of radiation-protective epoxy composite by the means of experiment designing analytical dependencies of average density and press resistance was derived.

The construction of Pareto set was carried out on the basis of the consecutive solution of nonlinear programming tasks together with penalty function methods:

I. $\rho(x_1, x_2) \rightarrow \max$, II. $R(x_1, x_2) \rightarrow \max$,

$\mathbf{x} = (x_1, x_2) \in G_X$, $\rho(x_1, x_2) = const.$ $\mathbf{x} = (x_1, x_2) \in G_X$, $R(x_1, x_2) = const$,

where x_1 and x_2 are concentration of plasticizer and rate of filling, respectively Curves of constant density $\rho(X_1, X_2) = conts$ (branch of hyperbola) and constant press resistance $R(X_1, X_2) = conts$ (parabola) derived from quadratic models of objective function shown on Fig. 2, where X_1 and X_2 are encoded (normalized) density and press resistance, respectively. The desired optimum position reached at point of $x_1 = 2{,}5$ and $x_2 = 10{,}2$. This point correspond to density *R*=3950 *kg/m*^{3} and resistance *R*=145 MPa.

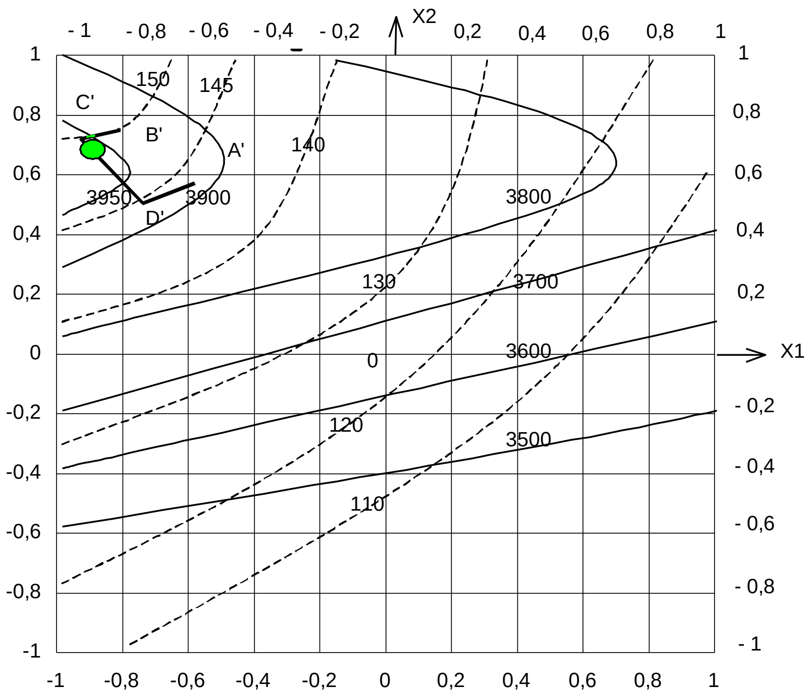

Figure 2. Curves of constant density and press resistance

The formalization of the partial criteria (properties)

The process of optimizing structure and properties of the radiation-protective material (absorption rate, resistance to radiation, durability) were performed on the base of parameters of kinetic processes (described, as stated above, by ordinary differential equations). During optimization, the analytic form for objective function were:

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

where $(-\lambda_i)$ are roots of characteristic polynomial, $\lambda_i > 0, i = \overline{1,k}$; *f, a, b, c* are weighting factors. In particular, for the second order models:

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

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

Lesser values of $\Phi(S)$ correspond greater quality of material. The solution of the task were performed by means of using areas of equal quality estimations of a material $d_{k-1} \le \Phi(S) < d_k$, where *k* - class of system; $k = \overline{1,N}$; *N* – range of a scale.

The boundaries of equal quality estimations areas were defined as $\Phi(S) = d_k = const$. The identification of equal quality estimations areas was made by a choice of numerical values d_k for class *k* on the basis of comparison with boundaries obtained from experiments. Thus, dependence between material characteristics and model parameters was derived from experimental data.
The choice of the mixture components and material characteristics was made on the basis of gradient optimization.

Charts and Pareto principle in quality control composites

The opportunity of using Pareto charts and Pareto principle for management materials' quality has been studied (it must be stated that such using of Pareto charts was unknown at the time). It's established that for radiation-protective glass dust composites kinetic of controllable parameters is that the initial 20% of formation time determines subsequent 80% together with stationary value of the parameters.

During optimization process were also used the objective function:

$$I = \int_0^T \left[\alpha\, y^2(t) + \beta\, \dot{y}^2(t)\right] dt .$$

It's shown that in common case zero value of α is acceptable (i.e. structure of a composite in the greater degree depends on speed of the energy flow, than on total energy charge). The numerous investigations was prove that by using of Pareto principle the mixture design (contents of components, grain size distribution) can be considerably facilitated. By using the given principle it's possible to discriminate mixture elements which determinate most of the operational characteristics of material. For the radiation-protective composites primary operational characteristics (durability and density) are determined mostly by a rate of filling and type of the modifier.

The Pareto principle also facilitates iterative improvement of material quality on the basis of consecutive Pareto charts construction at each stage of the development. It must be noted that shortly described here unified approach can be viewed also as a solution of control theory problem.

Conclusion

The use of systems engineering and mathematical modeling allowed us to obtain a number of unique composite materials for radiation protection (recognized at a number of international exhibitions). Have been achieved: the average density - 7500 kg / m^3, the compressive strength - 45 MPa, the coefficient of the radiation resistance up to 0.95, the linear attenuation coefficient gamma up to 0.5 cm^{-1}. The developed materials satisfy the requirements of practical application which are required for construction of the industrial objects, encapsulation of toxic and radioactive wastes [7].

References

[1] I. A. Garkina, A. M. Danilov, Quality management of the materials of special properties, Control Sciences, **6** (2008), 67-74.

[2] I. A. Garkina, A.M. Danilov, Y.V. Korolev, Building materials as systems, Building materials, **7** (2006), 55-58.

[3] I. A. Garkina, A. M. Danilov, Y. V. Korolev, Cognitive modeling of composite materials for the synthesis of complex systems, Proceedings of the universities. Construction, **3/4** (2009), 30-37.

[4] I. A. Garkina, A. M. Danilov, Management in complex technical systems: methodological principles of management, Regional architecture and construction, **1** (2012), 39-43.

[5] I. A. Garkina, A. M. Danilov, Y. V. Korolev, V. A. Smirnov, Overcoming uncertainty goals multicriteria optimization problems by the example of superheavy concrete for protection against radiation, Building materials, **8** (2006), 23-26.

[6] A. M. Danilov, I. A. Garkina, Methodology for the design of complex systems at development of special materials, Proceedings of the universities. Construction, **1** (2011), 80-85.

[7] I. A. Garkina, A. M. Danilov, Experience in the development of composite materials: some aspects of mathematical modeling, Proceedings of the universities. Construction, **8** (2013), 28-33.

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