IOP Conf. Series: Materials Science and Engineering **245** (2017) 062014 doi:10.1088/1757-899X/245/6/062014

Mathematical Methods of System Analysis in Construction Materials

Irina Garkina[1], **Alexander Danilov**[1]

[1]Penza State University of Architecture and Construction, Herman Titov Street, 28, Penza, 440028 Russia

i.a.naum@mail.ru

Abstract. System attributes of construction materials are defined: complexity of an object, integrity of set of elements, existence of essential, stable relations between elements defining integrative properties of system, existence of structure, etc. On the basis of cognitive modelling (intensive and extensive properties; the operating parameters) materials (as difficult systems) and creation of the cognitive map the hierarchical modular structure of criteria of quality is under construction. It actually is a basis for preparation of the specification on development of material (the required organization and properties). Proceeding from a modern paradigm (model of statement of problems and their decisions) of development of materials, levels and modules are specified in structure of material. It when using the principles of the system analysis allows to considered technological process as the difficult system consisting of elements of the distinguished specification level: from atomic before separate process. Each element of system depending on an effective objective is considered as separate system with more detailed levels of decomposition. Among them, semantic and qualitative analyses of an object (are considered a research objective, decomposition levels, separate elements and communications between them come to light). Further formalization of the available knowledge in the form of mathematical models (structural identification) is carried out; communications between input and output parameters (parametrical identification) are defined. Hierarchical structures of criteria of quality are under construction for each allocated level. On her the relevant hierarchical structures of system (material) are under construction. Regularities of structurization and formation of properties, generally are considered at the levels from micro to a macrostructure. The mathematical model of material is represented as set of the models corresponding to private criteria by which separate modules and their levels (the mathematical description, a decision algorithm) are defined. Adequacy is established (compliance of results of modelling to experimental data; is defined by the level of knowledge of process and validity of the accepted assumptions). The global criterion of quality of material is considered as a set of private criteria (properties). Synthesis of material is carried out on the basis of one-criteria optimization on each of the chosen private criteria. Results of one-criteria optimization are used at multicriteria optimization. The methods of developing materials as single-purpose, multi-purpose, including contradictory, systems are indicated. The scheme of synthesis of composite materials as difficult systems is developed. The specified system approach effectively was used in case of synthesis of composite materials with special properties.

1. Introduction

The theoretical basis of design of complex technical systems (including composite materials) is the creation and study of the most common ways to describe their functioning laws, methods of analysis and synthesis, including the behaviour of large collections of interrelated processes, elements and objects. In some cases, after the formalization and mathematical modelling of problem of system design is reduced to the determination of the global extremum of a function of many variables under restrictions. In the system study [1] are defined conditions under which it is possible execution by system of its tasks to achieve well-defined goals. It is assumed the possibility of decomposition (subdivision) system on relatively independent elements (subsystems) with description of significant structural and functional connections between them (specified inputs and outputs). Then the design will be to find the optimal settings based on multifunctionality and interconnections of subsystems (in terms of execution by the system of its functional purpose).

At each level of the hierarchy the optimal parameters of the system are determined based on mathematical modelling of the system; used quality criteria and their formalization must allow to carry out an objective assessment of the design results. Naturally, the system design is iterative and comprises a number of stages (feasibility study, preliminary design, technical design, etc.); at each subsequent stage using previous results.

System design of composite materials begins with the cognitive modelling (creating a directed graph) and build of hierarchical structure of the quality criteria. It becomes possible to determine the structure of a composite based on the formalization of inter-element links. The composite material is naturally represented in the form of a complex system with corresponding system attributes. Multicriteria and contradictory necessitate ranking quality criteria. Based on the specified accuracy of the simulation is determined the dimension of the criterion space; at each level is set kind of a given region of the factor space.

2. Materials as complex systems

Construction materials have the appropriate system attributes and they can be considered as a system[2,3]. Easily detected internal contradictions and paradoxical in the study of building materials as systems. The paradox of the integrity lies in the fact that the full description of the construction material is possible only with the "integrity" of its splitting apart (in the description of a certain integrity); knowledge as a building material integrity is impossible without analyzing its parts. With regard to the paradox of hierarchy, a description of the building material as the system is only possible if its description as part of the super-system (broader system) and back again, the description of the building material as a super-system element is possible only with the description of the actual building material.

There are two ways of decomposition of integrated system the «Building material». In the first method, after the breaking of an integrated system elements are obtained parts, which do not bear the holistic properties of the original system. Thus, when designing concrete (system) natural to the system partition on the individual components. However, this view does not allow with the necessary certainty to predict properties of concrete on the basis of studying the properties of the components (elements). This is also true for the decomposition of the material on the basis macro- and microstructure in polystructural theory (V.Solomatov). The second method involves the allocation of such parts (elementary education), which preserves the integrity of the specific form of the properties of the material ("holistic" partition). Thus, the material properties of the sample (elementary education) are determined by the properties of the components and the integrative properties of the entire system (material).

Without a holistic system approach it is impossible to study the material for the purpose of forecasting the possibility of its practical use. However, even the integrative property of system (as part of the structure) can be qualitatively examined outside the system (for example, surface wettability filler determined in a separate experiment). The results can serve as a qualitative description of structure formation process, but does not allow a complete description of the entire system.

The difference between the composite materials and of the mechanical mixture of the components (the properties of which are defined as the sum of the properties of the components) is the presence of

IOP Conf. Series: Materials Science and Engineering **245** (2017) 062014 doi:10.1088/1757-899X/245/6/062014

the phase boundary (determines the intensity of the processes of structuring and properties of the material (system)). At the phase boundary is formed by the contact layer: it provides traction components (adhesive strength, a new integrative properties that do not have the elements included in the system). Combining of the components at the phase boundary form a layers with altered properties. They influence on the properties the system which are different from the characteristics of components (for example, processes of curing cement in bulk and in thin layers at the phase boundary are different). As see, at the study of building materials have the paradox of integrity.

On the one hand, assessment and analysis of building materials can be made only on the basis of consideration of the material as an integrated and unified system; on the other hand - impossible to study the material without analysing its parts. That is why the study of the structure and properties of the material should be made on the basis the study of elements and of inter-element links while maintaining the integrity of the system (such as study kinetic processes of the formation of physical and mechanical characteristics of the material [3]). The quality of building materials is estimated taking into consideration their place as an element in the hierarchical structure of an integrated super system. Criteria of subsystem quality must be part of criteria quality of system (defined by integrative properties).

A complex system is divided into subsystems of different nature (decomposition of the system); are determined inter-element connections and relationships that give integrity. There is another way of extracting a system: description of individual aspects of the object not a whole object). Here, each system in one and the same object (building material) expresses only a certain facet of his nature. This use of the concept of the system allows a thorough and integrally study different aspects or facets of a single object (such as surface phenomena: wetting, capillary processes, etc.). Note, in many cases, a change in any element of the system has an effect on other components and it leads to a change in the whole system. Therefore, it is often impossible to produce of the building material decomposition (as a whole system) into individual components without loss of integrative properties.

The preliminary analysis of material is carried out on the basis of his representation as semistructured system with a set of the contradictory purposes and criteria. The qualitative analysis of materials as systems is made on the basis of creation of the cognitive map with the indication of relationships of cause and effect (including, on the basis of studying of results of interaction of structure-forming elements and mechanisms of flokulyation). The cognitive map allows to establish elementary prescription values (quantity, a specific surface, the chemical composition, etc.) for management of material manufacturing techniques. Naturally, it is always necessary to monitor the possible admission of some communications in the developed cognitive map by which in essence and the considered property of material (wrong representation of relationships of cause and effect) is defined.

By way of illustration in fig. 1 the hierarchical structure of criteria of efficiency of a radiation protective composite developed on the basis of cognitive modelling is given.

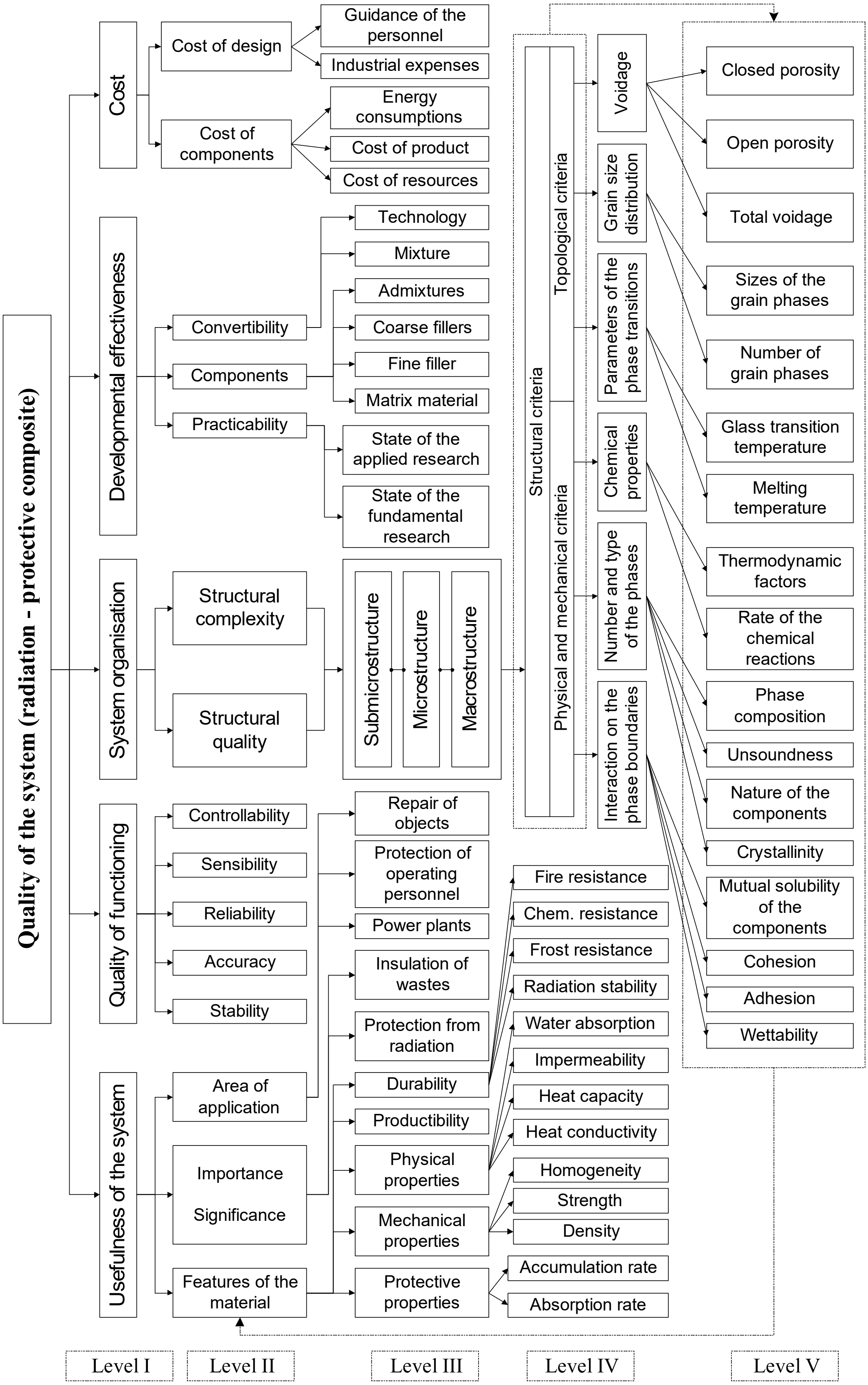

Fig. 1. Hierarchical structure of efficiency criteria

IOP Conf. Series: Materials Science and Engineering **245** (2017) 062014 doi:10.1088/1757-899X/245/6/062014

3. Scheme of synthesis of composite material

Algorithm (Fig. 2) is based on the main provisions of the optimality of systems:

- the system is optimized as a whole as a single object with the specified intended purpose;
- system consisting of optimal components (subsystems), it is not necessarily optimal (this does not mean that optimization by parts has no meaning);
- optimization is carried out by quantitative criteria, in general, the vector criterion (mathematically reflects the purpose of optimization, the absence of such a criterion, as a rule, shows a fuzzy understanding of the researcher of the task before them);
- optimality of system is relative: the optimization is carried out under conditions of quantitative restrictions on the optimized parameters.

Here are some comments on the choice of criteria for each level of design problems. The parameters and characteristics of each element of the subsystem to be chosen from the condition to ensure high efficiency of the whole system (organismic principle; subsystems quality criteria should not contradict the criterion of the quality of the entire system): if at all levels of the elements and subsystems are optimal (according to the criteria relevant systems of higher level), then the entire system will be optimal.In other words, at every stage of the design can be used its own criteria evaluation subsystems, but they must be consistent with the overall design goals.

As you can see, the most important part of the system design methodology is mathematical modelling of design problems: construction of the model and its research, the search for feasible solutions model sensitivity analysis and optimization. Construction of the model is a quantitative description of the characteristics (properties) from the selected system parameters (properties and parameters can be dependent on each other). The terms «parameters» and «characteristics» in the hierarchical system are relative: the top-level parameters for the lower level are the characteristics. If the current level of knowledge (the modern paradigm) cannot determine the relationship between the characteristics and parameters, they are excluded from the formal description of the model (to completion the required number of additional studies).

System design [4] is usually a modular; dismemberment system on modules based on the obtained hierarchy of quality criteria is ambiguous and contains elements of subjectivism (in particular, absorption by composite of ionizing radiation can be achieved by changing the ingredients and particle sizes, etc.).

Modular representation of complex systems is not always conducive to the understanding of how to achieve the ultimate goal of the system, depending on the physical state of the modules. Type of modules to a large extent determined by the partitions of the system, based on the different types of physical processes occurring in the system. Under no partition cannot reach the aggregation of modules presented in decomposition, in the real integrated system (identification is possible only with the specified accuracy, but not absolute).

Used models are often non-stationary; may depend on ambient parameters (summer, winter, etc.); at a small interval of time can be regarded as stationary. Optimization of the model parameters are based on the parametric identification, the development of a computational algorithm, including and the intermediate levels of the hierarchy.

Checking on the adequacy of the model by solving a test problem; eliminates the possibility of errors. If possible, simplified mathematical description and reduces the number of control parameters. In fact, optimization and is the final stage of system design.

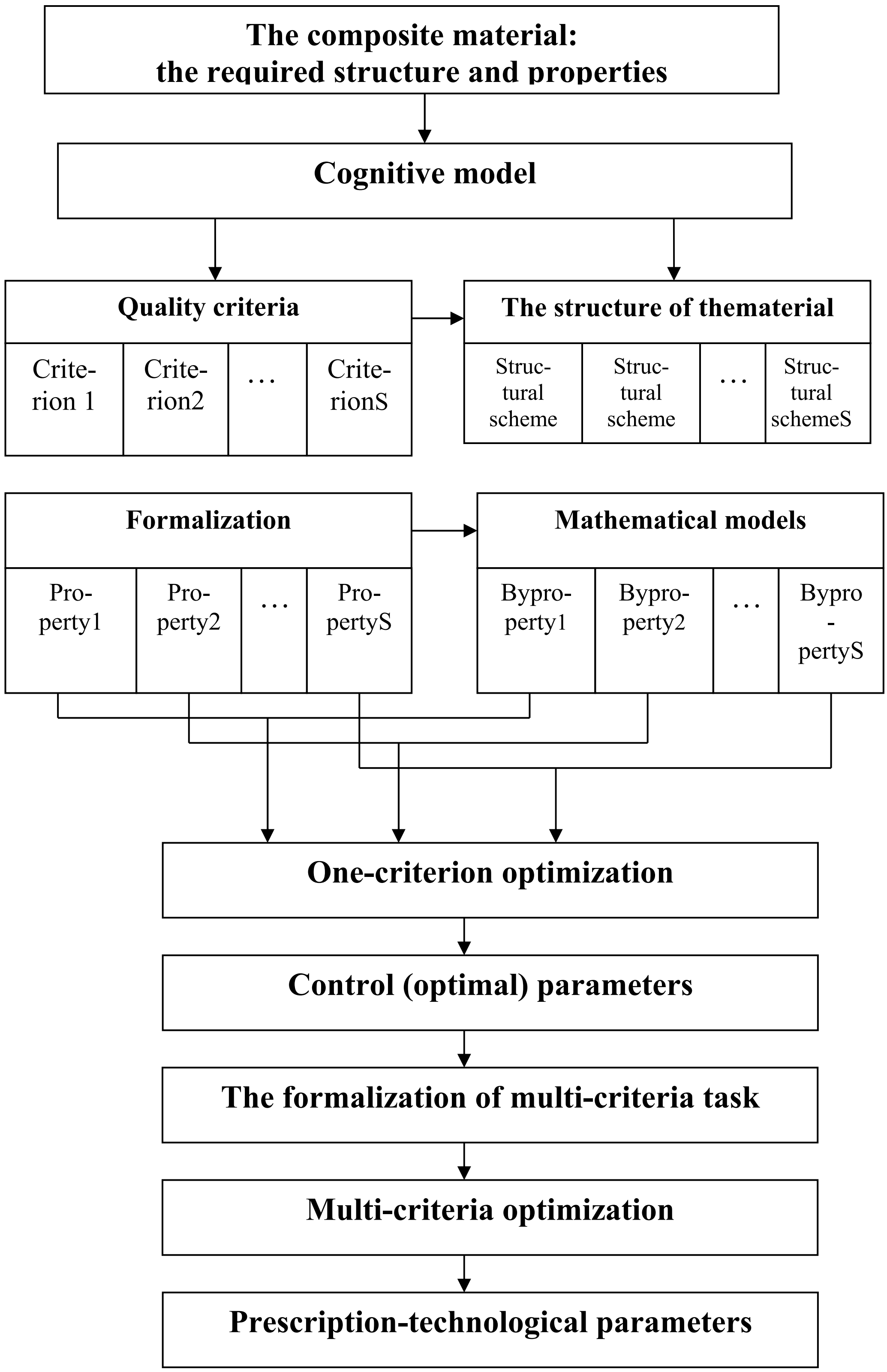

Figure 2. Scheme of synthesis of composite material

4. Mathematical modelling

In the design of a number of building materials are used the kinetic processes of formation of their physical and mechanical properties: strength development; changes in the modulus of elasticity; the kinetics of contraction and shrinkage; an increase of internal stresses; evolution of heat; kinetics of water absorption, water resistance and chemical resistance [5, 6]. It turned out, these processes are formally described by kinetic equations (identical): as the solution of the Cauchy problem for ordinary differential equation.

In homogeneous systems manifestation of the individual structural elements of the system is suppressed by global processes or the impact of these elements on the system slightly. For them, the kinetic processes are presented as a solution to of the Cauchy problem

$$\frac{dx}{dt} = -k(x - x_m);\ x(0) = 0, \tag{1}$$

x_m - the desired operational characteristics of the considered value. For the construction of composite materials (heterogeneous, disperse systems) this assumption is generally unacceptable. Kinetic processes $x(t)$ in heterogeneous systems is have inflection points: in homogeneous systems - are missing.

In heterogeneous systems with a single inflection point of the main characteristics of the material (is considered deviations $z = x - x_m$ from the equilibrium state) are the solution of differential equations

$$\ddot{z} + 2n\dot{z} + \omega_0^2 z = 0, (n > 0). \tag{2}$$

In the case $n^2 - \omega_0^2 > 0$ of kinetic process has the form

$$z = c_1 e^{-\lambda_1 t} + c_2 e^{-\lambda_2 t}, \tag{3}$$

$k_{1,2} = -\lambda_{1,2} = -\left(n \pm \sqrt{n^2 - \omega_0^2}\right), \lambda_1 > \lambda_2 > 0$ – the roots of the characteristic equation $k^2 + 2nk + \omega_0^2 = 0$.

When the initial conditions $z(0) = -x_m; \dot{z}(0) = 0$ is true:

$$x = \frac{x_m}{\lambda_1 - \lambda_2}\left(\lambda_2 e^{-\lambda_1 t} + \lambda_1 e^{-\lambda_2 t}\right) + x_m; \tag{4}$$

the abscissa of the inflection point

$$t_n = \frac{1}{\lambda_1 - \lambda_2}\ln\frac{\lambda_1}{\lambda_2}. \tag{5}$$

In the case of multiple roots

$$x = x_m\left[1 - (1 + nt)e^{-nt}\right];\ n = \omega_0; \tag{6}$$

$M_n\left(\frac{1}{n}; x_m\left(1 - \frac{2}{e}\right)\right)$ - inflection point.

For some processes, changes in physical and mechanical properties of building materials (in particular, changes in the internal pressure and heat; Fig. 1), the abscissa of points M_n and M_m (inflection and maximum), respectively, are defined as:

$$t_n = \frac{1}{\lambda_1 - \lambda_2}\ln\left[\left(-\frac{c_1}{c_2}\right)\left(\frac{\lambda_1}{\lambda_2}\right)^2\right];\ t_m = \frac{1}{\lambda_1 - \lambda_2}\ln\left[\left(-\frac{c_1}{c_2}\right)\left(\frac{\lambda_1}{\lambda_2}\right)\right];\ \left(\delta = t_n - t_m = \frac{1}{\lambda_1 - \lambda_2}\ln\frac{\lambda_1}{\lambda_2}\right). \tag{7}$$

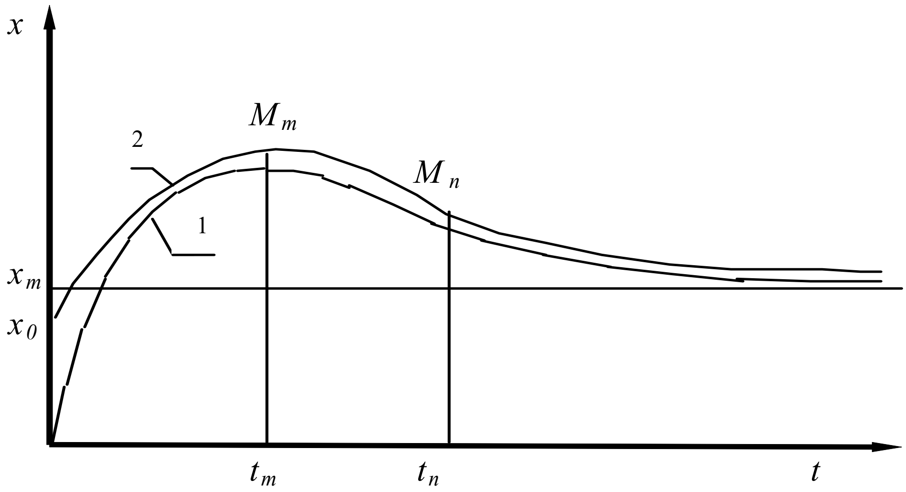

Figure 3. Typical types of kinetic dependences

Curve 1 (special case of curve 2; $x_0 = 0$) is a solution of the Cauchy problem

$$\ddot{z} + 2n\dot{z} + \omega_0^2 z = 0;\ z = x - x_m;\ z(0) = -x_m;\ \dot{z}(0) = x(0) \tag{8}$$

and has the form:

$$x = c_1 e^{-\lambda_1 t} + c_2 e^{-\lambda_2 t} + x_m(\lambda_1 > \lambda_2). \tag{9}$$

Parametric Identification of kinetic processes of this type is easily accomplished consistent definition λ2, δ, λ1, $\left(-\frac{c_1}{c_2}\right)$, $\dot{x}_0$ (so, for epoxy composite value of $\dot{x}_0$ determines the initial rate of polymerization).

Similarly, the identification process is carried out parametric type 2 (e.g. self-heating of epoxy composites):

$$\ddot{z} + 2n\dot{z} + \omega_0^2 = 0, \quad (z = x - x_m; \quad x = z + x_m) \tag{10}$$

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

Definition $\dot{x}_0$ is carried out using the known values λ_1, λ_2, x_m, $\left(-\frac{c_1}{c_2}\right)$, x_0.

Changes in the characteristics of processes depending on parameters of the dynamic model is shown in Fig. 3. Refinement of the dynamic model parameters was performed using the specified dependencies.

Thus, we propose a method of analytical design of the building materials based on the description of the kinetics of formation of the basic physical and mechanical properties of composite materials. As a generalized model is recommended to use a solution of the Cauchy problem for an ordinary fourth-order differential equation:

$$z^{(4)} + a_1 z^{(3)} + a_2 z^{(2)} + a_3 z^{(1)} + a_4 z = 0, \tag{11}$$

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

5. Conclusions

The annex to the development of composite materials proposed methodological principles of systems engineering of complex systems.

The structure of the composite material as a complex system is determined.

IOP Conf. Series: Materials Science and Engineering **245** (2017) 062014 doi:10.1088/1757-899X/245/6/062014

We present the implementation of the principle of modular design of complex systems.
Realization of system approach to development of materials as difficult systems in parameters of kinetic processes of formation of each of properties (private models) of composites is given.

References

[1] A. Danilov, I. Garkina, "Systems approach to the modelling and synthesis of building materials, "*Contemporary Engineering Sciences*, vol. 8, no. 5, pp. 219-225, 2015.
[2] I.A. Garkina, A.M. Danilov and V.P. Selyaev, "Materials as complex systems, " *Journal of Engineering and Applied Sciences,* vol. 11(11), pp. 2461-2464, 2016.
[3] I.Garkina, A. Danilov and Y. Skachkov, "Modelling of Building Materials as Complex Systems, "*Key Engineering Materials*, vol. 730, pp. 412-417, 2017.
[4] I.Garkina, A. Danilov**,** "Analytical design of building materials, "*Journal of Basic and Applied Research International*, vol.18, Issue 2, pp. 95-99, 2016.
[5] I.A.Garkina, "Modelling of kinetic processes in composite materials," *Contemporary Engineering Sciences*, vol. 8, no. 10, pp.421-425, 2015.
[6] I. Garkina, A. Danilov, "Parametric identification and optimization of properties of building materials as complex systems, " *J. Ponte*, vol. 73, issue 2, pp.119-125, 2017.