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# Modeling of Kinetic Processes in Composite Materials

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**Abstract**

Presented mathematical models of the kinetic processes in the class of ordinary differential equations. Given root locus, allowing to predict the structure and properties of materials.

**Keywords**: composite materials, modeling, kinetic processes, management of properties

## Introduction

Control of material properties is directly related to the mathematical modeling of kinetic processes of formation of physical and mechanical characteristics. It is necessary to define a set of numerical parameters, on which you can set the quality of kinetic processes and implement their optimization. Finally, for the objective estimation of the quality of the material (for each of the properties) should be designed functional quality. All of this will solve the problem of one-criterion optimization of material properties. The multiobjective optimization can be carried out using any of the known methods of overcoming uncertainties purposes. Below consistently are resolved the problems.

## Generalized kinetic model of the process

When designing composites [1 ... 4] to obtain needed properties is used of the generalized kinetic model of the process $x(t)$, which is a solution of the Cauchy problem:

$$z^{(4)} + a_1 z^{(3)} + a_2 z^{(2)} + a_3 z^{(1)} + a_4 z = 0\,,$$
$$z = x - x_m; \quad x(0) = x_0,\ \dot{x}(0) = \dot{x}_0,\ \ddot{x}(0) = \ddot{x}_0,\ \dddot{x}(0) = \dddot{x}_0;$$

$x_0, \dot{x}_0, \ddot{x}_0, \dddot{x}_0$ determined by the required views of the kinetic process and the defined steady-state value $x_m$ of the characteristic of the material.

For a second-order model; $\lambda_1 = \lambda_1(\omega_0, n)$, $\lambda_2 = \lambda_2(\omega_0, n)$ - roots of the characteristic polynomial.

The level curves $\lambda_2(\omega_0, n)$ defined by the equation (Figure 1a)

$$n - \sqrt{n^2 - \omega_0^2} = \lambda_2^{(0)} = \text{const}; \quad \sqrt{n^2 - \omega_0^2} = n - \lambda_2^{(0)}; \quad n = \frac{\lambda_2^{(0)}}{2} + \frac{1}{2\lambda_2^{(0)}}\omega_0^2\,.$$

Thus, when moving along a parabola $n = \frac{\lambda_2^{(0)}}{2} + \frac{1}{2\lambda_2^{(0)}}\omega_0^2$ to $\lambda_2$ is constant and equal $\lambda_2^{(0)}$.

Consider two line level $\lambda_2 = \lambda_2^{(1)} > 0$, $\lambda_2 = \lambda_2^{(2)} > 0$, $\lambda_2^{(2)} > \lambda_2^{(1)}$. The abscissa of the intersection point determined by the equation

$$\frac{\lambda_2^{(1)}}{2} + \frac{1}{\lambda_2^{(1)}}\omega_0^2 = \frac{\lambda_2^{(2)}}{2} + \frac{1}{2\lambda_2^{(2)}}\omega_0^2; \quad \omega_0^n = \sqrt{\lambda_2^{(1)} \cdot \lambda_2^{(2)}}.$$

If $\omega_0 = \sqrt{\lambda_2^{(1)} \cdot \lambda_2^{(2)}}$, the line-level $n = \frac{\lambda_2^{(2)}}{2} + \frac{1}{2\lambda_2^{(2)}}\omega_0^2$ passes above the level $n = \frac{\lambda_2^{(1)}}{2} + \frac{1}{2\lambda_2^{(1)}}\omega_0^2$, and for the values $\omega_0 > \sqrt{\lambda_2^{(1)} \cdot \lambda_2^{(2)}}$ the first line passes below the second level (Figure 1b).

Direction of steepest growth $\lambda_2$ coincides with the direction of $\mathbf{grad}\lambda_2(\omega_0, n)$ and perpendicular to the direction of the tangent to the level curve at a given point.

Similarly, we define the level curves $\lambda_1(\omega_0, n)$:

$$n = \frac{\lambda_1^{(0)}}{2} + \frac{1}{\lambda_1^{(0)}}\omega_0^2\,.$$

Line level $r = r_0 = const$ ($r = r(\omega_0, n)$) is determined from the condition

$$r = \left(\xi + \sqrt{\xi^2 - 1}\right)^2 = \left(\frac{n}{\omega_0} + \sqrt{\left(\frac{n}{\omega_0}\right)^2 - 1}\right)^2 = r_0\,.$$

Where the required level line: $n = \frac{1 + r_0}{2 \cdot \sqrt{r_0}} \cdot \omega_0 \quad (\omega_0,\ n > 0,\ r > 1)$.

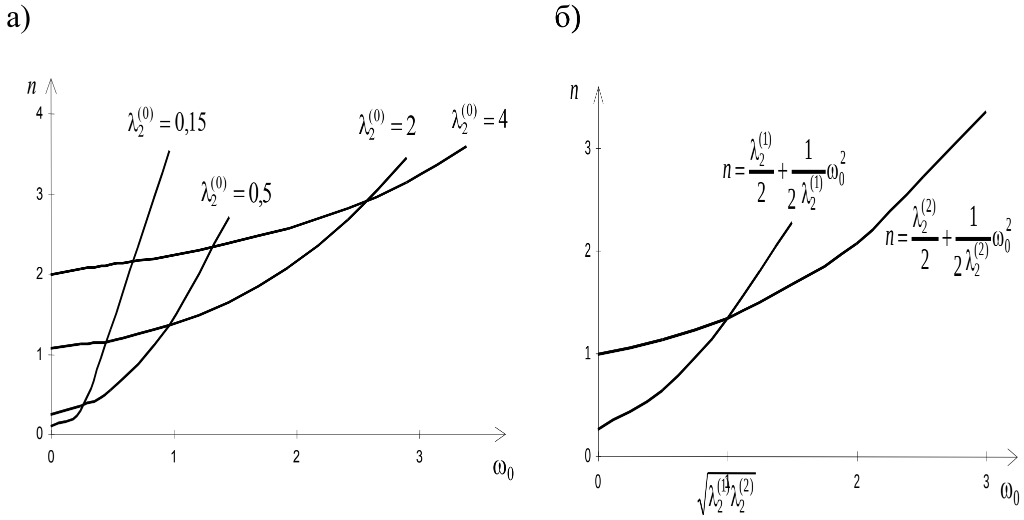


Figure 1. Location of the level lines: а) - $\lambda_2^{(0)} = \mathbf{const}$; б) – mutual.

If upon receipt of the material chosen direction, ensures that the condition $\xi = const$ then the roots $\lambda_1, \lambda_2$ (Figure 2) and the variable *r* become functions of only one variable $\omega_0$:

$$\frac{d\lambda_1}{d\omega_0} = \xi + \sqrt{\xi^2 - 1};$$

$$\frac{d\lambda_2}{d\omega_0} = \xi - \sqrt{\xi^2 - 1},$$

that is, the rate of change of the roots along the line $\xi = const$ constant when changing $\omega_0$; $r = \left(\frac{d\lambda_1}{d\omega_0}\right)^2$.

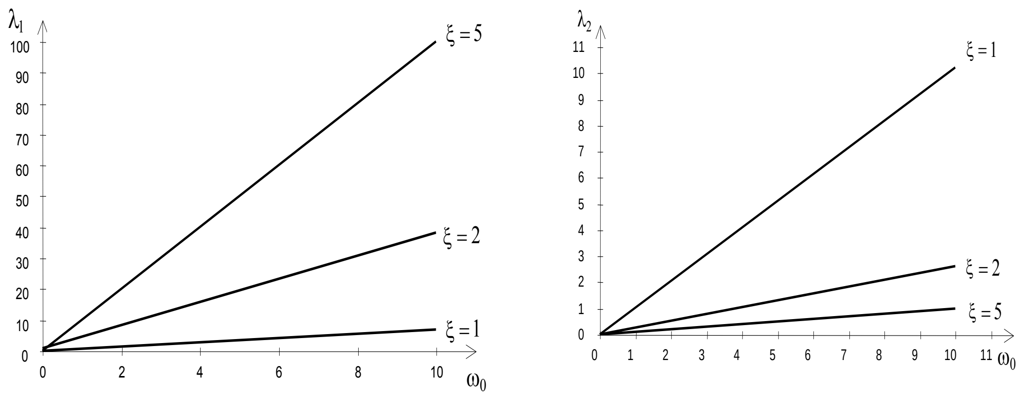


Figure 2. Depending $\lambda_1 = \lambda_1(\omega_0, \xi)$ and $\lambda_2 = \lambda_2(\omega_0, \xi)$

When changing ξ 10 times from 1 to 10 $\lambda_2$ change rate decreases 20 times, and the rate of change $\lambda_1$ increases by 20 times; *r* is increased by 400 times.

## Control of material properties

Let the reference point $M_0(\xi, \omega_0)$ is between the lines $\xi = \xi_1$ and $\xi = \xi_2$, $1 < \xi_1 < \xi_2$ (Figure 3,4).

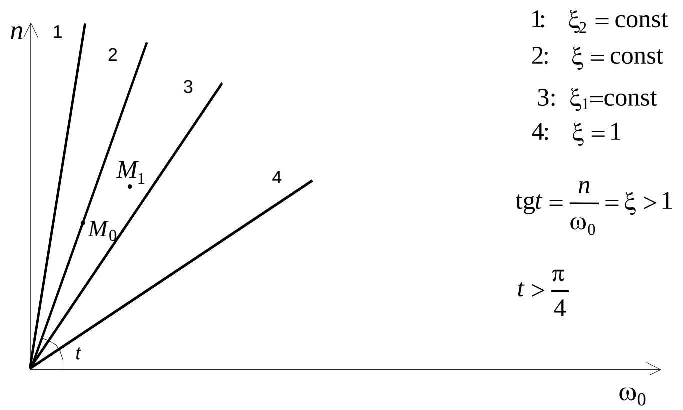


Figure 3. Location $M_1$ relative level lines $\xi = const$

Quality of the material for each of the properties individually may be evaluated in accordance with the functional quality of the form [2]:

$$\Phi(S) = f\lambda_m + a\frac{1}{\lambda_m} + br + c\frac{1}{r},$$

$$\lambda_m = \min_i \{\lambda_i\}, \quad r = \max_i \left\{\frac{\lambda_i}{\lambda_m}\right\},$$

where $(-\lambda_i)$ – the roots of the characteristic polynomial, $\lambda_1 > 0$, $i = \overline{1,k}$; $f, a, b, c$ – determine the significance of the terms in the functional. In particular, for a second order model

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

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

Material quality is higher, the less $\Phi(S)$. Let the boundary of the system is determined by the class level line $\Phi(\xi, \omega_0) = d$. Then, to improve the grade point $M_1$ system should take direction $\overline{M_0 N}$. While $M_1$ can be both left and right of the line $\xi = const$ and $\Phi = const$.

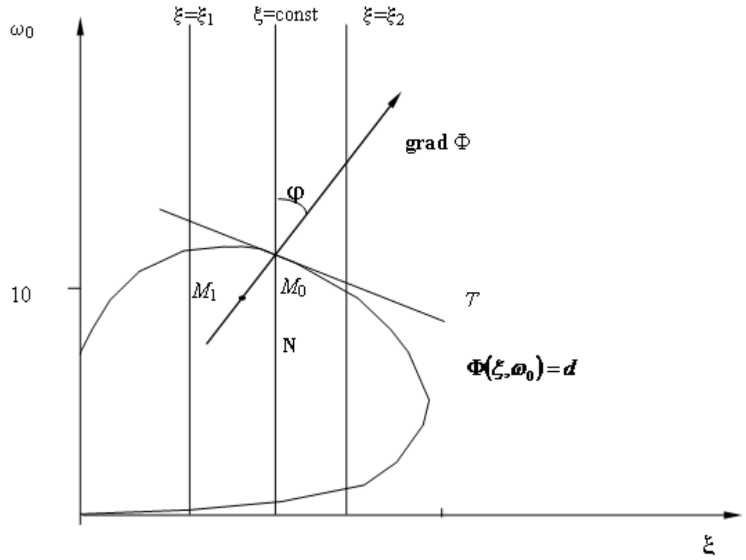


Figure 4. The mutual arrangement of regions in the plane of equal ranking $\xi 0 \omega_0$ and level lines $\xi = const$

## Conclusion

1. Is given the generalized kinetic model of the formation of physical and mechanical properties of the composites.
2. Is proposed the technique of one-criterion optimization of each of the properties individually on the basis of the functional of quality.
3. The effectiveness of the proposed method was confirmed in the development of chemically resistant sulfur composites, epoxy composites for protection against radiation and others.

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