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OPTIMIZATION OF THE MICROSTRUCTURE OF COMPOSITE MATERIALS TAKING INTO ACCOUNT THE CONSTRAINTS ON THEIR PROPERTIES

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Abstract. In the paper, an approach to optimizing the microstructure of composite materials under given restrictions on its properties has been put forward. The approach is based on the application of conditional optimization methods. The effective elastic properties were determined using the finite element homogenization procedure. As an example, the fiber-reinforced composite with ball-shaped inclusions was optimized taking into account the limitations on its thermal conductivity and elastic modulus at macro level using artificial intellect methods.

Keywords: composite material, homogenization, finite element method, conditional optimization, artificial intellect method

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ОПТИМИЗАЦИЯ МИКРОСТРУКТУРЫ КОМПОЗИЦИОННЫХ МАТЕРИАЛОВ С УЧЕТОМ ОГРАНИЧЕНИЙ НА ИХ СВОЙСТВА

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Аннотация. Предложен подход к оптимизации микроструктуры композиционных материалов с учетом накладываемых ограничений на их свойства. Подход основан на применении методов условной оптимизации. Определение эффективных упругих свойств осуществлялось с помощью метода конечно-элементной гомогенизации. Методами искусственного интеллекта выполнена оптимизация дисперсно-армированного композита с шарообразными включениями с ограничениями на коэффициент теплопроводности и модуль упругости материала на макроуровне.

Ключевые слова: композиционный материал, гомогенизация, метод конечных элементов, условная оптимизация, метод искусственного интеллекта

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Introduction

Composite materials have found applications in diverse fields. A wide variety of individual components of modern composites used industrially, as well as their possible combinations, augmented by extensive technologies to fabricate structures with diverse topologies, allow to produce materials with unique properties, often surpassing those of traditional materials. A richly varied selection of components, their volume ratios and composite material structures make it possible to further research the production of components with optimal properties.

An example is the development of novel materials for thermal protection of aerospace vehicles, which also need to have high thermal strength, low thermal conductivity and density. Another striking example are electrical insulating composites. Dielectric materials for electrical insulation systems in modern high-voltage electrical machines need to combine properties that are rather mutually exclusive, i.e., high insulation capability and high thermal conductivity.

A popular technique in modern industry is introducing dispersed particles with high thermal conductivity, such as aluminum oxide (Al_2O_3) or boron nitride (BN), into the polymer binder. Thus, the problem of conditional optimization can be formulated as selecting the concentration of dispersed inclusions ensuring maximum thermal conductivity of the composite with constraints on its electrical insulating properties.

The goal of this study is to develop methods for designing the optimal microstructure of composite materials, taking into account the constraints imposed on their properties.

Determination of effective properties of composite materials

Laboratory studies provide the most reliable data on the mechanical, thermophysical and diffusion properties, electrical conductivity, and other characteristics of composite materials. However, there is an almost unlimited number of possible combinations of components, while tests are expensive, so analytical or numerical estimates of the effective properties of composites need to be introduced.

An analytical estimate of elastic properties can be obtained based on the simplest estimates given by Reuss [4] or Voigt [5]; some approaches are based on solutions of the Eshelby problem [6–8] for an ellipsoidal inclusion in an infinite homogeneous elastic medium. Variational estimates of elastic properties were obtained by Hashin and Shtrikman [9–11]; asymptotic averaging methods have also gained much popularity [1, 11–13].

The thermal conductivity and diffusion properties of materials can be estimated by approaches proposed by Maxwell [14], Lord Rayleigh [15], Bruggerman [16], Mori and Tanaka [7], as well as other researchers [16–23]. The main disadvantage of analytical estimates is their low accuracy for composites with complex topology.

One of the most common methods for determining the effective properties is finite element (FE) homogenization [8, 24, 25]. This method is based on the concept of a representative volume element (RVE) containing all statistical information about the distribution and morphology of inhomogeneities in the material. The RVE of the material can be introduced assuming a statically homogeneous distribution of material characteristics and separable scales of inhomogeneities. Fig. 1 shows examples of RVEs for various types of polymer composite materials.

Finite element (FE) modeling of deformation, heat transfer, diffusion and other processes in an RVE allows to solve two main problems:

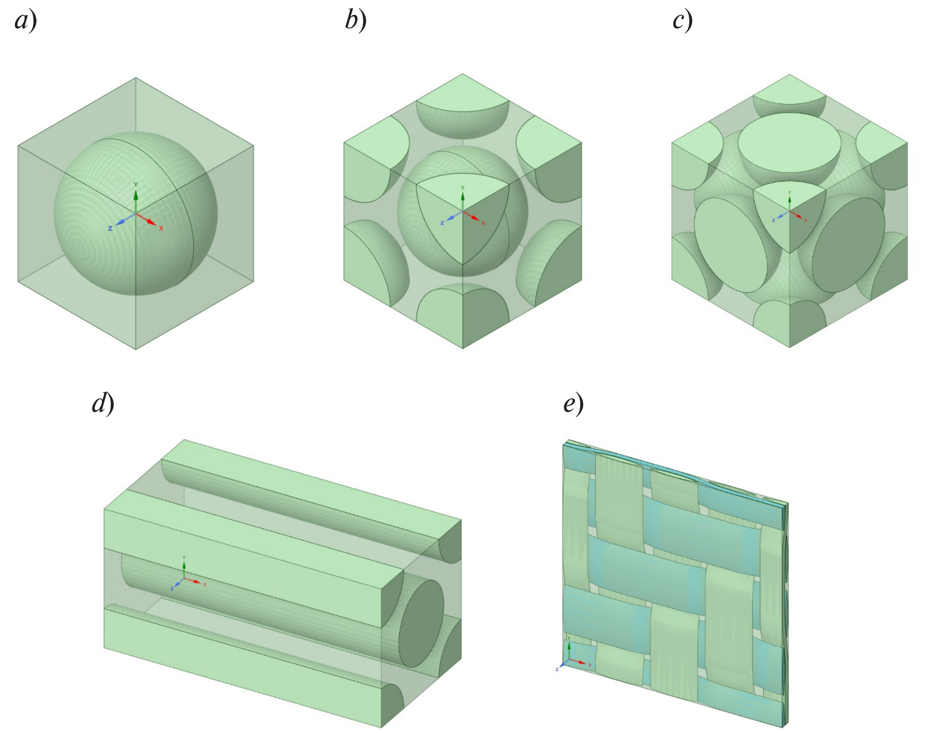

Fig. 1. Examples of RVEs for various types of polymer composite materials: dispersion-strengthened (*a*–*c*), unidirectional fiber (*d*) and woven (*e*)

determine the effective properties of a composite RVE (homogenization problem);

obtain the extreme values of the stress fields in a heterogeneous RVE for subsequent strength analysis (heterogenization problem).

The PANTOCRATOR software package [26] used for the calculations is based on the virtual work principle adopted for solving boundary value problems of elasticity theory:

$$\int_V \boldsymbol{\sigma} \cdot\cdot \delta\boldsymbol{\varepsilon} dV = \int_V \mathbf{f}_V \cdot \delta\mathbf{u} dV + \int_{S_\sigma} \mathbf{f}_S \cdot \delta\mathbf{u} dS, \tag{1}$$

where $\delta\boldsymbol{\varepsilon} = (\nabla\delta\mathbf{u})^S$, $\mathbf{f}_V$, $\mathbf{f}_S$ are the given body and surface forces.

Eq. (1) can be used to obtain the equilibrium equations $\nabla \cdot \sigma + \mathbf{f}_V = 0$ in the volume and static (force) boundary conditions $\mathbf{n} \cdot \boldsymbol{\sigma}|_{S_\sigma} = \mathbf{f}_S$.

Steady-state problems of thermal conductivity are solved in the following variational statement:

$$\int_V \left[\nabla \cdot \left(\mathbf{K} \cdot \nabla T\right) + q_v\right] \delta T dV =$$
$$= \int_{S_{II}} \left[n \cdot \left(\mathbf{K} \cdot \nabla T\right) + q_S\right] \delta T dS + \int_{S_{III}} \left[n \cdot \left(\mathbf{K} \cdot \nabla T\right) + a_S\left(T - T_\infty\right)\right] \delta T dS, \tag{2}$$

where q_v, q_s are the volume and surface heat fluxes, respectively; $\mathbf{K}$ is the thermal conductivity tensor; S_{II}, S_{III} are the surface areas where the boundary conditions of the second (Neumann condition) and third (Cauchy condition) kind are imposed, respectively.

Eq. (2) allows to obtain the equation of thermal conductivity

$$n \cdot \left(\mathbf{K} \cdot \nabla T\right) + q_S = 0$$

and natural Neumann and Cauchy boundary conditions:

$$-n \cdot \left(\mathbf{K} \cdot \nabla T\right) = q_S, \; -n \cdot \left(\mathbf{K} \cdot \nabla T\right) = a_S\left(T - T_\infty\right).$$

The stress-strain state corresponding to the homogenized material was calculated from the strain and stress tensors averaged over an RVE, obtained in the FE solution:

$$\bar{\boldsymbol{\varepsilon}} = \frac{1}{V_{REV}} \int_{V_{REV}} \boldsymbol{\varepsilon}\, dV, \tag{3}$$

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V_{REV}} \int_{REV} \boldsymbol{\sigma}\, dV. \tag{4}$$

The effective properties of the homogenized material were assumed to correspond to an orthotropic elastic material, for which Hooke's law can be written as follows:

$$\bar{\boldsymbol{\varepsilon}} = {}^4\bar{\mathbf{C}} \cdot\cdot\, \bar{\boldsymbol{\sigma}}, \tag{5}$$

where ${}^4\bar{\mathbf{C}}$ is the 4th-rank elastic compliance tensor, taking the following form for an orthotropic material (along the principal orthotropic directions):

$$\left[\bar{\mathbf{C}}\right] = \begin{bmatrix} \frac{1}{\bar{E}_1} & -\frac{\bar{\nu}_{21}}{\bar{E}_2} & -\frac{\bar{\nu}_{31}}{\bar{E}_3} & 0 & 0 & 0 \\ -\frac{\bar{\nu}_{12}}{\bar{E}_1} & \frac{1}{\bar{E}_2} & -\frac{\bar{\nu}_{32}}{\bar{E}_3} & 0 & 0 & 0 \\ -\frac{\bar{\nu}_{13}}{\bar{E}_1} & -\frac{\bar{\nu}_{23}}{\bar{E}_2} & \frac{1}{\bar{E}_3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\bar{G}_{12}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{\bar{G}_{23}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{\bar{G}_{31}} \end{bmatrix}, \tag{6}$$

where $\frac{\bar{\nu}_{12}}{\bar{E}_1} = \frac{\bar{\nu}_{21}}{\bar{E}_2}$, $\frac{\bar{\nu}_{13}}{\bar{E}_1} = \frac{\bar{\nu}_{31}}{\bar{E}_3}$, $\frac{\bar{\nu}_{23}}{\bar{E}_2} = \frac{\bar{\nu}_{32}}{\bar{E}_3}$.

The effective thermal conductivities are determined from Fourier's law, written as follows for a homogenized material:

$$\bar{\mathbf{q}} = -\bar{\mathbf{K}} \cdot \overline{\nabla T}, \tag{7}$$

where $\bar{\mathbf{q}} = -\frac{1}{V_{REV}} \int_{V_{REV}} \mathbf{K} \cdot \nabla T dV$ is the heat flux vector averaged over the volume; $\overline{\nabla T} = \frac{1}{V_{REV}} \int_{V_{REV}} \nabla T dV = \frac{1}{V_{REV}} \int_{S_{REV}} \mathbf{n} T dS$ is the averaged temperature gradient.

The thermal conductivity tensor $\bar{\mathbf{K}}$ for an orthotropic material has the form

$$\bar{\mathbf{K}} = \begin{bmatrix} \bar{\lambda}_1 & 0 & 0 \\ 0 & \bar{\lambda}_2 & 0 \\ 0 & 0 & \bar{\lambda}_3 \end{bmatrix}. \tag{8}$$

Three types of boundary conditions can be used to determine the effective elastic properties of a heterogeneous material:

kinematic

$$\mathbf{u}\big|_{S_u} = \bar{\boldsymbol{\varepsilon}}^* \cdot \mathbf{r}, \tag{9}$$

static

$$\mathbf{n}\cdot\boldsymbol{\sigma}\big|_{S_\sigma} = \mathbf{n}\cdot\bar{\boldsymbol{\sigma}}^* = \mathbf{f}_S, \tag{10}$$

and periodic conditions

$$\mathbf{u}\big|_{S_{u_1}} = \mathbf{u}\big|_{S_{u_2}} + \bar{\boldsymbol{\varepsilon}}^* \cdot \left(\mathbf{r}_1 - \mathbf{r}_2\right), \tag{11}$$

where $\mathbf{u}$ is the displacement vector; $\mathbf{r}$ is the radius vector; $\bar{\boldsymbol{\varepsilon}}^*$, $\bar{\boldsymbol{\sigma}}^*$ are the given constant symmetric tensors corresponding to various strain states (axial tension/compression and shear) and various stress states (axial tension/compression and shear), respectively.

It was found in [8, 27, 28] that imposing periodic conditions (11) yields satisfactory accuracy for RVEs including a smaller number (by 2–4 times) of unit cells compared to imposing boundary conditions (9), (10).

The effective thermal conductivities were found using first-kind boundary conditions (Dirichlet condition):

$$T\big|_{S_1} = T_1^*,\ T\big|_{S_2} = T_2^*, \tag{12}$$

where S_1, S_2 are the RVE surfaces where the temperature values T^*_1 and T^*_2 are set, so that $T^*_1 \neq T^*_2$.

It is assumed that the condition of ideal mechanical and thermal contact is satisfied at the interface of individual components of the composite material:

$$\mathbf{u}^{(i)} = \mathbf{u}^{(j)};\ \mathbf{n}^{(i)}\cdot\boldsymbol{\sigma}^{(i)} = \mathbf{n}^{(j)}\cdot\boldsymbol{\sigma}^{(j)}, \tag{13}$$

$$T^{(i)} = T^{(j)};\ \mathbf{n}^{(i)}\cdot\left(\mathbf{K}\cdot\nabla T^{(i)}\right) = -\mathbf{n}^{(j)}\cdot\left(\mathbf{K}\cdot\nabla T^{(j)}\right), \tag{14}$$

where the quantities with the superscript (i) correspond to one component, and the quantities with the superscript (j) correspond to the other.

Optimization problem statement

In general, a composite material consisting of a matrix and inclusions containing N different materials is considered. In the linear statement, each of the materials is characterized by elastic properties ${}^4\mathbf{C}_i$, density ρ_i, thermal conductivity $\mathbf{K}_i$ and has a volume V_i, where $i = \overline{1, N+1}$. Other characteristics can be considered similarly, such as strength, diffusion coefficient, permittivity, resistivity, etc. Each of these characteristics can be considered both as an objective function of the optimized material and as imposed constraints.

For certainty, we consider the mass minimization problem for a composite material with a given microstructure topology, with constraints on the values of Young's modulus and thermal conductivity along one of the orthotropic axes:

$$M = \sum_{i=1}^{N+1} \rho_i V_i \to \min; \tag{15}$$

$$\bar{E}_1\left(c_i\right) \geq E, \bar{K}_1\left(c_i\right) \leq K, \tag{16}$$

where $c_i = V_i/V$ are the volume fractions of the ith phase.

Such a problem can be formulated for example, for designing a cantilever beam of specific geometry with constraints on the maximum deflection or on the natural frequency, intended for mounting a thermal sensor sensor. Other optimization problems are constructed similarly.

The problem of unconditional minimization of functional (15) can be reduced to the problem of conditional minimization taking into account constraints (16) using AI methods [29, 30]. Let us briefly consider them.

Lagrange multiplier method:

$$L = \sum_{i=1}^{N+1} \rho_i c_i V + \lambda_1 \left(E - \overline{E}_1(c_i)\right) + \lambda_2 \left(\overline{K}_1(c_i) - K\right) \to \min, \quad (17)$$

where λ_1, λ_2 are Lagrange multipliers.

Penalty function method:

$$Q_k(c_i) = \sum_{i=1}^{N+1} \rho_i c_i V + r_1^k g_1 \left(E - \overline{E}_1(c_i)\right) + r_2^k g_2 \left(\overline{K}_1(c_i) - K\right) \to \min, \quad (18)$$

where r_1^k, r_2^k are coefficients of the penalty functions; $g_1\left(E - \overline{E}_1(c_i)\right)$, $g_2\left(\overline{K}_1(c_i) - K\right)$ are the penalty functions.

A distinct family of genetic optimization algorithms allows obtaining an optimal solution without a priori information about the behavior of the target function [31].

Selecting an optimization method is a fairly complex process. Thus, if the dependences of the target function and constraints on the system parameters are known, the Lagrange multiplier method allows to obtain an analytical solution to the conditional optimization problem in some cases. As for the widespread class of methods of penalty functions, applying it can result in 'valleys' appearing in the relief of the minimized potential. A wide class of problems can be solved by the Nelder—Mead method [32, 33], which does not require taking derivatives. Genetic algorithms can be considered the most universal. However, despite the variety of optimization methods, none of the algorithms guarantees finding a global extremum in an arbitrary case.

Optimization of dispersion-strengthened composite with spherical inclusions

Consider the mass minimization problem for a dispersion-strengthened composite with spherical inclusions (Fig. 1, *a*—*c*). Due to symmetry and stochastic arrangement of inclusions in the matrix, the resulting macro-properties of the material can be assumed to be isotropic with a high degree of confidence.

It is important to choose an RVE that adequately reflects the structure and properties of the given composite material. Regularized RVE models can be considered in the case of materials with randomly distributed inclusions. Otherwise, namely, for materials with a non-periodic structure, a stochastic problem should be considered with subsequent static processing of the results, which significantly increases the complexity and time-costs of determining the effective properties. It was established in [34] for the case of unidirectional fiber composites that the maximum differences between the elastic properties of the regularized model and the model with a random arrangement of reinforcing fibers do not exceed 10%.

If we assume the properties of the regularized model and the real dispersion-strengthened composite to be equivalent, the corresponding RVE should have the following properties:

the volume fraction of inclusions in the RVE should coincide with their concentrations in the real material;

the structure of the RVE should have the properties of central symmetry.

In the case of a dispersion-strengthened composite material, three approximations can be considered for the RVE: with a single inclusion (see Fig. 1,*a*), volume-centered cubic (see Fig. 1,*b*) and face-centered cubic (see Fig. 1,*c*) In this case, the most adequate model from the standpoint of isotropic isotropy of effective properties is a face-centered cubic RVE, however, it would result in significantly higher computational costs compared to the RVE with a single inclusion, so the RVE with a single inclusion was considered to solve the problem of microstructure optimization. .

Fig. 2 shows FE models of RVEs with different volume fractions of inclusions. Quadratic 8-node finite elements were used in the calculations.

For two-phase materials, it is convenient to reduce the mass minimization problem to the minimization problem for the volume fraction of the densest phase, in this case, the volume fraction of inclusions. Then the Lagrange functional (17) is written as

$$L = c + \lambda_1 \left(E - \overline{E}(c)\right) + \lambda_2 \left(\overline{\lambda}(c) - \lambda\right) \to \min. \quad (19)$$

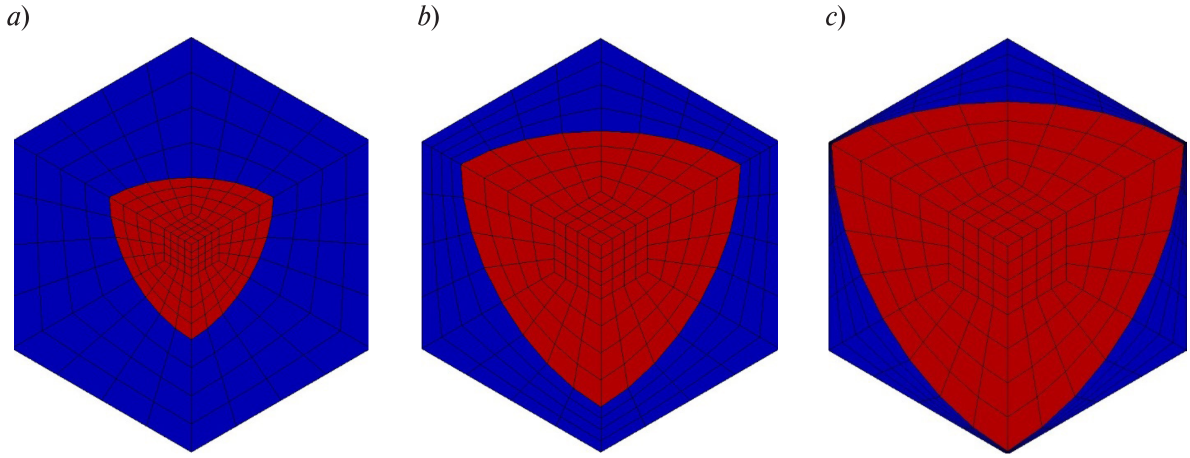

Fig. 2. Finite element models of RVEs with different volume fractions of inclusion c (1/8 of RVE is shown); c, %: 5 (*a*), 25 (*b*), 50 (*c*)

Minimization of this functional can be carried out by different techniques, such as the gradient descent method, the secant method (finite-difference approximation of the Newton method), the Levenberg–Marquardt algorithm, and many others. In this case, because the dependence of the effective properties on the volume fraction of inclusions is smooth and monotonic, we used the successive approximation method, which consists in approximating the constraint functions by the differentiable function. The stationary points of functional (19) are found by an iterative procedure constructed to successively calculate the derivatives, and next refine the coefficients of the approximating functions. This approach is also convenient for finding an initial approximation if other techniques are used.

Because the formulation is linear, the approximation dependences of Young's modulus and thermal conductivity can be found for a wide class of matrix and inclusion materials by introducing dimensionless parameters

$$e = \frac{E_m}{E_p},\ \bar{e} = \frac{\bar{E}}{E_p} \text{ and } l = \frac{\lambda_m}{\lambda_p},\ \bar{l} = \frac{\bar{\lambda}}{\lambda_p},$$

where the subscript m corresponds to the parameters of the matrix material, p is the inclusion material.

Monotonic conditions were imposed on the considered relations over the entire variation range of the parameters. We considered the following parameters describing the dependences studied:

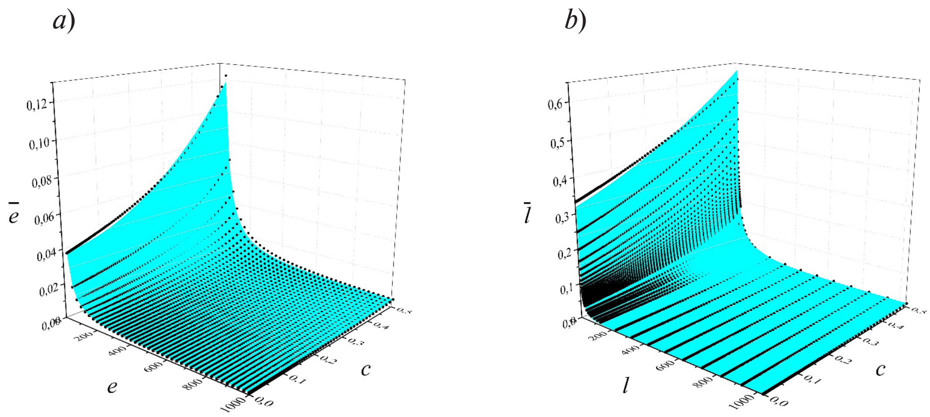

Fig. 3. Dependences of effective Young's modulus (*a*) and thermal conductivity (*b*) of the composite material on the relations for $\bar{e}$ and l (see Eqs. (20) and (21)), as well as on the volume fraction of inclusions c.
The points correspond to the values from the database of calculated cases.

$$\overline{e}\left(e,c\right)=A_E\left[\exp\left(-B_E e^{C_E}\right)+D_E\right]\left[E_E c^2+F_E c+1\right] \quad (20)$$

$$\overline{l}\left(l,c\right)=A_\lambda\left[\exp\left(-B_\lambda l^{C_\lambda}\right)+D_\lambda\right]\left[E_\lambda\left(1+G_\lambda l\right)c^2+F_\lambda c+1\right]. \quad (21)$$

Multivariate computational experiments were carried out to accumulate a database of calculated effective Young's moduli and thermal conductivity. The parameters of models (20), (21) were determined using the least squares method by the Levenberg–Marquardt algorithm. The values of the parameters of both models and the correlation coefficients R^2 are given in Table 1. Evidently, the correlation coefficient is close to unity for both models, which confirms their adequacy. The comparison of the initial data and their approximation is shown in Fig. 3.

Thus, in the case of the parameters given for the materials of the matrix and the inclusion, functional (19) is written as follows taking into account Eqs. (20), (21):

$$L=c+\lambda_1\left(E-\overline{A}_E\left[E_E c^2+F_E c+1\right]\right)+\lambda_2\left(\overline{A}_\lambda\left[\overline{E}_\lambda c^2+F_\lambda c+1\right]-\lambda\right)\to \min, \quad (22)$$

where $\overline{A}_E$, $\overline{A}_\lambda$ and $\overline{E}_\lambda$ are the parameters depending on the properties of the matrix and the inclusion materials:

$$\begin{aligned}\overline{A}_E&=A_E\left[\exp\left(-B_E e^{C_E}\right)+D_E\right]\ {}_p,\\ \overline{A}_\lambda&=A_\lambda\left[\exp\left(-B_\lambda l^{C_\lambda}\right)+D_\lambda\right]\lambda_p,\\ \overline{E}_\lambda&=E_\lambda\left(1+G_\lambda l\right).\end{aligned} \quad (23)$$

The stationary points of functional (22) can be found from the following conditions:

$$\begin{aligned}\frac{\partial L}{\partial c}&=1+\lambda_1\overline{A}_E\left[2E_E c+F_E\right]+\lambda_2\overline{A}_\lambda\left[2\overline{E}_\lambda c+F_\lambda\right]=0,\\ \frac{\partial L}{\partial \lambda_1}&=\left(E-\overline{A}_E\left[E_E c^2+F_E c+1\right]\right)=0,\\ \frac{\partial L}{\partial \lambda_2}&=\left(\overline{A}_\lambda\left[\overline{E}_\lambda c^2+F_\lambda c+1\right]-\lambda\right)=0.\end{aligned} \quad (24)$$

For definiteness, we consider an organosilicon binder as the matrix materials, with glass as the inclusion material. The characteristics of both materials are given in Table 2 [29]. The following constraints on thermal conductivity λ and Young's modulus E are taken: $\lambda \le 0.3$ W/(m·K), $E \ge 3$ GPa.

Table 1

Parameter values of approximating functions in two equations

Equation parameter	Parameter value in equation	
	(20)	(21)
A	32.40	9.85
B	0.13	0.23
C	4.36	2.66
D	$2\cdot10^{-5}$	$3\cdot10^{-6}$
E	6.69	0.05
f	0.66	1.17
G	–	9.00
Correlation coefficient R^2	0.997	0.998

Notations: ρ is the density, *E* is Young's modulus, ν, λ are Poisson's ratio and thermal conductivity.

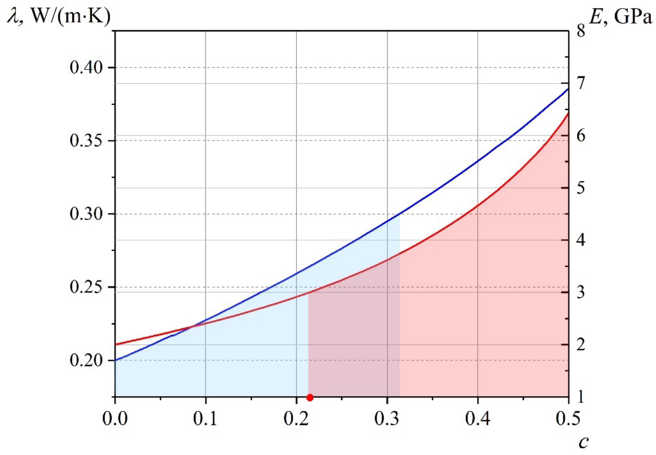

Fig. 4. Dependences of effective values of thermal conductivity (blue curve) and Young's modulus (red curve) on the concentration of inclusions

Due to the simplicity of the functional to be minimized, the search for the optimal ratio between the matrix and the inclusions can be illustrated by plotting the dependences of effective values of the material parameters, on which constraints are imposed, on the concentration of inclusions (Fig. 4).

Table 2

Characteristics of materials considered

Parameter	Parameter value	
	Matrix	Inclusion
ρ, kg/m^3	1100	2600
E, GPa	2.0	70
ν	0.20	0.35
λ, W/(m·K)	0.7	0.2

Based on the above optimization procedure, we obtained the optimal value of glass inclusion concentration in the organosilicon matrix of the composite ensuring the minimum mass of the composite under the imposed constraints; it amounts to 21.3%.

Importantly, it is generally impossible to guarantee the existence of a solution that satisfies all of the imposed constraints. In this case, a solution can be found by substituting the materials, changing the structure of the composite or loosening the constraints imposed.

Conclusion

The paper introduces an approach to determining the optimal parameters of composite materials with constraints imposed on their properties. The approach is based on the finite element homogenization method, making it possible to find the effective characteristics of heterogeneous materials, as well as on conditional optimization methods. We considered a particular case, solving a problem on minimizing the density of a composite dispersion-strengthened by spherical inclusions, with constraints on the elastic modulus and the thermal conductivity of the matrix and the inclusions. The conditional optimization problem was solved using the Lagrange multiplier method and the successive approximation method. Approximating dependences were proposed to adequately describe the variation in the effective thermal conductivity and Young's modulus (correlation coefficient $R^2 \geq 0.99$).

The developed algorithm can be used for multicriterial optimization of composite materials with different reinforcement topologies, to subsequently accumulate a database for training neural networks. This approach and algorithm will accelerate the search for an initial approximation of the optimization problem.

REFERENCES

1. **Dimitrienko Yu. I., Sokolov A. P.,** Development of automated technology of calculation of effective elastic characteristics of composites by method of asymptotic averaging, Herald of the Bauman Moscow State Techn. Univ. Natur. Sci. (2) (2008) 56–67 (in Russian).
2. **Mannanov E. R.,** About dielectric materials with high thermal conductivity for electrical insulation systems of high-voltage electric machines: a review of domestic and foreign literature, Mater. Sci. Power Eng. 27 (4) (2021) 42–67 (in Russian).
3. **Ngo I. L., Byon C.,** Thermal conductivity of particle-filled polymers, Polymer Science Book Series. No. 1: Research advances, practical applications and educational aspects, Edit. by A. Méndez-Vilas, A. Solano, Formatex Research Center, Badajoz (Spain) (2016) 554–565.
4. **Reuss A.,** Berechnung der Fliessgrenze von Mischkristallen auf Grund der Plastizitдtsbedingung für Einkristalle, ZAMM – J. Appl. Math. Mech. /Z. Angew. Math. Mech. 9 (1) (1929) 49–58.
5. **Voigt W.,** Ьber die Beziehung zwischen den beiden Elasticitдtsconstanten isotroper Körper, Ann. Phys. 274 (12) (1889) 573–587.
6. **Eshelby J. D.,** The determination of the elastic field of an ellipsoidal inclusion and related problems, Proc. R. Soc. London, Ser. A. 241 (1226) (1957) 376–396.
7. **Mori T., Tanaka K.,** Average stress in matrix and average elastic energy of materials with misfitting inclusions, Acta Metallurg. 21 (5) (1973) 571–574.
8. **Grishchenko** A. I., **Semenov A. S., Semenov S. G., Melnikov B. E.,** Influence of structural parameters of the masonry on effective elastic properties and strength, Mag. Civ. Eng. 49 (5) (2014) 95–106.
9. **Hashin Z., Shtrikman S.,** A variational approachto the theory of elastic behavior of multiphase materials, J. Mech. Phys. Solids. 11 (2) (1963) 127–140.
10. **Svetashkov A. A., Kupriyanov N. A., Manabaev K. K.,** Modifications of effective moduli Hashin – Strickmann type for two-component isotropic composite, Physical Mesomechanics. 18 (6) (2015) 57–65 (in Russian).
11. **Pobedrya B. E.,** Mechanics of composite materials, Publishing House of Moscow State University, Moscow, 1984 (in Russian).
12. **Gorbachev V. I.,** The homogenization method of Bakhvalov – Pobedrya in the composite mechanics, Moscow Univ. Mech. Bull. 71 (2016) 137–141.
13. **Bakhvalov N. S., Panasenko G. P.,** Homogenization: Averaging processes in periodic media: Mathematical problems in the mechanics of composite materials (Mathematics and Its Applications, Vol. 36) Springer, New York, 1989.
14. **Maxwell J. C.,** A treatise on electricity and magnetism, Oxford University Press, Oxford, 1904.
15. **Lord Rayleigh J. S.,** On the influence of obstacles arranged in rectangular order upon the properties of a medium, Philos. Mag. 34 (5) (1892) 481–502.
16. **Bruggeman D. A. G.,** Berechnung verschiedener physikalischer Konstanten von heterogenen Substanzen. I. Dielektrizitдtskonstanten und Leitfдhigkeiten der Mischkörper aus isotropen Substanzen, Ann. Phys. 416 (7) (1935) 636–664.
17. **Pashkovsky D. M., Frolova K. P., Vilchevskaya E. N.,** Effective diffusion properties of a polycrystal, St. Petersburg Polytechnical State University Journal. Physics and Mathematics. 15 (3) (2022) 154–168.
18. **Barrer R. M.,** Diffusion and permeation in heterogeneous media, In book: Diffusion in polymers, Ed. by J. Crank and G. S. Park, Academic Press, London, 1968.
19. **Bell G. E., Crank J.,** Influence of imbedded particles on steady-state diffusion, J. Chem. Soc. Farad. Trans. 70 (2) (1974) 1259–2732.
20. **Meredith R. E., Tobias C. W.,** Conductivities of emulsions, J. Electrochem. Soc. 108 (3) (1961) 286.
21. **Fricke H.,** A mathematical treatment of the electric conductivity and capacity of disperse systems. I. The electric conductivity of a suspension of homogeneous spheroids, Phys. Rev. 24 (5) (1924) 575–587.
22. **Epov M. I., Terekhov V. I., Nizovtsev M. I., et al.,** Effective thermal conductivity of dispersed materials with contrast inclusions, High Temperature. 53 (1) (2015) 45–50.
23. **Zarubin V. S., Kuvyrkin G. N., Savelyeva I. Yu.**, Effective thermal conductivity of a composite in case of inclusions shape deviations from spherical ones, Mat. Mod. Chisl. Met. (4) (2014) 3–17 (in Russian).
24. **Borovkov A. I., Sabadash V. O.,** Finite element multiscale homogenization and equential heterogenization of composite structures, Proc. 10th Int. ANSYS’2002 Conf., Pittsburgh, USA, 2002.

25. **Borovkov A. I., Klich A. E.,** Computational micromechanics of composites. Finite element homogenization methods, Appl. Math. Mech. (Z. Angew. Math. Mech. – ZAMM). 78 (Suppl. 1) (1998) S295–S296.

26. **Semenov A. S.,** PANTOCRATOR – konechno-elementnyy programmnyy kompleks, oriyentirovannyy na resheniye nelineynykh zadach mekhaniki [PANTOCRATOR – finite-element program specialized on the solution of non-linear problems of solid body mechanics], In: Proc. The V-th Int. Conf. "Scientific and engineering problems of reliability and service life of structures and methods of their decision", St. Petersburg Polytechnical University Publishing, St. Petersburg (2003) 466–480.

27. **Semenov A. S., Grishchenko A. I., Melnikov B. E.,** Finite-element modeling of bone tissue deformation at the submicroscopic level, St. Petersburg State Polytechnical University Journal. Physics and Mathematics. (3 (201)) (2014). 20–34 (in Russian).

28. **Grishchenko A. I., Semenov A. S.,** Modeling of the elastoplastic deformation process of single crystal superalloys, PNRPU Mechanics Bulletin. (2) (2022) 58–72 (in Russian).

29. **Maalawi K.,** Introductory chapter: An introduction to the optimization of composite structures, in book: Optimum Composite Structures. Edit. by K. Maalawi. IntechOpen. Publ. Nov. 5-th, 2018.

30. **Dimitrienko Yu. I., Drogolyub A. N., Sokolov A.P., Shpakova Yu. V.,** Metod resheniya zadachi optimizatsii struktury dispersno-armirovannykh kompozitov pri ogranicheniyakh na teplovye i prochnostnye svoistva [Method for solving an optimization problem of the structure of fiber reinforced composites under restrictions on thermal and strength properties], Science and Education (Bauman State Technical University) (11) (2013) 415–430 (in Russian).

31. **Hamdia K. M., Zhuang, X., Rabczuk T.,** An efficient optimization approach for designing machine learning models based on genetic algorithm, Neural Comput. Applic. 33 (6) (2021), 19231933.

32. **Nelder J. A., Mead R.,** A simplex method for function minimization, Comput. J. 7 (4) (1965) 308–313.

33. **Getsov L. B., Semenov A. S., Golubovsky E. R., et al.,** Features and uniform description of I, II, and III stages of the creep in single-crystal superalloys, Industrial Laboratory. Diagnostics of materials. 86 (3) (2020) 44–54 (in Russian).

34. **Borovkov A. I., Aleman Mesa D.,** Homogenization of unidirectional fiber and granular elastic composites, St. Petersburg State Polytechnical University Journal. (3 (84)) (2009) 135–153 (in Russian).

СПИСОК ЛИТЕРАТУРЫ

1. **Димитриенко Ю. И., Соколов А. П.** Разработка автоматизированной технологии вычисления эффективных упругих характеристик композитов методом асимптотического осреднения // Вестник Московского государственного технического университета им. Н. Э. Баумана. Серия «Естественные науки». 2008. № 2. С. 56–67.

2. **Маннанов Э. Р.** О диэлектрических материалах с высокой теплопроводностью для систем электрической изоляции высоковольтных электрических машин: обзор отечественной и зарубежной литературы // Материаловедение. Энергетика. 2021. Т. 27. № 4. С. 42–67.

3. **Ngo I. L., Byon C.** Thermal conductivity of particle-filled polymers // Polymer Science Book Series. No. 1: Research advances, practical applications and thermal conductivity of particle-filled polymers. Edited by A. Méndez-Vilas, A. Solano. Badajoz (Spain): Formatex Research Center, 2016. Pp. 554–565.

4. **Reuss A.** Berechnung der Fliessgrenze von Mischkristallen auf Grund der Plastizitдtsbedingung für Einkristalle // ZAMM – Journal of Applied Mathematics and Mechanics /Zeitschrift für Angewandte Mathematik und Mechanik. 1929. Vol. 9. No. 1. Pp. 49–58.

5. **Voigt W.** Ьber die Beziehung zwischen den beiden Elasticitдtsconstanten isotroper Körper // Annalen der Physik. 1889. Vol. 274. No. 12. Pp. 573–587.

6. **Эшелби Дж.** Определение поля упругих напряжений, создаваемого эллипсоидальным включением, и задачи, связанные с этой проблемой // Сборник переводов статей 1956 – 62 гг. М.: Изд-во иностранной литературы, 1963. 248 с.

7. **Mori T., Tanaka K.** Average stress in matrix and average elastic energy of materials with misfitting inclusions // Acta Metallurgica. 1973. Vol. 21. No. 5. Pp. 571–574.

8. **Grishchenko A. I., Semenov A. S., Semenov S. G., Melnikov B. E.** Influence of structural parameters of the masonry on effective elastic properties and strength // Инженерно-строительный журнал. 2014. № 5 (49). С. 95–106.

9. **Hashin Z., Shtrikman S.** A variational approachto the theory of elastic behavior of multiphase materials // Journal of the Mechanics and Physics of Solids. 1963. Vol. 11. No. 2. Pp. 127–140.

10. **Светашков А. А., Куприянов Н. А., Манабаев К. К.** Модификации эффективных модулей типа Хашина – Штрикмана для двухкомпонентного изотропного композита // Физическая мезомеханика. 2015. Т. 18. № 6. С. 57–65.

11. **Победря Б. Е.** Механика композиционных материалов. М.: Изд-во МГУ, 1984. 336 с.

12. **Горбачёв В. И.** Метод осреднения Бахвалова – Победри в механике композитов // Вестник Московского университета. Серия 1: Математика. Механика. 2016. № 6. С. 41–46.

13. **Бахвалов Н. С., Панасенко Г. П.** Осреднение процессов в периодических средах. М.: Наука, 1984. 352 с.

14. **Maxwell J. C.** A treatise on electricity and magnetism. Oxford: Oxford University Press, 1904. 435 p.

15. **Lord Rayleigh J. S.** On the influence of obstacles arranged in rectangular order upon the properties of a medium // The Philosophical Magazine. 1892. Vol. 34. 5-th Series. Pp. 481–502.

16. **Bruggeman D. A. G.** Berechnung verschiedener physikalischer Konstanten von heterogenen Substanzen. I. Dielektrizitдtskonstanten und Leitfдhigkeiten der Mischkörper aus isotropen Substanzen // Annalen der Physik. 1935. Vol. 416. No. 7. Pp. 636–664.

17. **Пашковский Д. М., Фролова К. П., Вильчевская Е. Н.** Эффективные диффузионные свойства поликристалла // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2022. Т. 15. № 3. С. 154–168.

18. **Barrer R. M.** Diffusion and permeation in heterogeneous media // Diffusion in polymers, Ed. by J. Crank and G. S. Park, Academic Press, London, 1968. 452 p.

19. **Bell G. E., Crank J.** Influence of imbedded particles on steady-state diffusion // Journal of the Chemical Society, Faraday Transactions. 1974. Vol. 70. No. 2. Pp. 1259–2732.

20. **Meredith R. E., Tobias C. W.** Conductivities of emulsions // Journal of the Electrochemical Society. 1961. Vol. 108. No. 3. P. 286.

21. **Fricke H.** A mathematical treatment of the electric conductivity and capacity of disperse systems. I. The electric conductivity of a suspension of homogeneous spheroids // Physical Review. 1924. Vol. 24. No. 5. Pp. 575–587.

22. **Эпов М. И., Терехов М. И., Низовцев М. И., Шурина Э. Л., Иткина Н. Б., Уколов Е. С.** Эффективная теплопроводность дисперсных материалов с контрастными включениями // Теплофизика высоких температур. 2015. Т. 53. № 1. С. 48–53.

23. **Зарубин В. С., Кувыркин Г. Н., Савельева И. Ю.** Эффективная теплопроводность композита в случае отклонений формы включений от шаровой // Математическое моделирование и численные методы. 2014. № 4. С. 3–17.

24. **Borovkov A. I., Sabadash V. O.** Finite element multiscale homogenization and equential heterogenization of composite structures // Proceedings of 10th International ANSYS'2002 Conference, Pittsburgh, USA, 2002. 15 p.

25. **Borovkov A. I., Klich A. E.** Computational micromechanics of composites. Finite element homogenization methods, Appl. Math. Mech. (Z. Angew. Math. Mech. – ZAMM). 1998. Vol. 78. Pp. 295–296.

26. **Семенов А. С.** PANTOCRATOR – конечно-элементный программный комплекс, ориентированный на решение нелинейных задач механики // Труды V-ой Международной конференции «Научно-технические проблемы прогнозирования надежности и долговечности конструкций». СПб.: Изд-во СПбГПУ, 2003. С. 466–480.

27. **Семенов А. С., Грищенко А. И., Мельников Б. Е.** Конечно-элементное моделирование деформирования костной ткани на субмикроскопическом уровне // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2014. № 3 (201) С. 20–34.

28. **Грищенко А. И., Семенов А. С.** Моделирование процессов упругопластического деформирования монокристаллических сплавов // Вестник Пермского политехнического университета. Механика. 2022. № 2. С. 58–72.

30. **Димитриенко Ю. И., Дроголюб А. Н., Соколов А. П., Шпакова Ю. В.** Метод решения задачи оптимизации структуры дисперсно-армированных композитов при ограничениях на тепловые и прочностные свойства // Наука и образование (МГТУ им. Н. Э. Баумана). 2013. № 11. С. 415–430.

31. **Hamdia K. M., Zhuang, X., Rabczuk T.** An efficient optimization approach for designing machine learning models based on genetic algorithm // Neural Computing and Applications. 2021. Vol. 33. No. 6. Pp. 1923–1933.

32. **Nelder J. A., Mead R.** A simplex method for function minimization // The Computer Journal. 1965. Vol. 7. No. 4. Pp. 308–313.

33. **Гецов Л. Б., Семенов А. С., Голубовский Е. Р., Грищенко А. И., Семенов С. Г.** Особенности и единое описание I, II и III стадий ползучести монокристаллических жаропрочных сплавов // Заводская лаборатория. Диагностика материалов. 2020. Т. 86. № 3. С. 44–54.

34. **Боровков А. И., Алеман Меза Д.** Гомогенизация однонаправленных волокнистых и гранулированных упругих композитов // Научно-технические ведомости Санкт-Петербургского государственного политехнического университета. 2009. № 3 (84) **С**. 135–153.

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