

SOME FINITE ELEMENT APPROACHES FOR MODELING OF ANISOTROPIC THERMOELASTIC MIXTURE AND PERIODIC COMPOSITES WITH INTERNAL MICROSTRUCTURE

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Abstract: *The paper considers an integrated approach to the determination of the material properties of thermoelastic bulk (mixture) and periodic composites of an arbitrary anisotropy class with account for their internal microstructure.*

1 INTRODUCTION

Nowadays the problems of the effective moduli calculation for thermoelastic composite media are studied quite extensively. These issues are covered in the monographs that has already become classical ([2, 14], etc.), as well as in many other publications. Nevertheless, various aspects of thermoelastic composite modeling continue to be developed in recent publications. For example, we can note [1, 4, 5, 10, 11, 15, 17] and others, in which porous thermoelastic materials were considered.

The present paper develops the approach based on the effective moduli method for the composite mechanics, computer modeling of the representative volumes with account for their microstructure and application of finite element technologies of solving coupled problems of thermoelasticity for anisotropic mixture two-phase composites and porous bodies. Numerical results have shown that thermoelastic effective moduli can significantly depend on the representative volume structure of the composite material.

2 EFFECTIVE MODULI METHOD FOR THERMOELASTIC COMPOSITES

Let $\Omega \in \mathbb{R}^3$ be a representative volume of composite body, $\Gamma = \partial\Omega$ is its boundary, \mathbf{n} is the outward unit normal vector to Γ , $\mathbf{x} = \{x_1, x_2, x_3\}$ is the vector of the special coordinates. We will consider heterogeneous anisotropic thermoelastic material without bulk mechanical and thermal sources in a volume Ω . Then in the framework of linear static theory of thermoelasticity we have the following system of differential equations

$$\sigma_{ij,j} = 0, \quad \sigma_{ij} = c_{ijkl}\varepsilon_{kl} - \beta_{ij}\theta, \quad \varepsilon_{ij} = (u_{i,j} + u_{j,i})/2, \quad (1)$$

$$q_{j,j} = 0, \quad q_i = -k_{ij}\theta_{,j}, \quad (2)$$

where σ_{ij} are the components of the stress tensor $\boldsymbol{\sigma}$; ε_{ij} are the components of the strain tensor $\boldsymbol{\varepsilon}$; u_i are the components of the displacement vector \mathbf{u} ; θ is the temperature increment from natural state, c_{ijkl} are the forth

rank tensor of elastic stiffness moduli; β_{ij} are the thermal stress coefficients; q_i are the components of the heat flux vector \mathbf{q} ; k_{ij} are the components of the tensor \mathbf{k} of thermal conductivities.

In vector-matrix symbols in R^3 the formulas (1), (2) can be rewritten in the form

$$\mathbf{L}^*(\nabla) \cdot \mathbf{T} = 0, \quad \mathbf{T} = \mathbf{c} \cdot \mathbf{S} - \beta \theta, \quad \mathbf{S} = \mathbf{L}(\nabla) \cdot \mathbf{u}, \quad (3)$$

$$\nabla^* \cdot \mathbf{q} = 0, \quad \mathbf{q} = -\mathbf{k} \cdot \nabla \theta, \quad (4)$$

where

$$\mathbf{L}^*(\nabla) = \begin{bmatrix} \partial_1 & 0 & 0 & 0 & \partial_3 & \partial_2 \\ 0 & \partial_2 & 0 & \partial_3 & 0 & \partial_1 \\ 0 & 0 & \partial_3 & \partial_2 & \partial_1 & 0 \end{bmatrix}, \quad \nabla = \begin{Bmatrix} \partial_1 \\ \partial_2 \\ \partial_3 \end{Bmatrix}, \quad (5)$$

$\mathbf{T} = \{\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{23}, \sigma_{13}, \sigma_{12}\}$ is the stress (pseudo-) vector; $\mathbf{S} = \{\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, 2\varepsilon_{23}, 2\varepsilon_{13}, 2\varepsilon_{12}\}$ is the strain (pseudo-) vector; \mathbf{c} is the 6×6 matrix of elastic moduli; $c_{\alpha\beta} = c_{ijkl}$, $\alpha, \beta = 1, \dots, 6$, $i, j = 1, 2, 3$ with correspondence law $\alpha \leftrightarrow (ij)$, $\beta \leftrightarrow (kl)$, $1 \leftrightarrow (11)$, $2 \leftrightarrow (22)$, $3 \leftrightarrow (33)$, $4 \leftrightarrow (23) = (32)$, $5 \leftrightarrow (13) = (31)$, $6 \leftrightarrow (12) = (21)$; $\beta = \{\beta_{11}, \beta_{22}, \beta_{33}, \beta_{23}, \beta_{13}, \beta_{12}\}$; $(\dots)^*$ is the transpose operation; and $(\dots) \cdot (\dots)$ is the scalar product operation.

Setting the appropriate boundary conditions at $\Gamma = \partial\Omega$, we can find the solutions of the problems (1), (2) or (3), (4) for heterogeneous medium in the representative volume Ω . Then the comparison of the solution characteristics averaged over Ω (such as stresses, etc.) with analogous values for homogeneous medium (the comparison medium) will permit to determine the effective moduli for the composite material. We note that for anisotropic media in order to determine the full set of the effective moduli it is necessary to solve several problems of the considered types for different boundary conditions.

Here the main difficulties consist in the choice of the representative volume and boundary problems for the heterogeneous medium and the comparison medium, as well as the technologies for solving the problems for heterogeneous media. According to the previously developed methods of modeling the piezoelectric active materials [3, 6, 8], we consider analogous approaches for the problems of thermoelasticity.

For thermoelastic homogeneous comparison medium we adopt that the same equations (1), (2) or (3), (4) are satisfied with constant modules \mathbf{c}^{eff} , β^{eff} , \mathbf{k}^{eff} , which are to be determined. Let us assume that at the boundary Γ the following boundary condition take place

$$\mathbf{u} = \mathbf{L}^*(\mathbf{x}) \cdot \mathbf{S}_0, \quad \theta = \theta_0, \quad \mathbf{x} \in \Gamma, \quad (6)$$

where $\mathbf{S}_0 = \{\varepsilon_{011}, \varepsilon_{022}, \varepsilon_{033}, 2\varepsilon_{023}, 2\varepsilon_{013}, 2\varepsilon_{012}\}$; ε_{0ij} , θ_0 are some values that do not depend on \mathbf{x} . Then $\mathbf{u} = \mathbf{L}^*(\mathbf{x}) \cdot \mathbf{S}_0$, $\mathbf{S} = \mathbf{S}_0$, $\theta = \theta_0$, $\mathbf{T} = \mathbf{T}_0 = \mathbf{c}^{eff} \cdot \mathbf{S}_0 - \beta^{eff} \theta_0$ will give the solution for the problem (3)–(6) in the volume Ω for the homogeneous comparison medium. Note, that for $\theta = \theta_0$ the equations (4) are satisfied identically, if $\mathbf{q} = \mathbf{q}_0 = 0$, but this pure thermal problem is not actually used here.

Let us solve now the same problem (3)–(6) for heterogeneous medium and assume that for this medium and for the comparison medium the averaged stresses are equal $\langle \mathbf{T} \rangle = \langle \mathbf{T}_0 \rangle$, where hereinafter the angle brackets $\langle (\dots) \rangle$ denote the averaged by the volume values $\langle (\dots) \rangle = (1/|\Omega|) \int_{\Omega} (\dots) d\Omega$. Therefore we obtain that for the effective moduli of the composite the equation $\mathbf{c}^{eff} \cdot \mathbf{S}_0 - \beta^{eff} \theta_0 = \langle \mathbf{T} \rangle$ is satisfied, where \mathbf{S}_0 and θ_0 are the given values from the boundary conditions (6). Hence, even in the assumption of the anisotropy of the general form for the comparison medium, all the stiffness modules $c_{\alpha\zeta}^{eff}$ and thermal stress coefficients β_{α}^{eff} can be computed. Indeed, setting in (6) $\mathbf{S}_0 = \varepsilon_0 \mathbf{h}_{\zeta}$, $\varepsilon_0 = \text{const}$, $\theta_0 = 0$, where ζ is some fixed index mark (\mathbf{h}_{ζ} is the vector from six-dimensional basic set for the components for strain tensor basic set; $\mathbf{h}_j = \mathbf{e}_j \mathbf{e}_j$, $j = 1, 2, 3$; $\mathbf{h}_4 = (\mathbf{e}_2 \mathbf{e}_3 + \mathbf{e}_3 \mathbf{e}_2)/2$; $\mathbf{h}_5 = (\mathbf{e}_1 \mathbf{e}_3 + \mathbf{e}_3 \mathbf{e}_1)/2$; $\mathbf{h}_6 = (\mathbf{e}_1 \mathbf{e}_2 + \mathbf{e}_2 \mathbf{e}_1)/2$; \mathbf{e}_j are the orts of the Cartesian coordinate system), we get the computation formulas for the elastic modules $c_{\alpha\zeta}^{eff}$: $c_{\alpha\zeta}^{eff} = \langle T_{\alpha} \rangle / \varepsilon_0$. If in (6) we set $\mathbf{S}_0 = 0$, $\theta_0 \neq 0$, than from the boundary problem (3)–(6) the thermal stress effective modules can be obtained: $\beta_{\alpha}^{eff} = -\langle T_{\alpha} \rangle / \theta_0$. An important justification of the choice of the boundary condition $\mathbf{u} = \mathbf{L}^*(\mathbf{x}) \cdot \mathbf{S}_0$ for $\mathbf{x} \in \Gamma$ lays in the fact that with this boundary condition between the stress and strain fields of heterogeneous medium and comparison medium the equalities $\langle \mathbf{S} \rangle = \langle \mathbf{S}_0 \rangle$, $\langle \mathbf{T}^* \cdot \mathbf{S} \rangle = \langle \mathbf{T}_0^* \cdot \mathbf{S}_0 \rangle$ also take place. Therefore with such boundary condition for two media under consideration their mechanical potential energies appear to be equal. We would like to note, that the proof of this fact completely repeats the well know proof from classical theory of elasticity [12].

In order to determine the effective coefficients of the tensor \mathbf{k} it is sufficient to consider the thermal conductivity equation (4). For the formulation of the corresponding boundary-value problem we adopt the boundary conditions in the form

$$\theta = \mathbf{x}^* \cdot \mathbf{G}_0, \quad \mathbf{x} \in \Gamma, \quad (7)$$

where \mathbf{G}_0 is some constant vector that does not depend on \mathbf{x} . It is obvious that $\theta = \mathbf{x}^* \cdot \mathbf{G}_0$, $\mathbf{G} = \nabla\theta$, $\mathbf{G} = \mathbf{G}_0$, $\mathbf{q} = \mathbf{q}_0 = -\mathbf{k}^{eff} \cdot \mathbf{G}_0$ will give the solution of the problem (4), (7) in the volume Ω for the homogeneous comparison medium. Then having solved the problem (4), (7) for heterogeneous medium, we can set that for this medium and for the comparison medium the averaged heat fluxes are equal $\langle \mathbf{q} \rangle = \langle \mathbf{q}_0 \rangle$. As a result we get the equation for the effective moduli of the composite $\mathbf{k}^{eff} \cdot \mathbf{G}_0 = -\langle \mathbf{q} \rangle$, where \mathbf{G}_0 is the vector known from the boundary conditions (7)). Then for the comparison medium with anisotropy of general form it is not difficult to obtain computation formulas for thermal conductivity moduli k_{il}^{eff} . Indeed, setting in (7) $\mathbf{G}_0 = G_0 \mathbf{e}_l$, $G_0 = \text{const}$, where $l = 1, 2, 3$ is some fixed index, we get computation formulas for the moduli k_{il}^{eff} : $k_{il}^{eff} = -\langle \mathbf{q}_i \rangle / G_0$. The choice of the boundary condition $\theta = \mathbf{x}^* \cdot \mathbf{G}_0$ in (7) can be justified by the fact that in this case between the heat flux and temperature gradient fields for the heterogeneous medium and the comparison medium the following equalities take place $\langle \mathbf{G} \rangle = \langle \mathbf{G}_0 \rangle$, $\langle \mathbf{q}^* \cdot \mathbf{G} \rangle = \langle \mathbf{q}_0^* \cdot \mathbf{G}_0 \rangle$, where the last relation has the energy sense.

The approaches described above are associated with the averaging of the moduli \mathbf{c} , β , \mathbf{k} . Further we will mark the effective moduli obtained by this method with the superscript "I": $\mathbf{c}^{eff} = \mathbf{c}^{Ieff}$, $\beta^{eff} = \beta^{Ieff}$, $\mathbf{k}^{eff} = \mathbf{k}^{Ieff}$.

The second way of determination of the effective moduli is related to another type of the boundary conditions. In this case it is convenient to change the form of the governing equations in the thermoelastic problem (3), (4)

$$\mathbf{S} = \mathbf{s} \cdot \mathbf{T} + \alpha \theta = 0, \quad \mathbf{G} = -\mathbf{r} \cdot \mathbf{q}, \quad \mathbf{G} = \nabla\theta, \quad (8)$$

where $\mathbf{s} = \mathbf{c}^{-1}$ is the matrix of elastic compliances, $\alpha = \mathbf{s} \cdot \beta$ is the six-dimensional (pseudo-) vector of thermal expansion coefficients, $\mathbf{r} = \mathbf{k}^{-1}$ is the matrix of the inverse thermal conductivities coefficients.

Let us assume that at the boundary $\Gamma = \partial\Omega$ the following boundary conditions take place

$$\mathbf{L}^*(\mathbf{n}) \cdot \mathbf{T} = \mathbf{L}^*(\mathbf{n}) \cdot \mathbf{T}_0, \quad \theta = \theta_0, \quad \mathbf{x} \in \Gamma, \quad (9)$$

where \mathbf{T}_0 , θ_0 are some values that do not depend on \mathbf{x} . Then for homogeneous comparison medium the fields $\mathbf{T} = \mathbf{T}_0$, $\mathbf{S} = \mathbf{S}_0 = \mathbf{s}^{eff} \cdot \mathbf{T}_0 + \alpha^{eff} \theta_0$, $\mathbf{u} = \mathbf{L}^*(\mathbf{x}) \cdot \mathbf{S}_0$, $\theta = \theta_0$ in Ω satisfy the equilibrium equation from (3) and the constitutive equation from (8) with $\mathbf{s} = \mathbf{s}^{eff}$, $\alpha = \alpha_0$. At that the thermal equation is satisfied identically with $\mathbf{q} = \mathbf{q}_0$.

For solution of the problem (3), (4), (9) for heterogeneous medium the relation $\langle \mathbf{T} \rangle = \langle \mathbf{T}_0 \rangle$ will take place, and therefore for the effective moduli determination it makes sense to require that the equality $\langle \mathbf{S} \rangle = \mathbf{S}_0 = \mathbf{s}^{eff} \cdot \mathbf{T}_0 + \alpha^{eff} \theta_0$ is satisfied. This condition enables to determine the compliances $s_{\alpha\beta}^{eff}$ and coupling coefficients α_{β}^{eff} for anisotropic comparison medium. Setting in (9) $\mathbf{T}_0 = T_0 \mathbf{h}_{\zeta}$, $T_0 = \text{const}$, $\theta_0 = 0$ for fixed index ζ , we get the computation formulas for effective elastic compliances: $s_{\alpha\zeta}^{eff} = \langle S_{\alpha} \rangle / T_0$. The solutions of the problems (3), (4), (9) with $\mathbf{T}_0 = 0$, $\theta_0 \neq 0$ permit to obtain the effective coefficients of thermal expansions $\alpha_{\beta} = \langle S_{\beta} \rangle / \theta_0$. At that for the solution of the problems (3), (4), (9) for heterogeneous medium and homogeneous comparison material the mechanical energies will also be equal $\langle \mathbf{T}^* \cdot \mathbf{S} \rangle = \langle \mathbf{T}_0^* \cdot \mathbf{S}_0 \rangle$, that additionally justifies the choice of the boundary condition (9).

In order to determine the effective inverse thermal conductivities coefficients r_{il}^{eff} we adopt the following boundary conditions for the thermal conductivity equation (4)

$$\mathbf{n}^* \cdot \mathbf{q} = \mathbf{n}^* \cdot \mathbf{q}_0, \quad \mathbf{x} \in \Gamma, \quad (10)$$

where \mathbf{q}_0 is some constant vector that does not depend on \mathbf{x} . Then $\mathbf{q} = \mathbf{q}_0$, $\theta = \mathbf{x}^* \cdot \mathbf{G}_0$, $\mathbf{G} = \nabla\theta$, $\mathbf{G} = \mathbf{G}_0$, $\mathbf{G}_0 = -\mathbf{r}^{eff} \cdot \mathbf{q}_0$ give the solution of the problem (4), (10) for the homogeneous comparison medium, moreover, for any solution of the problem (4), (10) with heterogeneous coefficients $\mathbf{k}(\mathbf{x}) = \mathbf{r}^{-1}(\mathbf{x})$ the following equality holds $\langle \mathbf{q} \rangle = \langle \mathbf{q}_0 \rangle$. Therefore for the determination of the effective coefficients r_{il}^{eff} we can set: $\langle \mathbf{G} \rangle = \langle \mathbf{G}_0 \rangle$, where \mathbf{G} is the gradient of the temperature field, calculated for heterogeneous medium. This condition leads to the relation $\mathbf{r}^{eff} \cdot \mathbf{q}_0 = -\langle \mathbf{G} \rangle$, from which, assuming in (10) $\mathbf{q}_0 = q_0 \mathbf{e}_i$, $q_0 = \text{const}$, we get the computation formulas for the effective reduced impermeability coefficients: $r_{il}^{eff} = -\langle G_i \rangle / q_0$. As for the first variant, the choice of the boundary condition $\mathbf{n}^* \cdot \mathbf{q} = \mathbf{n}^* \cdot \mathbf{q}_0$ in (10) can be justified by the equality of the potential energies in the heterogeneous medium and the comparison medium: $\langle \mathbf{q}^* \cdot \mathbf{G} \rangle = \langle \mathbf{q}_0^* \cdot \mathbf{G}_0 \rangle$.

It can be seen that the second approach is related to the averaging of the moduli \mathbf{s} , $\boldsymbol{\alpha}$, \mathbf{r} . Therefore we will call mark the effective moduli obtained by the superscript "II" $\mathbf{s}^{eff} = \mathbf{s}^{IIeff}$, $\boldsymbol{\alpha}^{eff} = \boldsymbol{\alpha}^{IIeff}$, $\mathbf{r}^{eff} = \mathbf{r}^{IIeff}$.

Both approaches enable to determine the full sets of the effective moduli for thermoelastic media of arbitrary anisotropy class: \mathbf{c}^{Ieff} , $\boldsymbol{\beta}^{Ieff}$, \mathbf{k}^{Ieff} , and then, if necessary, $\mathbf{s}^{Ieff} = (\mathbf{c}^{Ieff})^{-1}$, $\boldsymbol{\alpha}^{Ieff} = \mathbf{s}^{Ieff} \cdot \boldsymbol{\beta}^{Ieff}$, $\mathbf{r}^{Ieff} = (\mathbf{k}^{Ieff})^{-1}$; \mathbf{s}^{IIeff} , $\boldsymbol{\alpha}^{IIeff}$, \mathbf{r}^{IIeff} , and after that, if necessary, $\mathbf{c}^{IIeff} = (\mathbf{s}^{IIeff})^{-1}$, $\boldsymbol{\beta}^{IIeff} = \mathbf{c}^{IIeff} \cdot \boldsymbol{\alpha}^{IIeff}$, $\mathbf{k}^{IIeff} = (\mathbf{r}^{IIeff})^{-1}$. Generally speaking, the obtained sets will differ, and in fact we can confine ourselves to one of the approaches presented. The benefit of the use of both approaches can be seen in the split of the values of the effective moduli that makes it possible to verify these values in analogy with classical mechanics of composites in the elasticity theory.

3 FINITE ELEMENT APPROXIMATIONS

For solving problems for thermoelastic body in weak forms we will use classical finite element approximation techniques. Let Ω_h be a region of the corresponding finite element mesh $\Omega_h \subseteq \Omega$, $\Omega_h = \cup_m \Omega^{em}$, where Ω^{em} is a separate finite element with number m . On the finite element mesh we will find the approximation to the weak solution $\{\mathbf{u}_h \approx \mathbf{u}, \theta_h \approx \theta\}$ for static problem in the form

$$\mathbf{u}_h(\mathbf{x}) = \mathbf{N}_u^*(\mathbf{x}) \cdot \mathbf{U}, \quad \theta_h(\mathbf{x}) = \mathbf{N}_\theta^*(\mathbf{x}) \cdot \boldsymbol{\theta}, \quad (11)$$

where \mathbf{N}_u^* is the matrix of the shape functions for displacements, \mathbf{N}_θ^* is the row vector of the shape functions for temperature, \mathbf{U} , $\boldsymbol{\theta}$ are the global vectors of nodal displacements and temperature, respectively.

According to usual finite element technique we approximate the continuum weak formulation of the thermoelasticity problem by the problem in finite-dimensional spaces. Substituting (11) and similar representations for project functions into weak formulation for Ω_h , we obtain the following finite element system

$$\mathbf{K}_{uu} \cdot \mathbf{U} - \mathbf{K}_{u\theta} \cdot \boldsymbol{\theta} = \mathbf{F}_u, \quad (12)$$

$$\mathbf{K}_{\theta\theta} \cdot \boldsymbol{\theta} = \mathbf{F}_\theta. \quad (13)$$

Here $\mathbf{K}_{uu} = \sum^a \mathbf{K}_{uu}^{em}$, $\mathbf{K}_{u\theta} = \sum^a \mathbf{K}_{u\theta}^{em}$, $\mathbf{K}_{\theta\theta} = \sum^a \mathbf{K}_{\theta\theta}^{em}$ are the global finite element matrices, obtained from the element matrices as a result of the assembling process (\sum^a); \mathbf{F}_u , \mathbf{F}_θ are the vectors that are defined by external influences and the main boundary conditions. The element matrices are given by the formulas: $\mathbf{K}_{uu}^{em} = \int_{\Omega^{em}} \mathbf{B}_u^{e*} \cdot \mathbf{c} \cdot \mathbf{B}_u^e d\Omega$, $\mathbf{K}_{u\theta}^{em} = \int_{\Omega^{em}} \mathbf{B}_u^{e*} \cdot \boldsymbol{\beta} \cdot \mathbf{N}_\theta^{e*} d\Omega$, $\mathbf{K}_{\theta\theta}^{em} = \int_{\Omega^{em}} \mathbf{B}_\theta^{e*} \cdot \mathbf{k} \cdot \mathbf{B}_\theta^e d\Omega$, $\mathbf{B}_u^e = \mathbf{L}^*(\nabla) \cdot \mathbf{N}_u^{e*}$, $\mathbf{B}_\theta^e = \nabla \mathbf{N}_\theta^{e*}$, where \mathbf{N}_u^{e*} , \mathbf{N}_θ^{e*} are the matrix and the row vector of approximating shape functions, respectively, defined at separate finite elements.

Note that the vector $\mathbf{T} = \mathbf{T}_0$ has the solution of Eq. (7) for the problems (3)–(5) and (3), (4), (9), where \mathbf{T}_0 is the vector with identical values θ_0 on all nodes. Then for calculation of nodal displacements from (12) we obtain: $\mathbf{K}_{uu} \cdot \mathbf{U} = \mathbf{F}_u + \mathbf{K}_{u\theta} \cdot \boldsymbol{\theta}$. It can be also note that the problem (2), (4) for determination of thermal conductivities moduli is decoupled, i.e. for this problem it can be solve the finite element equations (13).

4 MODELING OF REPRESENTATIVE VOLUMES FOR BINARY COMPOSITES

At microlevel we consider the models of thermoelastic skeleton of the representative volumes that take into account important characteristics of porous composite structures. Ideally a representative volume should be a region large enough compared to the sizes of the inhomogeneity (such as inclusions or pores) but small enough compared to the distances where the slow variables change considerably. Let us consider a binary composite the first phase of which is the coherent structural skeleton and the second phase of which are isolated or connected with each other inclusions or pores of the size large enough at microlevel. The first case according to the classification of R.E. Newnham [9] corresponds to 3-0 connectivity and the second case corresponds to 3-3 connectivity (closed and open inclusions or pores, respectively).

In the case of irregular stochastic structure composite with a low concentration of the material of the second phase we can suggest a model of a cubic lattice consisting of identical elements - elementary cube, some of which are randomly declared as the material of the second phase (inclusions or pores). We assume that each of the elementary cubes is a separate thermoelastic finite element, and in the case of a porous material we can specify for pores the

negligible stiffness moduli and the thermal conductivities coefficients equal to thermal conductivities for air. Note that the random cubic lattice model can be easily constructed, but it does not support the connectivity of the composite (closed or open pores), and in the case of a porous material with a large percentage of porosity, this model can lose the skeleton connectivity.

Special cubic lattice model (method of connected skeletons) was developed by S.V. Bobrov purposely to building of the connected structures (clusters) [7]. In this model the basic cell is a cube of $10 \times 10 \times 10$ the same cubic finite elements. In the basic cell the skeleton consists of a parallelepiped represented by its edges (linear dimensions are pointed out by the randomizer) as well as of elements chains connecting the corners of the parallelepiped with the corners of the main cell. Linear dimensions of the parallelepiped are defined in the selected range of the random numbers generator, and the connecting chain elements are also generated randomly. The skeleton occupies 10 % of the cell volume. So, the maximum possible quantum of second phase material or porosity that can be achieved in this model runs up to 90%.

Figure 1 shows two variants of the generated skeletons of basic cells. On the left in Fig. 1 a box inside the cell has the dimensions $7 \times 4 \times 5$ and on the right – $4 \times 5 \times 3$. In both cases, the elements of parallelepipeds painted a darker color compared to the elements of the connecting chains.

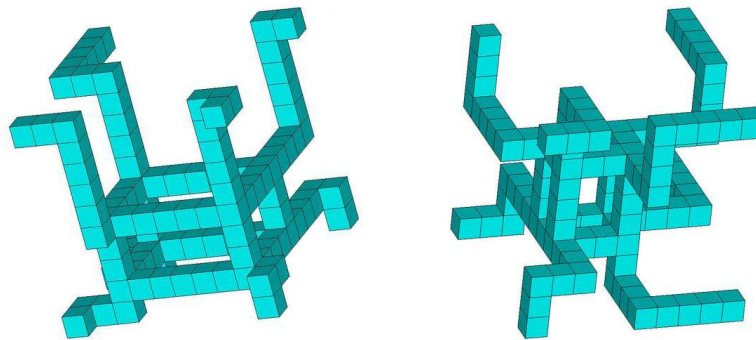


Figure 1: Method of connected skeletons. Two variants of basic cells

Representative volumes with a large number of elements are obtained by repeating the procedure of creating the basic cells of the size $10 \times 10 \times 10$ by three axes. At that each of the cells is generated randomly within the above-described procedures.

A smaller fraction of the second phase material or porosity (down to zero) is ensured by applying the following algorithm. For constructed in the previous step representative volume two elements are randomly selected, and if at least one of them is not represented the second phase material, these elements are connected by some arbitrary connected path. The resulting set is then added to the previously built skeleton consisting of solid (thermoelastic) elements. After that we calculate the quantum of the second phase material or porosity and compare it to the given value. If the calculated quantum of the second phase material or porosity is less than the given value, the step of the algorithm should be repeated, i.e. again two cells should be randomly chosen in the representative volume, and so on.

Two versions of the built skeletons are shown in Figure 2 for 10% of the first phase material (without elements of the second phase material at the left and with elements of the second phase material at the right). The sizes of these volumes are $30 \times 30 \times 30$. Thus, here the cubic structures of $10 \times 10 \times 10$ size generally were generated in different ways $30^3/10^3 = 27$ times.

Thus, the described algorithm of the representative volume construction generates the composite structures in the form of binary cubic lattices and supports the coupling of the structural matrix up to 90 % proportion of the first phase of the material. Here it is possible to build cubic lattices of the size $10m \times 10m \times 10m$, where m is an integer. Repeated passes of the algorithm lead to various representative volumes, as at different stages of the algorithm work we use the random number generator.

The cluster structures in the cubic lattice can be obtained with the use of the algorithms of the percolation theory. In the case of porous composites for small porosity it is logical to build clusters from pores and for large porosity we can build the clusters from the material of the structural skeleton. A range of such methods was implemented

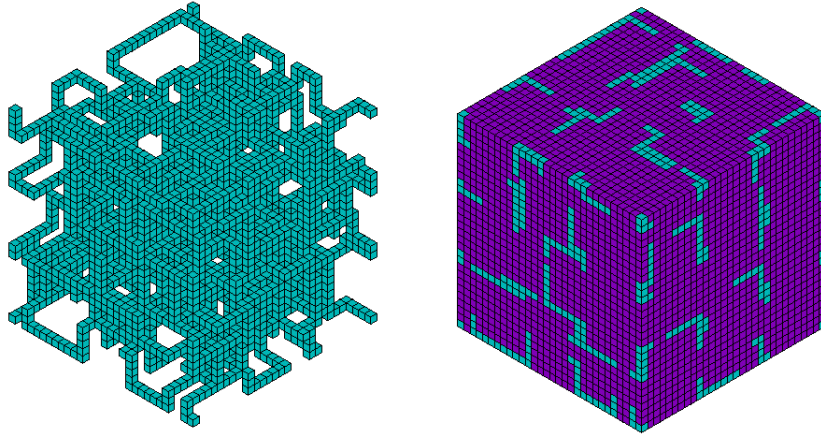


Figure 2: Method of connected skeletons. Representative volume with the size $30 \times 30 \times 30$ for 10% of the first phase material

in programs and analyzed in [3] with application to porous piezoelectric materials. But it is obvious that these methods can be also used for the representative volumes of porous thermoelastic composites.

For example, the diffusion limited aggregation method of the Witten-Sander method [16] enables to obtain cluster of the fractal type. In a standard version of this method inside the original cubic lattice consisting of the material of the first phase we select an arbitrary particle (elementary cube) which will be the embryo for the future second phase. Then far from the embryo a new particle is born which wanders through the lattice in random reflecting from its boundaries. When the particle comes closely to the particles of this new phase, it sticks to them and thus the motion of the particle stops. After that a new particle of the first phase is selected and the step of the algorithm with the particle wandering repeats unless the required percentage between the phases of the binary composite is reached. As the result of the work of this algorithm, all the particles of the second phase will be connected to each other, i. e. only one cluster of the particles of the second phase is formed. For large sizes of the lattice the resulting cluster has an advanced branching structure with signs of fractals. However, the coupling of the particles of the first phase can not be guaranteed in this case.

For the composites with significant surface inhomogeneity the modification of the described algorithm can be useful, which differs only in the growth of the particles of the second phase from the specific plane. Here the particles are launched, for example, from the upper part of the lattice and in the process of their random movement they are reflected by lateral and upper edges of the lattice, settling on its lower surface and on the growing clusters of a new phase. As a result, the growth of the "particle trees" of the second phase also occurs on the lower surface of the binary composite. In contrast with standard Witten-Sander method, in the "growth from the plane" method there can be several clusters, but the coupling of the particles of the first phase is not guaranteed either.

Fig. 3 shows the variants of the constructed clusters of the material of the second phase for the representative volumes of the size $30 \times 30 \times 30$ for the porosity of 5 %. The cluster on the left is generated by the Witten-Sander method, and the clusters on the right are generated by the "growth from the plane" method. In Fig. 3 only the elements of the second phase are shown, and the elements of the first phase (thermoelastic matrix) are not represented. Besides, as the clusters from the elements of the second phase here are mainly located inside, then for convenience in Fig. 3 the visible edges of the representative volumes are also presented.

In [3] other percolation algorithms were also presented such as the method of initial concentration and the methods of longitudinal and transverse fiber arrangement. All these methods enable to build the models of the representative volumes of binary composites of various microstructure, and in particular the models of porous anisotropic thermoelastic composites.

In the case of the composites of periodic structure, such as the masonry fragments, for the representative volume we can select a set of periodicity cells and then apply the approaches described in Sections 2, 3.

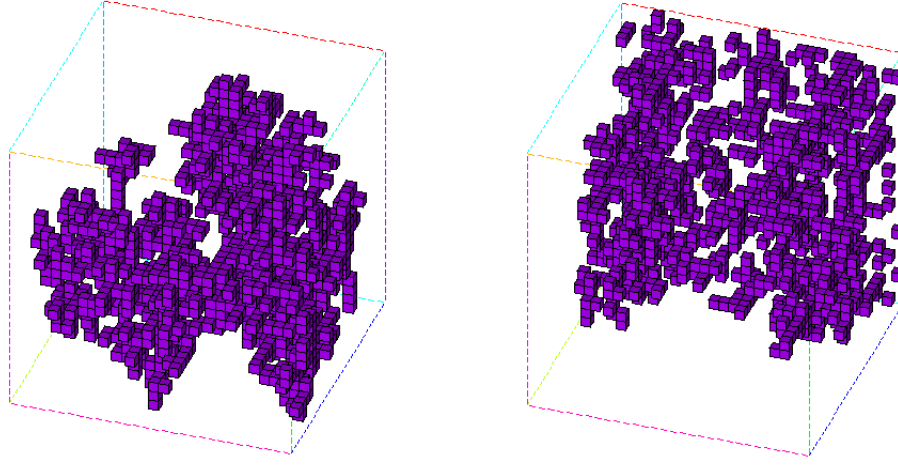


Figure 3: Witten-Sander method (left) and growth from the plane method (right). Representative volume with the size $30 \times 30 \times 30$ for 5% of the second phase material

5 NUMERICAL EXAMPLES

The finite element lattices described in the previous section were obtained with the help of the programs in C++. Further calculation of the material modules were carried out using the methodology of Section 2 and 3 in ANSYS finite element complex. In order to do that the finite element models of the representative volumes were translated in ANSYS together with the arrays of the signs of the material properties of the finite elements (1 is the material of the first phase, 2 is the material of the second phase). To solve the boundary value problems of thermoelasticity (3)–(6), we used the elements SOLID226 with the options of thermoelastic analysis and to solve the problems of thermal conductivity (4), (7)) we used the elements SOLID90 for thermal analysis. These elements are hexahedrons with 20 nodes which in total ensure quadratic approximations by canonic variables for the displacement and temperature fields.

As an example let us consider a porous silicon [8]. As it is known [13], silicon is an anisotropic material of cubic system, and we assume the following values of the non-zero materials moduli of a silicon with zero porosity ([13] at the temperature $T = 300$): $c_{11} = c_{12} = 16.56 \cdot 10^{10}$ (N/m²), $c_{12} = c_{13} = c_{23} = 6.39 \cdot 10^{10}$ (N/m²), $c_{21} = c_{12}$, $c_{31} = c_{13}$, $c_{32} = c_{23}$, $c_{44} = c_{55} = c_{66} = 7.95 \cdot 10^{10}$ (N/m²), $\alpha = 2.62 \cdot 10^{-6}$ (K⁻¹), $\beta = \alpha(c_{11} + 2c_{12})$, $\beta_{11} = \beta_{22} = \beta_{33} = \beta$, $k_{11} = k_{22} = k_{33} = k$, $k = 156$ (W/(m · K)).

The material constants for the pores (marked by "tilde") were taken equal to the following values: $\tilde{c}_{ij} = \kappa c_{ij}$, $\alpha = \kappa \alpha$, $\kappa = 1 \cdot 10^{-10}$, $\tilde{k} = 0.025$ (W/(m · K)).

As it can be seen, the considered thermoelastic material in stationary problems is characterized by five material moduli: the elastic stiffness moduli c_{11} , c_{12} , c_{44} ; thermal stress module β and thermal conductivity module k .

Let us assume that the models of the representative volumes do not have explicit geometric anisotropy and hence the porous silicon also belongs to the class of anisotropic materials of cubic system. Then for the full set of effective stiffness moduli and thermal stresses it is enough to solve three problems (3)–(6) with various boundary conditions in (6)

$$\text{I } \mathbf{S}_0 = \varepsilon_0 \mathbf{h}_1, \quad \theta_0 = 0 \quad \Rightarrow \quad c_{1j}^{eff} = \langle T_j \rangle / \varepsilon_0 = \langle \sigma_{jj} \rangle / \varepsilon_0, \quad j = 1, 2, 3, \quad (14)$$

$$\text{II } \mathbf{S}_0 = \varepsilon_0 \mathbf{h}_4, \quad \theta_0 = 0 \quad \Rightarrow \quad c_{44}^{eff} = \langle T_4 \rangle / \varepsilon_0 = \langle \sigma_{23} \rangle / \varepsilon_0, \quad (15)$$

$$\text{III } \mathbf{S}_0 = 0, \quad \theta_0 \neq 0 \quad \Rightarrow \quad \beta_{44}^{eff} = \langle T_1 \rangle / \theta_0 = \langle \sigma_{11} \rangle / \theta_0, \quad (16)$$

where in (14) for the computations it should be $c_{12}^{eff} \approx c_{13}^{eff}$.

Finally, the fourth problem (4), (7) enables to determine an effective thermal conductivity coefficient k^{eff}

$$\text{IV } \mathbf{G}_0 = G_{01} \mathbf{e}_1 \quad \Rightarrow \quad k^{eff} = -\langle q_1 \rangle / G_{01}. \quad (17)$$

Thus, four boundary-value problems for the representative volumes (three problems (3)–(6), that differ by their boundary conditions and one problem (4), (7)) in total by (14)–(17) enable to calculate five main material thermoelastic constants of porous silicon: c_{11}^{eff} , c_{12}^{eff} , c_{44}^{eff} , β^{eff} and k^{eff} . By these values we can find other important constants: the elastic compliances $s_{11}^{eff} = (c_{11}^{eff} + c_{12}^{eff})/\Delta_c^{eff}$, $s_{12}^{eff} = -c_{12}^{eff}/\Delta_c^{eff}$, $\Delta_c^{eff} = (c_{11}^{eff})^2 + c_{11}^{eff}c_{12}^{eff} - 2(c_{12}^{eff})^2$; the Young's modulus $E^{eff} = 1/s_{11}^{eff}$; the Poisson's ratio $\nu^{eff} = -s_{12}^{eff}/s_{11}^{eff} = c_{12}^{eff}/(c_{11}^{eff} + c_{12}^{eff})$; the bulk modulus $K^{eff} = E^{eff}/[3(1 - 2\nu^{eff})]$ and the coefficient of thermal expansion $\alpha^{eff} = \beta^{eff}/(c_{11}^{eff} + 2c_{12}^{eff})$.

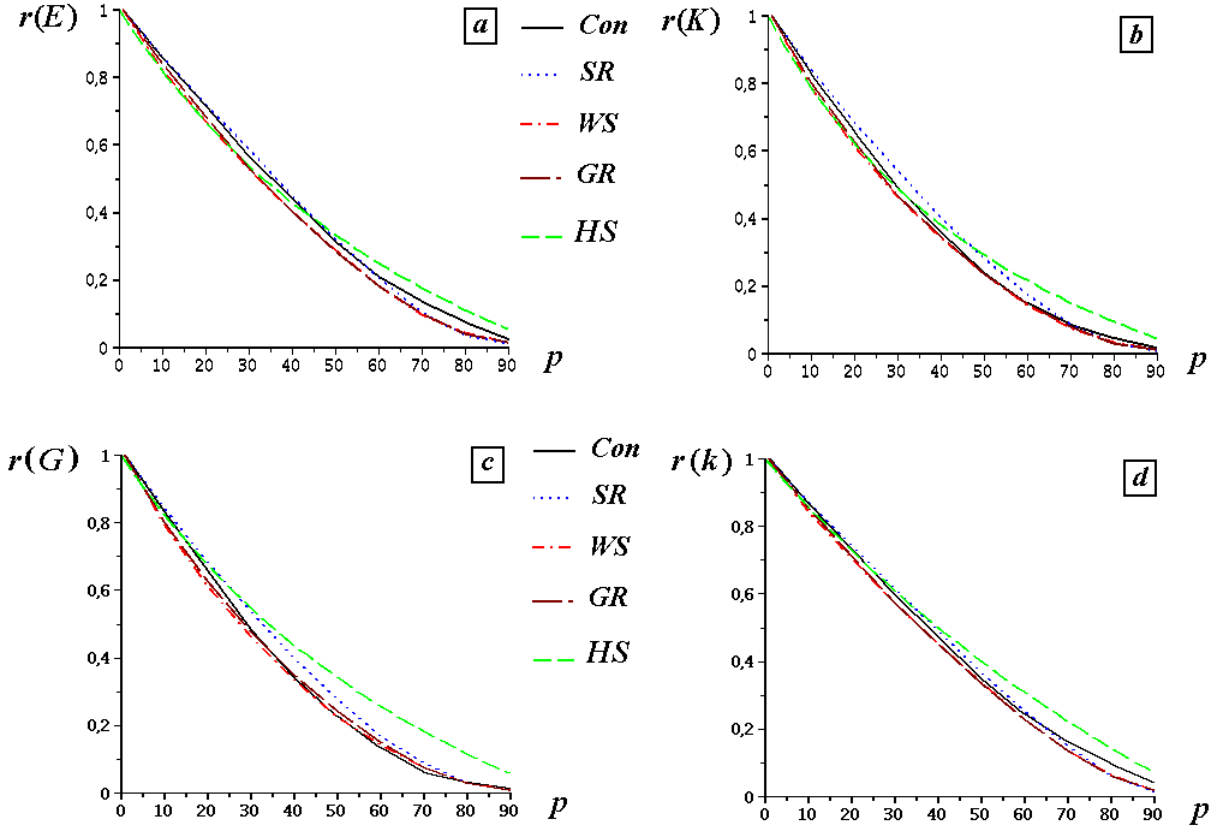


Figure 4: Dependences of the relative values of the effective moduli on the porosity

Fig. 4 shows some computation results of the relative values of the effective moduli $r(\dots)$ with respect to the porosity p (in percents). Here the values of the effective moduli are related to the corresponding values of the material moduli for zero porosity, for example $r(E) = E^{eff}(p)/E$, and by analogy for the relative values of the bulk modulus K , the shear modulus $G = c_{44}$ and the thermal conductivity coefficient k . Everywhere in Fig. 4 the curves of various types correspond to the results obtained for different methods of the representative volume generation: *Con* is the method that supports the coupling of the structural framework up to 90 % porosity, *SR* is the simple random method, *WS* is the Witten-Sander method and *GR* is the "growth from the plane" method. Besides, in Fig. 4 the dashed curves (*HS*) show the calculations by the approximate formulas of Hashin-Shtrikman for isotropic porous composites [6]: $r(E_{HS}) = r(K_{HS})r(G_{HS})(3 + \kappa)/[3r(K_{HS}) + \kappa r(G_{HS})]$; $r(K_{HS}) = 1 - (3 + 4\kappa)c/(3c + 4\kappa)$; $r(G_{HS}) = 1 - (15 + 20\kappa)c/[9 + 8\kappa + (6 + 12\kappa)c]$; $r(k_{HS}) = (1 - c)/(1 + c/2)$; $c = p/100$; $\kappa = 3(1 - 2\nu)/2/(1 + \nu)$.

Before analyzing the curves in Fig. 4 let us make some notes. All computations were carried out with the use of cubic lattices of size $20 \times 20 \times 20$ described in the previous section. For the simple random method three sets of computations were performed and after that the average values were calculated. While theoretically this method can give any structures of the representative volumes in the frames of the considered cubic lattices, the composites obtained in result of numerical experiments did not show the signs of the structures generated by three other methods from Section 4. Finally, as the coupling of the skeleton was not supported in the simple random method, Witten-Sander method and "growth from the plane" method, these methods gave lower results for the effective moduli that decrease with the porosity increase.

The results shown in Fig. 4 show that almost in all cases the Witten-Sander and "growth from the plane" method

give close values of the effective moduli. When the porosity value is not large, the values of the Young's effective moduli and thermal conductivity coefficients obtained by the method that supports the coupling of the structural skeleton, and by the simple random method are quite close to each other and significantly differ from the values obtained by the Witten-Sander and "growth from the plane" methods. Meanwhile, the values of the bulk modulus and the shear modulus obtained by the method that supports the coupling of the structural skeleton, are closer to the values obtained by the Witten-Sander and "growth from the plane" method than to the values obtained by the simple random method. The values calculated by analytical formulas of Hashin-Shtrikman for isotropic porous composites for small porosity are quite close to the values obtained by the Witten-Sander and "growth from the plane" method, but even for an average porosity value significantly differ from the values of the effective moduli calculated with the use of finite element programs for all considered types of the representative volumes. For large porosity among all the methods described we can recommend only the method that supports the coupling of the structural skeleton, as other methods can lead to disparate parts of the material matrix and eventually give results that correspond to the models with significantly larger porosity.

6 CONCLUSIONS

The paper considers an integrated approach to the determination of the material properties of thermoelastic bulk (mixture) stochastic distributed and periodic composites of an arbitrary anisotropy class with account for their internal microstructure. According to the classical effective moduli method of the mechanics of composites it is necessary to choose a set of stationary boundary value problems for a representative volume or for a periodical cell, which enables to determine effective properties of an equivalent anisotropic material. The representative volumes or cells are simulated with account for its internal microstructure, and the thermoelastic boundary value problems obtained for inhomogeneous media are solved numerically by the finite element method. The postprocessing of the solutions obtained gives averaged characteristics of the stress-strain state and thermal fields that enable to compute the effective moduli of the composite.

For bulk (mixture) binary composites two types of structures are investigated, namely, a mixture composite consisting of two fractions (phases) and a porous composite, for which the first fraction is a structure matrix, and the second fraction is a pore. Various models of representative volumes with selectable values of the phase entry parts are considered. These models are generated randomly, but at the same time under certain determinacy laws. The following approaches were implemented into computer models: the random generation of the entry for one of the phases (pores); the method that supports the skeleton connectivity for one of the phases for up to 90% entry for the second volume fraction of the second phase; the diffusion limited aggregation (DLA) method or the Witten-Sander method; the DLA "growth from the plane" and a range of other methods.

Among the sets of the boundary conditions, two basic types of boundary conditions were considered, namely, the boundary conditions of the first kind (for displacements and temperature) and the boundary conditions of the second kind (for stresses and heat flow). These known forms of boundary conditions permit to obtain constant fields of stresses, strains, temperature gradients and heat flows for homogeneous media. For porous thermoelastic composites only the boundary conditions of the first kind were taken.

Numeric implementation of the approach required to develop the set of programs in C++ language, which enables to generate the structures of the representative volumes by the chosen methods. The resulting sets of data on the properties of the elements of the cubic lattices of binary composites were further transferred to the programs in APDL language for ANSYS finite element package. This package allowed to solve the sets of thermoelastic problems under special sets of boundary conditions and to calculate the effective moduli of anisotropic thermoelastic composites.

To provide some examples, we have considered thermoelastic materials of porous silicon and copper-tungsten alloy (presented at the conference only). The described approaches are extended for the periodic masonry with porous bricks. A periodic part of masonry with porous bricks was chosen as a representative cell with thermoelastic tetrahedral and hexahedral finite elements. Various models of representative cells with different porous bricks, thickness of mortar and periodic structure are considered. (Also presented at the conference only.)

The results of numerical experiments showed that the structures of the representative volumes or cells could significantly affect the values of the effective moduli for the considered thermoelastic composites, especially for large inclusion parts of one of the phases or especially for large porosity of the brick structures.

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References

- [1] Cho, J.R., Kang, Y.J., Jeong, K.Y., Noh, Y.J., Lim, O.K. (2012), "Homogenization and thermoelastic analysis of heterogeneous materials with regular and random microstructures", *Composites: Part B.*, Vol. 43, pp. 2313–2323.
- [2] Christensen, R.M. (1979), *Mechanics of Composite Materials*, Wiley, New York.
- [3] Domashenkina, T.V., Nasedkin, A.V., Remizov, V.V. and Shevtsova, M.S. (2011), "Finite element modeling of porous piezocomposite materials with different connectivity and applications for analysis of ultrasonic transducers", *Proc. 7th GRACM Int. Congr. Comput. Mechanics*, Athens, Greece, June 30 - July 2, 2011, CD format, 2011, Paper 141, 10 p.
- [4] Giraud, A., Hoxha, D., Do, D.P. and Magnenet, V. (2008), "Effect of pore shape on effective porothermoelastic properties of isotropic rocks", *Int. J. Solids Struct.*, Vol. 45, pp. 1–23.
- [5] Martini, R., Depauw, V., Gonzalez, M., Vanstreels, K., Nieuwenhuysen, K.V., Gordon, I. and Poortmans, J. (2012), "Mechanical properties of sintered meso-porous silicon: a numerical model", *Nanoscale Res. Lett.*, Vol. 7(1), p. 597.
- [6] Nasedkin, A., Rybjanets, A., Kushkuley, L., Eshel, Y. and Tasker, R. (2005), "Different approaches to finite element modelling of effective moduli of porous piezoceramics with 3-3 (3-0) connectivity", *Proc. 2005 IEEE Ultrason. Symp.*, Rotterdam, Sept. 18 -21, 2005, pp. 1648–1651.
- [7] Nasedkin, A.V. and Shevtsova, M.S. (2011), "Improved finite element approaches for modeling of porous piezocomposite materials with different connectivity", In: *Ferroelectrics and Superconductors: Properties and Applications*, Ed. I.A. Parinov, Nova Science Publ., N.-Y., ch. 7, pp. 231–254.
- [8] Nasedkin, A.V., Nasedkina, A.A. and Remizov, V.V. (2014), "Finite element modeling of porous thermoelastic composites with account for their microstructure", *Computational continuum mechanics*, Vol. 71, pp. 100–109. (in Russian)
- [9] Newnham, R.E., Skinner, D.P. and Cross, L.E. (1978), "Connectivity and piezoelectric pyroelectric composites", *Mater. Res. Bull.*, Vol. 13(5), pp. 525–536.
- [10] Öchsner, A., Tane, M. and Nakajima, H. (2006), "Prediction of the thermal properties of lotus-type and quasi-isotropic porous metals: Numerical and analytical methods", *Materials Letters*, Vol. 60, pp. 2690–2694.
- [11] Pabst, W. and Gregorova, E. (2007), "A cross-property relation between the tensile modulus and the thermal conductivity of porous materials", *Ceramics International*, Vol. 33, pp. 9–12.
- [12] Pobedria, B.E. (1984), *Mechanics of Composite Materials*, Moscow State University Press. (in Russian)
- [13] Hull, R. (Ed.) (1999), *Properties of crystalline silicon*, London: INSPEC.
- [14] Shermegor, T.D. (1977), *Theory of elasticity of microin-homogeneous media*, Moscow, Nauka Publ. (in Russian)
- [15] Vel, S.S. and Goupee, A.J. (2010), "Multiscale thermoelastic analysis of random heterogeneous materials. Part I: Microstructure characterization and homogenization of material properties", *Comput. Mater. Sci.*, Vol. 48, pp. 22–38.
- [16] Witten, T.A. and Sander, L.M. (1981), "Diffusion-limited aggregation, a kinetic critical phenomenon", *Phys. Rev. Lett.*, Vol. 47, pp. 1400–1403.
- [17] Zhang, S., Yang, D.S., Zhang, H.W. and Zheng, Y.G. (2013), "Coupling extended multiscale finite element method for thermoelastic analysis of heterogeneous multiphase materials", *Comput. and Structures*, Vol. 121, pp. 32–49.