ECONTECHMOD. AN INTERNATIONAL QUARTERLY JOURNAL – 2015, Vol. 04, No. 2, 03–12

Effective Thermal Characteristics Synthesis Microlevel Models in the Problems of Composite Materials Optimal Design

Nazariy Jaworski

Lviv Polytechnic National Univesity
e-mail: Nazariy.Jaworski@gmail.com

Received May 06 2015; accepted June 30 2015

Abstract. The composite materials optimal design problem which taking into account the thermal characteristics is the part of an actual structural design task. A wide range of variety of such material structures and the complexity of modeling some physical phenomena (such as the phenomenon of those structures effective characteristics percolation threshold appearing) requires a high level of detail in physico-mathematical models. Here, in this paper, were analyzed the role and place of physico-mathematical microlevel models in problems of composite materials optimal design. The methods of such materials representative volume elements construction within the model calculations, which are the key step in the modeling of complex structures variety, also were analyzed. Basing on the usage of finite element method for modeling of stationary heat conduction and elasticity linear problems was proposed the combined formalization of coupled thermoelasticity problems simulation method in complex structured composite materials, which is especially useful when used in engineering applications which provide a high level of abstraction. Basing on the analogy method and theory of similarity were developed the complex structured composite materials microlevel models, which allow one to synthesize and then re-use in the problems of composite materials optimal design, such effective thermal characteristics as thermal conduction coefficient, Young's modulus, Poisson's ratio and temperature coefficient of linear expansion. This gives the ability to avoid of classical complex mathematical homogenization processes or real experiments. The method and models were successfully implemented by using of high-performance parallel and distributed computing technologies in heterogeneous computing environments, as evidenced by the simulation results.

Key words: composite materials, optimal design, microlevel models, finite element method, coupled problems, multiphysics problems.

INTRODUCTION

The composite materials (CM) optimal design problem which taking into account the thermal characteristics [1] is the part of an actual structural design task. Volumes of research in this field are growing every year, as evidenced by the increase in the number of published papers. A wide range of variety of such material structures [2] and the complexity of modeling some physical phenomena (such as the phenomenon of those structures effective characteristics percolation threshold appearing) requires a high level of detail in microlevel physico-mathematical models. To solve the described problems is appropriate to use numerical modeling techniques, such as finite element method.

In this paper, one has gotten the further development of numerical microlevel effective thermal characteristics synthesis models of composite materials with complex structure. Basing on the usage of finite element method for modeling coupled thermoelasticity problems and analogies method were developed microlevel models of composite materials. Models allow one to synthesize effective thermal characteristics such as thermal conduction coefficient, Young's modulus, Poisson's ratio and temperature coefficient of linear expansion. The main difference from other models is combined formalization of coupled multiphysics problems, which allows one to simultaneously take into account boundary conditions in the form of heat flows, surface loads, given surface temperatures and movements, if they are present. This approach is especially useful when used in engineering applications which provide a high level of abstraction. The models successfully implemented by technologies of high-performance parallel and distributed computing, which opens the possibility of direct effective usage in problems of CM optimal design.

THE ANALYSIS OF RECENT RESEARCHES AND PUBLICATIONS

Microlevel composite materials models

Composite materials or composites – materials composed from two or more components, and have specific properties that are different from the properties of their component sum [3]. There are two fundamentally different approaches of building models in the tasks of CM analysis or synthesis – consideration of material as a system of interacting elementary physical component, and consideration of material as some abstract continuous environment. The combination of both approaches in the model allows one to define the structural element order relative to the entire CM system. Under this order, any CM model can be attributed to such classes as empirical, structural, microlevel [4, 5]. The most promising in terms of research, automation, and further practical use, is the microlevel models class that allows one to describe irregularities of base elements, and gives the ability to describe real physical and spatial CM structures most adequately. Models of this class are using numerical methods for solving problems of analysis such as finite element method [6 – 8], thus, allow one to cover almost the entire range of phenomena known to modern science. Here the analysis of physical processes is considered in the so-called representative volume element (RVE) [4, 9]. Determination of its size is usually carried out by a series of numerical experiments [10].

In general case, CM optimal design algorithm, which is considering microlevel models, consists of the following stages:

1. Pre-design phase [11]:
   - select the model parameters that vary (components, structure formation options),
   - set the ranges of variation (maximum or minimum allowable concentrations of components, ranges of acceptable characteristics),
   - select optimal criteria (a set of characteristics that should be optimal – minimum or maximum, depending on the specific task).
2. Optimization phase:
   - formulate optimization problem, basing on pre-design phase,
   - problem solving:
     - o build representative volume element (model of the CM structure),
     - o do the model analysis by physico-mathematical problems numerical simulation,
     - o basing on the results, synthesize a set of model effective characteristics,
     - o check optimality criteria (selected effective characteristics), stop or continue the search, depending on the result.
3. The result – solution with optimal (for specific task) characteristics.

Representative volume element construction

Unlike the mathematical models and homogenization methods for constructing effective field as a superposition of each composite material constituent element contribution (e.g. Hashin polydisperse model [18]), microlevel models involve the construction so-called representative volume element (RVE) – usually a volume $\Omega \subset \Re^3$ of heterogeneous material, sufficiently large to describe it statistically, i.e. to effectively include a sampling of all microstructural heterogeneities that occur in the composite.

Another definition that is used in this paper and doesn't consider possible statistical fluctuations – the smallest composite material volume $\Omega \subset \Re^3$, for which macroscopic representation of spatial characteristics is sufficiently accurate model of effective response on corresponding outer influence [10]. In construction of the RVEs under problems of CM optimal design is convenient enough to use the cellular structure models [9], in the form of a large number of regular voxel-cells that simultaneously represent a regular finite-element discretization. Advantages of approach include:

- simplicity and relatively small number of computations in discretization [14, 15];
- the possibility of direct usage of domain decomposition methods for calculations and corresponding effective implementation on devices with big number of computing nodes [6];
- universality, which allow one to construct in one way such composite material complex structure models, as a model of random scalar fields, random cellular models, models with deterministic inclusions, and the combination of these models with the ability to build functional transition layers.

Construction of the RVE is the task of composite materials structure modeling that prior to physical processes analysis in these materials [12]. Classically, the heterogeneous systems microlevel model differential balance equations that describe physical processes, consider the structure of the CM as a combination of component material characteristics that are represented by equations coefficients and topology of the material, which is described by the integration borders where these equations are defined. Pair:

$$(\Omega, \mathbf{D}) = \bigcup_p \left(\Omega_p, \mathbf{D}_p\right), \tag{1}$$

where: $\mathbf{D}_p$ – the set of characteristics of p-th component, and Ω_p – corresponding geometric area, i.e. its topology; completely describes the composite material microlevel structure model. By using this formalization, the RVE can be conveniently presented as a cubic matrix of scalar intensities, i.e. cells that accept scalar values in a certain range, for example from 0 to 1. With a large number of cells, by defining the intensities intervals as a separate composite phases Ω_p and giving them an appropriate characteristics set $\mathbf{D}_p$, it is possible to construct the model of complex structure (Fig. 1).

OBJECTIVES

The main objectives of this paper are: development of complex structured composite materials microlevel models basing on multiphisics problems numerical simulation by finite element method, which gives the ability to avoid of classical complex mathematical homogenization processes or real experiments; as the consequence, development of materials effective thermal characteristics synthesis models that can be used in the problems of composite materials optimal design.

COMPOSITE MATERIALS ANALYSIS BASING ON PHYSICO-MATHEMATICAL PROBLEMS NUMERICAL SIMULATION

The stationary heat conduction linear problem

Numerical simulation of stationary heat conduction problems in CM RVEs is the basis which allows one to synthesize the effective thermal conduction coefficient λ_{eff}. A standardized [19, 20] λ_{eff} finding method of some material sample with thickness d is taken as the starting point:

$$\lambda_{eff} = \frac{d \cdot q}{\Gamma_q \Delta T} = \frac{d \cdot q}{\Gamma_q (T_{\Gamma_q} - T_\infty)}, \tag{2}$$

where: heat flux $\partial T / \partial \mathbf{n} = q$, i.e. Neumann boundary condition on a RVE side $\Gamma_q \subset \Re^2$, and outer environment temperature T_∞, i.e. Dirichlet boundary condition on the opposite RVE side $\Gamma_{T_\infty} \subset \Re^2$, are known. In fact, there are no boundary conditions on other sides – they are, so-called, "floating" sides ($\partial T/\partial \mathbf{n} = 0$):

$$\begin{cases} \mathcal{L}(T(\mathbf{x})) = 0 \Rightarrow \lambda \dfrac{\partial^2 T}{\partial x^2} + \lambda \dfrac{\partial^2 T}{\partial y^2} + \lambda \dfrac{\partial^2 T}{\partial z^2} = 0, \\ \ell_q(T(\mathbf{x}))\Big|_{\Gamma_q} = q \Rightarrow \dfrac{\partial T}{\partial \mathbf{n}}\Big|_{\Gamma_q} = q, \quad \mathbf{n} \perp \Gamma, \\ \ell_{T_\infty}(T(\mathbf{x}))\Big|_{\Gamma_{T_\infty}} = T_\infty \Rightarrow T\Big|_{\Gamma_{T_\infty}} = T_\infty. \end{cases} \tag{3}$$

It should be noted that the temperature field must be uninterrupted between the composite phases. It is necessary to specify, so-called, fourth type boundary conditions, also called as ideal contact. However, with the further numerical problem simulation by finite element method, this condition is automatically satisfied by the finite-element basis consistency requirement [13], and visibly not specified.

Approximate test solution can be built as:

$$T(\mathbf{x}) \approx \tilde{T}(\mathbf{x}) = \sum_{j=1}^{M} T_j \varphi_j(\mathbf{x}), \tag{4}$$

where: T_j – unknown temperature at RVE cells that should be found; φ_j – some simple polynomial basis function.

Putting the test solution into boundary value problem, gives residuals:

$$\mathcal{L}(\tilde{T}(\mathbf{x})) = R^{\Omega}(\mathbf{x}) \neq 0, \quad \ell_q(\tilde{T}(\mathbf{x}))\Big|_{\Gamma_q} = R^{\Gamma_q}(\mathbf{x}) \neq q,$$
$$\ell_{T_\infty}(\tilde{T}(\mathbf{x}))\Big|_{\Gamma_{T_\infty}} = R^{\Gamma_{T_\infty}}(\mathbf{x}) = T_\infty, \tag{5}$$

note that the last residual is exactly matched.

The best approximation of the true solution $T(\mathbf{x}) \in \mathcal{H}^\infty(\Omega)$ is an orthogonal projection $\tilde{T}(\mathbf{x})$ into subspace $C^1 \subset \mathcal{H}^\infty(\Omega)$ that is defined by functions φ:

$$\left\langle R^{\Omega}(\mathbf{x}), \varphi_i^{\Omega}(\mathbf{x}) \right\rangle + \left\langle R^{\Gamma_q}(\mathbf{x}), \varphi_i^{\Gamma_q}(\mathbf{x}) \right\rangle = 0,$$
$$i = 1, 2, \ldots, M, \quad \varphi_i^{\Omega} = -\varphi_i^{\Gamma_q}, \tag{6}$$

or:

$$\iiint_{\Omega} \varphi_i^{\Omega}(\mathbf{x}) \left[\sum_{j=1}^{M} T_j \mathcal{L}(\varphi_j(\mathbf{x})) \right] d\Omega +$$
$$+ \iint_{\Gamma_q} \varphi_i^{\Gamma_q}(\mathbf{x}) \left[\sum_{j=1}^{M} a_j \ell(\varphi_j(\mathbf{x})) - q \right] d\Gamma = 0, \quad 1 \le i, j \le M. \tag{7}$$

Smoothness C^1 of the test solution is minimum permissible, because in the original equation are presenting maximum second order derivatives.

Resulting expression can be rewritten in a weak form, and thus one can weaken the requirements for basis functions smoothness ($\varphi \in C^1 \Rightarrow \varphi \in C^0$). For example, by using the rule of integration by parts and divergence theorem, last expression can include Neumann boundary conditions, which are natural for it ($\varphi_i^{\Omega} = -\varphi_i^{\Gamma_q}$):

$$\left[\iiint_{\Omega} \left[\frac{\partial \varphi_i}{\partial x}\frac{\partial \varphi_j}{\partial x} + \frac{\partial \varphi_i}{\partial y}\frac{\partial \varphi_j}{\partial y} + \right.\right.$$
$$\left.\left. + \frac{\partial \varphi_i}{\partial z}\frac{\partial \varphi_j}{\partial z} \right] dxdydz \right] T_j = -\iint_{\Gamma_q} q \varphi_i d\Gamma. \tag{8}$$

Let change notation to known stiffness matrix and loads vector $[\mathbf{K}]\{\mathbf{u}\} = \{\mathbf{f}\}$ (brackets – matrix; braces – vector).

Let split RVE $\Omega \subset \Re^3$ into tetrahedral finite elements (i.e. simplex elements) $\Omega_i \subset \Omega \subset \Re^3$, $i = 1, 2, \ldots, P$.

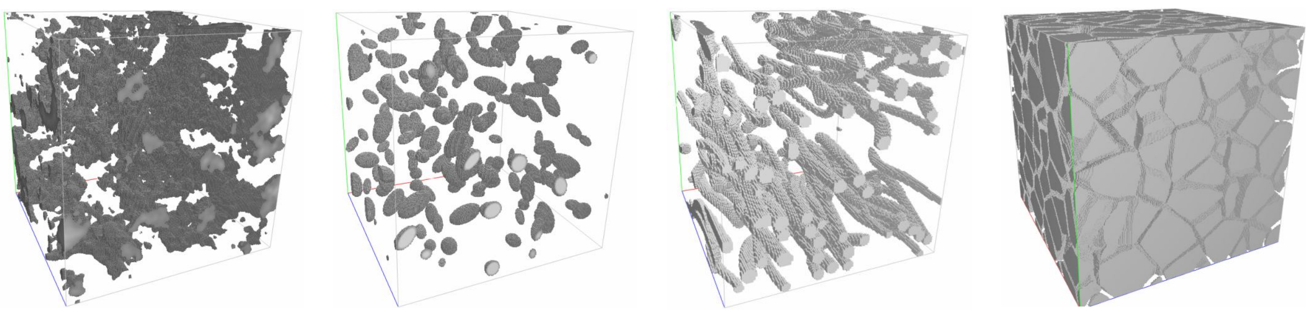
Using the simplex elements is permissible since such basis is C^0 smooth and easily consistent with neighboring (temperature will be uninterrupted between elements). For this is using a simple template method in which every four adjacent RVE cells form a cube, which can be divided into six tetrahedrons.

Now all "local" stiffness matrices $[\mathbf{K}]_i$ and load vectors $\{\mathbf{f}\}_i$ should be found. For linear simplex finite element basis functions are its barycentric coordinates:

$$\lambda_i \sum_{j=1}^{4} T_{i,j} N_{i,j}(\mathbf{x}) = \lambda_i \left[N_{i,1} \; N_{i,2} \; N_{i,3} \; N_{i,4} \right] \cdot$$
$$\cdot \left\{ T_{i,1} \; T_{i,2} \; T_{i,3} \; T_{i,4} \right\}^{\mathbf{T}} = [\mathbf{N}]_i \{\mathbf{u}\}_i, \tag{9}$$

where:

$$[\mathbf{N}] = \begin{bmatrix} 1 & x & y & z \end{bmatrix} \begin{bmatrix} 1 & x_1 & y_1 & z_1 \\ 1 & x_2 & y_2 & z_2 \\ 1 & x_3 & y_3 & z_3 \\ 1 & x_4 & y_4 & z_4 \end{bmatrix}^{-1}. \tag{10}$$



a) b) c) d)

Fig.1. Example of representative volume elements in the form of a 256x256x256 elements matrix that represents composite materials microlevel structure models:
a) scalar random fields; b) random ellipsoid particles; c) fibers; d) cellular structures

The boundary of any tetrahedron is a triangle – 2D simplex. Here can be found each local load vector, for example, for firs three nodes of tetrahedron:

$$\{\mathbf{f}\}_i = \iint_{\Gamma_q} [\mathbf{N}]^{\mathbf{T}} q d\Gamma = q \int_{\Gamma_q} \begin{Bmatrix} N_1 \\ N_2 \\ N_3 \\ 0 \end{Bmatrix} d\Gamma =$$

$$= q \int_0^1 \int_0^{1-N_1} \int_0^{1-N_1-N_2} \begin{Bmatrix} N_1 \\ N_2 \\ N_3 \\ 0 \end{Bmatrix} \left|[\mathbf{Jac_N x}]\right| dN_3 dN_2 dN_1 = q\frac{(\Gamma_q)_i}{3}. \tag{11}$$

If finite element doesn`t contain boundary triangle, its load vector will be empty – local boundary value problem is not correct i.e. “floating”, and can’t be solved without considering neighbor problems. To take into account Dirichlet boundary conditions is enough to modify the local system of equations, taking border nodal temperature equal to the given T_∞, i.e. exactly satisfy the residual $R^{\Gamma_{T_\infty}}$.

After recording weak form (8), its weak operator can be expressed in matrix form:

$$[\mathcal{L}] = \nabla(.) = \begin{bmatrix} \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \end{bmatrix}^{\mathbf{T}}. \tag{12}$$

As a result each local problem can be written as:

$$\left[\iiint_{\Omega_i} \left([\mathcal{L}][\mathbf{N}]_i\right)^{\mathbf{T}} [\mathbf{D}]_i \left([\mathcal{L}][\mathbf{N}]_i\right) dxdydz\right] \{\mathbf{u}\}_i = \{\mathbf{f}\}_i,$$

$$[\mathbf{D}]_i = \begin{bmatrix} \lambda_i & 0 & 0 \\ 0 & \lambda_i & 0 \\ 0 & 0 & \lambda_i \end{bmatrix}. \tag{13}$$

Values of each matrix $[\mathbf{D}]_i$ depends on which subarea Ω_p is located the finite element. Expression $[\mathcal{L}][\mathbf{N}]_i$ gives 3x4 matrix that contains only constants:

$$[\mathbf{K}]_i \{\mathbf{u}\}_i = \{\mathbf{f}\}_i,$$
$$[\mathbf{K}]_i = \left([\mathcal{L}][\mathbf{N}]_i\right)^{\mathbf{T}} [\mathbf{D}]_i \left([\mathcal{L}][\mathbf{N}]_i\right)\Omega_i. \tag{14}$$

When all local stiffness matrices and load vectors are found, they should be assembled into global SLAE, which describes initial boundary value problem (3). The solution can be conveniently found by conjugate gradient stabilized (to computational errors) method.

The stationary elasticity linear problem

Elasticity problem numerical simulation in CM RVEs allows one to synthesize effective Young's modulus E_{eff} and Poisson's ratio μ_{eff}. Together with the previous, this problem is the basis for the coupled thermoelasticity problem. Young's modulus can be found as:

$$E_{eff} = \frac{d \cdot f_x}{\Gamma_{\mathbf{f}} \Delta u_x} = \frac{d \cdot f_x}{\Gamma_{\mathbf{f}}(u_{x\mathbf{f}} - u_{x\infty})}, \quad f_y, f_z = 0, \tag{15}$$

where: $u_x, u_y, u_z = \mathbf{u}$ – mechanical displacements along coordinate axes x, y, z; $f_x, f_y, f_z = \mathbf{f}$ – components of the surface loads, i.e. Neumann boundary condition on a RVE side $\Gamma_f \subset \Re^2$; $u_{x\infty}$ – known starting displacement along chosen axis, i.e. Dirichlet boundary condition on the opposite RVE side $\Gamma_{u_\infty} \subset \Re^2$. Note that components $u_{y\infty}$ and $u_{z\infty}$ are no imposed in fact.

Poisson's ratio describes object transverse resizing under described conditions:

$$\mu_{eff} = \frac{\Delta u_y}{\Delta u_x} = \frac{\Delta u_z}{\Delta u_x}. \tag{16}$$

According to the classical linear elasticity theory [21, 22], there is a connection between displacements and deformation – strain tensor:

$$[\boldsymbol{\varepsilon}] = \begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \gamma_{xy} \\ \gamma_{xz} \\ \gamma_{yz} \end{bmatrix} = \begin{bmatrix} \partial u_x/\partial x \\ \partial u_y/\partial y \\ \partial u_z/\partial z \\ \partial u_x/\partial y + \partial u_y/\partial x \\ \partial u_x/\partial z + \partial u_z/\partial x \\ \partial u_y/\partial z + \partial u_z/\partial y \end{bmatrix} = [\mathcal{L}]\{\mathbf{u}\},$$

$$[\mathcal{L}] = \begin{bmatrix} \partial/\partial x & 0 & 0 \\ 0 & \partial/\partial y & 0 \\ 0 & 0 & \partial/\partial z \\ \partial/\partial y & \partial/\partial x & 0 \\ \partial/\partial z & 0 & \partial/\partial x \\ 0 & \partial/\partial z & \partial/\partial y \end{bmatrix}, \quad \{\mathbf{u}\} = \begin{Bmatrix} u_x \\ u_y \\ u_z \end{Bmatrix}. \tag{17}$$

According to Hooke's law relationship between the strain tensor and the stress tensor is expressed through the environment characteristics matrix:

$$[\boldsymbol{\sigma}] = \left(\sigma_x \ \sigma_y \ \sigma_z \ \tau_{xy} \ \tau_{xz} \ \tau_{yz}\right)^{\mathbf{T}} = [\mathbf{D}][\boldsymbol{\varepsilon}] = [\mathbf{D}][\mathcal{L}]\{\mathbf{u}\}, \tag{18}$$

where:

$$[\mathbf{D}] = G \cdot \begin{bmatrix} A & B & B & 0 & 0 & 0 \\ B & A & B & 0 & 0 & 0 \\ B & B & A & 0 & 0 & 0 \\ 0 & 0 & 0 & C & 0 & 0 \\ 0 & 0 & 0 & 0 & C & 0 \\ 0 & 0 & 0 & 0 & 0 & C \end{bmatrix},$$

$$G = E/(1+\mu)/(1-2\mu), \quad A = 1-\mu,$$
$$B = \mu, \quad C = (1-2\mu)/2. \tag{19}$$

Let consider the boundary value problem:

$$\begin{cases} \mathbf{u}(\mathbf{x}) = \{u_x(\mathbf{x}) \quad u_x(\mathbf{x}) \quad u_z(\mathbf{x})\}, \quad \mathbf{x} = \{x, y, z\} \in \Omega, \\ \mathcal{L}(\mathbf{u}(\mathbf{x})) = 0 \Rightarrow \begin{cases} \partial\sigma_x/\partial x + \partial\tau_{xy}/\partial y + \partial\tau_{xz}/\partial z = 0 \\ \partial\tau_{xy}/\partial x + \partial\sigma_y/\partial y + \partial\tau_{yz}/\partial z = 0, \\ \partial\tau_{xz}/\partial x + \partial\tau_{yz}/\partial y + \partial\sigma_z/\partial z = 0 \end{cases} \\ \ell_{\mathbf{f}}(\mathbf{u}(\mathbf{x}))\Big|_{\Gamma_{\mathbf{f}}} = \mathbf{f} \Rightarrow \begin{cases} \sigma_x l_x + \tau_{xy} l_y + \tau_{xz} l_z & = f_x \\ \tau_{xy} l_x + \sigma_y l_y + \tau_{yz} l_z & = 0 \\ \tau_{xz} l_x + \tau_{yz} l_y + \sigma_z l_z \Big|_{\Gamma_{\mathbf{f}}} & = 0 \end{cases}, \\ \ell_{\mathbf{u}_\infty}(\mathbf{u}(\mathbf{x}))\Big|_{\Gamma_{\mathbf{u}_\infty}} = \mathbf{u}_\infty \quad \Rightarrow \quad u_x\big|_{\Gamma_{\mathbf{u}_\infty}} = u_{x\infty}. \end{cases} \tag{20}$$

In matrix form the basic equation takes the form:

$$\mathcal{L}(\mathbf{u}(\mathbf{x})) = 0 \Rightarrow [\mathcal{L}]^{\mathbf{T}}[\mathbf{D}][\mathcal{L}]\{\mathbf{u}\} = 0. \tag{21}$$

Let construct an approximation by finite element method, similar to the previous heat conduction problem. One gets the weighted residuals equation:

$$\iiint_{\Omega_i}[\mathbf{N}]_i^{\mathbf{T}}\left([\mathcal{L}]^{\mathbf{T}}[\mathbf{D}]_i[\mathcal{L}]\{\tilde{\mathbf{u}}\}_i\right)d\Omega - \\ -\iint_{\Gamma_{\mathbf{f}i}}[\mathbf{N}]_i^{\mathbf{T}}\frac{\partial\{\tilde{\mathbf{u}}\}_i}{\partial\mathbf{n}}d\Gamma+\iint_{\Gamma_{\mathbf{f}i}}[\mathbf{N}]_i^{\mathbf{T}}\mathbf{f}_i d\Gamma=0. \quad (22)$$

It can also be reduced to a weak form that includes Neumann boundary conditions:

$$\left(\iiint_{\Omega_i}\left([\mathcal{L}][\mathbf{N}]_i\right)^{\mathbf{T}}[\mathbf{D}]_i\left([\mathcal{L}][\mathbf{N}]_i\right)d\Omega\right)\{\mathbf{u}\}_i = \\ =\iint_{\Gamma_{\mathbf{f}i}}[\mathbf{N}]_i^{\mathbf{T}}\mathbf{f}_i d\Gamma. \quad (23)$$

Unlike the previous problem, the matrix of basis functions is sparse. For simplex elements it can be written as:

$$[\mathbf{N}]=\left[[\mathbf{M}]_1,[\mathbf{M}]_2,[\mathbf{M}]_3,[\mathbf{M}]_4\right], \\ [\mathbf{M}]_k=\begin{bmatrix}N_k & 0 & 0\\ 0 & N_k & 0\\ 0 & 0 & N_k\end{bmatrix}, \quad (24)$$

wherefrom the expression $[\mathcal{L}][\mathbf{N}]$ for all elements can be written as:

$$[\mathcal{L}][\mathbf{N}]=\left[[\mathbf{M}]_1,[\mathbf{M}]_2,[\mathbf{M}]_3,[\mathbf{M}]_4\right], \\ [\mathbf{M}]_k=\begin{bmatrix}b_k & 0 & 0 & c_k & d_k & 0\\ 0 & c_k & 0 & b_k & 0 & d_k\\ 0 & 0 & d_k & 0 & b_k & c_k\end{bmatrix}^{\mathbf{T}}, \quad (25)$$

$$\begin{bmatrix}1 & x_1 & y_1 & z_1\\ 1 & x_2 & y_2 & z_2\\ 1 & x_3 & y_3 & z_3\\ 1 & x_4 & y_4 & z_4\end{bmatrix}^{-1}=\begin{bmatrix}a_1 & a_2 & a_3 & a_4\\ b_1 & b_2 & b_3 & b_4\\ c_1 & c_2 & c_3 & c_4\\ d_1 & d_2 & d_3 & d_4\end{bmatrix}.$$

Last expression again contains only constants and that's why the local 12x12 stiffness matrix finding is a trivial task (14). Finding of the local loads vectors differs from the previous case in part that the vector expands to 12 elements – three load components per node, each of which should be multiplied by one-third of that tetrahedron side area.

When all local stiffness matrices and load vectors are found, they should be assembled into global SLAE, which describes initial boundary value problem (20).

The solution can be conveniently found by conjugate gradient stabilized method.

THE MAIN RESULTS OF THE RESEARCH

The coupled thermoelasticity problem

Coupled problems are multiphysics problems and usually can be solved in two steps – firstly separately one finds a temperature field, and then a displacement field, which based on temperature, or vice versa, depending on given boundary conditions [23].

Here, basing on previously described linear stationary heat conduction and elasticity problems, is proposed the combined numerical model of thermoelasticity problem simulation in composite materials with complex structure, that unlike to traditional, gives the ability to take into account boundary conditions in the form of heat flows, surface loads, given surface temperatures and movements, if they are present. Combination is made by using a single differential matrix operator.

This approach is especially useful when used in engineering applications which provide a high level of abstraction, e.g. FEMLab/COMSOL or FreeFem++ [24].

Coupled thermoelasticity problem numerical simulation allows one to synthesize an effective thermal conduction coefficient λ_{eff} and temperature coefficient of linear expansion α_{eff} (LCTE).

The LCTE describes a thermal expansion within solid materials, according to which the linear sizes and body shape are changing by body temperature change under fixed environment pressure. In the general case LCTE can be found as:

$$\alpha_{eff}=\frac{1}{d}\frac{\Delta u_x}{\Delta T}, \quad (26)$$

with given heat flux q (Neumann b.c. on $\Gamma_f \subset \Re^2$) and outer environment temperature T_∞ (Dirichlet b.c. on the opposite side $\Gamma_{u_\infty} \subset \Re^2$). In addition, all displacement components $u_x = u_y = u_z = 0$ on $\Gamma_{\mathbf{u}_\infty}$, and transverse displacements $u_y = u_z = 0$ on flanks, should be limited, leaving the ability to deform in only one direction.

Let build the numerical model. In every point within RVE are unknown a value of temperature and displacements along coordinate axes:

$$\mathbf{u}(\mathbf{x})=\{T\ u_x\ u_y\ u_z\}^{\mathbf{T}}.$$

Let combine strain tensor and temperature gradient into single tensor:

$$[\boldsymbol{\varepsilon}]=\left\{q_x\ q_y\ q_z\ \varepsilon_x\ \varepsilon_y\ \varepsilon_z\ \gamma_{xy}\ \gamma_{xz}\ \gamma_{yz}\right\}^{\mathbf{T}}= \\ =\left\{\frac{\partial T}{\partial x}\ \frac{\partial T}{\partial y}\ \frac{\partial T}{\partial z}\ \frac{\partial u_x}{\partial x}\ \frac{\partial u_y}{\partial y}\ \frac{\partial u_z}{\partial z}\right. \quad (27) \\ \left.\frac{\partial u_x}{\partial y}+\frac{\partial u_y}{\partial x}\ \frac{\partial u_x}{\partial z}+\frac{\partial u_z}{\partial x}\ \frac{\partial u_y}{\partial z}+\frac{\partial u_z}{\partial y}\right\}^{\mathbf{T}}=[\mathcal{L}]\{\mathbf{u}\},$$

where: $[\mathcal{L}]$ – given problem differential operator matrix (in weak form), which is equal to:

$$[\mathcal{L}]=\begin{bmatrix}A & B & C & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & A & 0 & 0 & B & C & 0\\ 0 & 0 & 0 & 0 & B & 0 & A & 0 & C\\ 0 & 0 & 0 & 0 & 0 & C & 0 & A & B\end{bmatrix}^{\mathbf{T}} \quad (28) \\ A=\partial/\partial x,\quad B=\partial/\partial y,\quad C=\partial/\partial z.$$

Let combine the relation between strain tensor and stress tensor (Hooke's law) and between temperature gradient and heat flow (Fourier law) by single environment characteristics matrix:

$$[\mathbf{D}]=\begin{bmatrix} \lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \lambda & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & A & B & B & 0 & 0 & 0 \\ 0 & 0 & 0 & B & A & B & 0 & 0 & 0 \\ 0 & 0 & 0 & B & B & A & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & C & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & C & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & C \end{bmatrix}, \quad (29)$$

$$A = E(1-\mu)/(1+\mu)/(1-2\mu),$$

$$B = \mu E/(1+\mu)/(1-2\mu), \quad C = E/2+2\mu.$$

Given problem balance differential equations can be written as:

$$[\mathcal{L}]^{\mathrm{T}}[\mathbf{D}][\mathcal{L}]\{\mathbf{u}\}+\{\mathbf{X}\}=0, \quad (30)$$

where: $\{\mathbf{X}\}$ – inner heat sources or inner forces. By known LCTE α of the body components, can be found the inner forces:

$$X=\frac{\alpha E}{1-2\mu}\frac{\partial T}{\partial x}, \quad Y=\frac{\alpha E}{1-2\mu}\frac{\partial T}{\partial y}, \quad Z=\frac{\alpha E}{1-2\mu}\frac{\partial T}{\partial z}. \quad (31)$$

In other side, the material is warming under influences of the stress – it is equivalent to presence of the inner heat source that is equal to:

$$Q=\frac{\alpha E}{1-2\mu}\frac{\partial u_x}{\partial x}+\frac{\alpha E}{1-2\mu}\frac{\partial u_y}{\partial y}+\frac{\alpha E}{1-2\mu}\frac{\partial u_z}{\partial z}, \quad (32)$$

wherefrom:

$$\{\mathbf{X}\}=\{Q \quad X \quad Y \quad Z\}^{\mathrm{T}}=[\mathcal{L}]^{\mathrm{T}}[\mathbf{J}]\{\mathbf{u}\}, \quad (33)$$

where: $\{\mathbf{J}\}$ – matrix in form:

$$[\mathbf{J}]=\frac{\alpha E}{1-2\mu}\begin{bmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^{\mathrm{T}}. \quad (34)$$

Now can be written the weighted residual equation:

$$\iiint\limits_{\Omega_i}[\mathbf{N}]_i^{\mathrm{T}}\left([\mathcal{L}]^{\mathrm{T}}[\mathbf{D}]_i[\mathcal{L}]\{\tilde{\mathbf{u}}\}_i\right)d\Omega+$$
$$+\iiint\limits_{\Omega_i}[\mathbf{N}]_i^{\mathrm{T}}\left([\mathcal{L}]^{\mathrm{T}}\left([\mathbf{J}]\{\tilde{\mathbf{u}}\}_i\right)\right)d\Omega- \quad (35)$$
$$-\iint\limits_{\Gamma_{fi}}[\mathbf{N}]_i^{\mathrm{T}}\frac{\partial\{\tilde{\mathbf{u}}\}_i}{\partial\mathbf{n}}d\Gamma+\iint\limits_{\Gamma_{fi}}[\mathbf{N}]_i^{\mathrm{T}}\mathbf{f}_i d\Gamma=0,$$

which can be reduced to the weak form by including Neumann boundary conditions:

$$\left(\iiint\limits_{\Omega_i}\left([\mathcal{L}][\mathbf{N}]_i\right)^{\mathrm{T}}[\mathbf{D}]_i\left([\mathcal{L}][\mathbf{N}]_i\right)d\Omega-\right. \quad (36)$$
$$\left.-\iiint\limits_{\Omega_i}[\mathbf{N}]_i^{\mathrm{T}}\left([\mathcal{L}]^{\mathrm{T}}[\mathbf{J}][\mathbf{N}]_i\right)d\Omega\right)\{\mathbf{u}\}_i=\iint\limits_{\Gamma_{fi}}[\mathbf{N}]_i^{\mathrm{T}}\mathbf{f}_i d\Gamma.$$

As in the previous case, the matrix of basis functions is 4x16 sparse matrix. Expression $[\mathcal{L}][\mathbf{N}]$ for all elements can be written as:

$$[\mathcal{L}][\mathbf{N}]=\left[[\mathbf{M}]_1,[\mathbf{M}]_2,[\mathbf{M}]_3,[\mathbf{M}]_4\right],$$

$$[\mathbf{M}]_k=\begin{bmatrix} b_k & c_k & d_k & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & b_k & 0 & 0 & c_k & d_k & 0 \\ 0 & 0 & 0 & 0 & c_k & 0 & b_k & 0 & d_k \\ 0 & 0 & 0 & 0 & 0 & d_k & 0 & b_k & c_k \end{bmatrix}^{\mathrm{T}}. \quad (37)$$

The second term of stiffness matrix describes the inner heat force sources. For simplex elements it can be found same as loads vector, basing on tetrahedron barycentric coordinates, with the difference that the result should be multiplied by a quarter of the tetrahedron volume:

$$\iiint\limits_{\Omega_i}[\mathbf{N}]_i^{\mathrm{T}}\left([\mathcal{L}]^{\mathrm{T}}[\mathbf{J}][\mathbf{N}]_i\right)d\Omega=\frac{\Omega_i}{4}\frac{\alpha E}{1-2\mu}\cdot$$

$$\cdot\begin{bmatrix} [\mathbf{M}]_1 & [\mathbf{M}]_2 & [\mathbf{M}]_3 & [\mathbf{M}]_4 \\ [\mathbf{M}]_1 & [\mathbf{M}]_2 & [\mathbf{M}]_3 & [\mathbf{M}]_3 \\ [\mathbf{M}]_1 & [\mathbf{M}]_2 & [\mathbf{M}]_3 & [\mathbf{M}]_3 \\ [\mathbf{M}]_1 & [\mathbf{M}]_2 & [\mathbf{M}]_3 & [\mathbf{M}]_3 \end{bmatrix}, [\mathbf{M}]_k=\begin{bmatrix} 0 & b_k & c_k & d_k \\ b_k & 0 & 0 & 0 \\ c_k & 0 & 0 & 0 \\ d_k & 0 & 0 & 0 \end{bmatrix}. \quad (38)$$

Finding of the local loads vectors differs from the previous case in the part that vector expands to 16 elements, four components (heat flux + loads) per node, each of which should be multiplied by one-third of that tetrahedron side. When all local stiffness matrices and load vectors are found, they should be assembled into global SLAE, which describes initial boundary value problem (30).

The feature of this problem is that the differential operator and according SLAE are asymmetric, thanks to the contribution of inner heat and force sources. Since this term in the expression of stiffness matrix is standing with a minus sign, one can make sure that the system and its differential operator always be positively defined and bounded (doesn't give infinity under integration). These properties are sufficient for the convergence of computational model. An important difference in the practical realization is the impossibility of usage such approximate SLAE solving method as conjugate gradient method that may be used only for symmetric systems. However, in this case, can be used the biconjugate gradient stabilized method, which is a generalization of the previous.

Effective thermal characteristics synthesis

Approximate solution of physico-mathematical problems in the complex structured CM RVEs allows one to synthesize their effective characteristics, i.e. to do the homogenization procedure by numerical simulation. For this can be used thermoelectricity analogy method and theory of similarity [16, 17, 25 – 27]. Let consider the problem of non-stationary heat conduction described by parabolic equation:

$$c\rho\frac{\partial T}{\partial\tau}=\lambda\nabla^2 T, \quad (39)$$

where: specific heat capacity c [J/kg°C], when [J = kg·m^2/s^2]; density ρ [kg/m^3]; heat conduction coefficient λ [W/m°C], when [W = kg·m^2/s^3]; time τ [s]; distance x, y, z, or, ignoring the differential operator, some characteristic distance l [m] and temperature T [°C]. Let find the similarity criterion by reducing the equation to non-dimensional:

$$\pi_1 = \frac{\lambda \frac{T}{l^2}}{c\rho \frac{T}{\tau}} = \frac{\lambda \tau}{c\rho l^2}, \quad [\pi_1] = \mathrm{kg^0 m^0 s^0 C^0} = 1. \qquad (40)$$

This criterion is known as Fourier criterion. To determine the next criterion it can be used the Robin boundary conditions (Newton-Richman), i.e. temperature driving force:

$$\lambda \frac{\partial T}{\partial \mathbf{n}}\bigg|_\Gamma = \xi \Delta T\big|_\Gamma, \qquad (41)$$

where: ξ – heat transfer coefficient [W/m^2°C]. Let reduce the last equation to non-dimensional:

$$\pi_2 = \frac{\alpha T}{\lambda \frac{T}{l}} = \frac{\alpha l}{\lambda}, \quad [\pi_2] = \mathrm{kg^0 m^0 s^0 C^0} = 1. \qquad (42)$$

This criterion is known as Biot criterion.

Now, the electric conduction problem, which describes the commutation in some electrical device, can be considered. This problem is also determined by parabolic equation [28, 29]:

$$c\frac{\partial U}{\partial \tau} = \sigma \nabla^2 U, \qquad (43)$$

where: σ – specific electrical conductivity [m^{-3}kg^{-1}s^{3}A^2]; c – electric capacity per volume [F/m^3 = A^{2}s^{4}kg^{-1}m^{-5}]; U – electric potential [m^{2}kg^{1}s^{-3}A^{-1}]. The corresponding similarity criteria for this equation are:

$$\pi_1 = \frac{\sigma \frac{U}{l^2}}{c\frac{U}{\tau}} = \frac{\sigma\tau}{cl^2}, \quad \pi_2 = \frac{\zeta U}{\sigma \frac{U}{l}} = \frac{\zeta l}{\sigma}. \qquad (44)$$

By the selection of model (43) parameters, in which its similarity criteria are respectively the same for all of original (39) similarity criteria, the problems be similar and analogical. This condition is easy to perform in numerical mathematical models. Expansion the analogy on stationary problem is trivial.

Let consider the modification process of continuous system to its discrete analog. To ensure the unambiguousness of the conditions and matching of third similarity theorem [25], it is necessary to analyze the geometric properties of both systems. It can be considered the linear two-dimensional simplex elements in the problem of stationary heat conduction, for example. Stiffness matrix describes the relation between element nodes:

$$[\mathbf{K}] = \iint ([\mathcal{L}][\mathbf{N}])^{\mathrm{T}} [\mathbf{D}]([\mathcal{L}][\mathbf{N}])\, d\Omega. \qquad (45)$$

It can be noted that coefficients of gradients matrix $[\mathcal{L}][\mathbf{N}]$ have direct geometric meaning – element side projections on the coordinate axes:

$$[\mathbf{K}] = \frac{1}{2\Omega}\begin{bmatrix} b_1 & c_1 \\ b_2 & c_2 \\ b_3 & c_3 \end{bmatrix} \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix} \frac{1}{2\Omega}\begin{bmatrix} b_1 & c_1 \\ b_2 & c_2 \\ b_3 & c_3 \end{bmatrix}^{\mathrm{T}} \Omega =$$
$$= \frac{\lambda}{4\Omega}\begin{bmatrix} b_1^2 + c_1^2 & b_1 b_2 + c_2 c_2 & b_1 b_3 + c_1 c_3 \\ b_1 b_2 + c_1 c_2 & b_2^2 + c_2^2 & b_2 b_3 + c_2 c_3 \\ b_1 b_3 + c_1 c_3 & b_2 b_3 + c_2 c_3 & b_3^2 + c_3^2 \end{bmatrix}. \qquad (46)$$

The triangle area can be written by the last matrix coefficients, e.g. by taking a first node as the basis:

$$2\Omega = \begin{vmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{vmatrix} = \begin{vmatrix} x_2 - x_1 & y_2 - y_1 \\ x_3 - x_1 & x_3 - y_1 \end{vmatrix} = \begin{vmatrix} c_3 & -b_3 \\ -c_2 & b_2 \end{vmatrix}. \qquad (47)$$

By repeating these steps for the other nodes one gets:

$$2\Omega = b_1 c_2 - b_2 c_1 = b_1 c_3 - b_3 c_1 = b_2 c_3 - b_3 c_2. \qquad (48)$$

Taking into account the last expression, relationship between element nodes can be expressed by conductivities Y, or inverse to them values – resistors R:

$$[\mathbf{K}]_{1,2} = [\mathbf{K}]_{2,1} = Y_{1,2} = \frac{1}{R_{1,2}} = \frac{1}{2}\lambda \frac{b_1 b_2 + c_1 c_2}{b_1 c_2 - b_2 c_1},$$
$$[\mathbf{K}]_{1,3} = [\mathbf{K}]_{3,1} = Y_{1,3} = \frac{1}{R_{1,3}} = \frac{1}{2}\lambda \frac{b_1 b_3 + c_1 c_3}{b_1 c_3 - b_3 c_1}, \qquad (49)$$
$$[\mathbf{K}]_{2,3} = [\mathbf{K}]_{3,2} = Y_{2,3} = \frac{1}{R_{2,3}} = \frac{1}{2}\lambda \frac{b_2 b_3 + c_2 c_3}{b_2 c_3 - b_3 c_2}.$$

The local stiffness matrix now can be written as:

$$[\mathbf{K}] = \begin{bmatrix} -Y_{1,2} - Y_{1,3} & Y_{1,2} & Y_{1,3} \\ Y_{1,2} & -Y_{1,2} - Y_{2,3} & Y_{2,3} \\ Y_{1,3} & Y_{2,3} & -Y_{1,3} - Y_{2,3} \end{bmatrix}. \qquad (50)$$

The resulting matrix is nothing else than a combination of diagonal conductance matrix and Boolean connections matrix from the node potential method – the electrical circuits analysis method that uses SLAE, where nodal potentials are unknown [29]. In matrix form this SLAE can be written as:

$$[\mathbf{A}][\mathbf{Y}][\mathbf{A}]^{\mathrm{T}}\{\mathbf{U}\} = -[\mathbf{A}](\{\mathbf{J}\} + [\mathbf{Y}]\{\mathbf{E}\}), \qquad (51)$$

where: $[\mathbf{A}]$ – connections matrix (nodes to the edges incidence matrix); $[\mathbf{Y}]$ – diagonal conductance matrix; $\{\mathbf{U}\}$ – unknown nodal potentials; $\{\mathbf{J}\}$ – electric power sources; $\{\mathbf{E}\}$ – voltage source. By using the analogy, this system can be reduced to:

$$[\mathbf{K}]\{\mathbf{u}\} = \{\mathbf{f}\}, \quad [\mathbf{K}] = [\mathbf{A}][\mathbf{Y}][\mathbf{A}]^{\mathrm{T}},$$
$$\{\mathbf{f}\} = -[\mathbf{A}](\{\mathbf{J}\} + [\mathbf{Y}]\{\mathbf{E}\}). \qquad (52)$$

Where, one concludes that the elements of the analogy between physical processes are directly embedded in the linear finite element basis functions – they reflect the parameters of resistance/conductivity for similar discrete systems. If one considers the elasticity problem, stiffness matrix describes the behavior of simplex element where each edge of which is idealized spring with stiffness coefficient analogical to discrete mechanical system. And so on for other similarities, including multiphysics problems.

After numerical simulation of thermo-mechanical processes in RVE the resulting potential field on chosen volume sides can be inhomogeneous. To determine the effective characteristics it can be used described analogy method, i.e. analogy with parallel or serial conductivities connection [12, 26]. It is shown [16] that under the usage of simplex elements an effective heat conduction coefficient can be found as:

$$\lambda_{eff}=\frac{d\cdot q}{\Gamma_q(T_{\Gamma_q}-T_\infty)}=\frac{q}{\Gamma_q}\sum_{j=1}^{P_{\Gamma_q}}\frac{3(\Gamma_q)_j}{\sum_{i=1}^{3}\left(T_{qi,j}-T_\infty\right)}. \quad (53)$$

Extending this formalization to similar mechanical and coupled thermo-mechanical problems, one can get the expressions for effective thermal characteristics synthesis of complex structured composite materials microlevel model. For elasticity problem:

$$E_{eff}=\frac{d\cdot f_x}{\Gamma_{\mathbf{f}}(u_{x\mathbf{f}}-u_{x\infty})}=\frac{f_x}{\Gamma_{\mathbf{f}}}\sum_{j=1}^{P_{\Gamma_{\mathbf{f}}}}\frac{3(\Gamma_{\mathbf{f}})_j}{\sum_{i=1}^{3}\left(u_{x\mathbf{f}i,j}-u_{x\infty}\right)},$$

$$\mu_{eff}=\frac{\Delta u_y}{\Delta u_x}=\frac{\sum_{k=1}^{P_\Gamma}\left|u_{y_1k}-u_{y_2k}\right|}{\Gamma_{\mathbf{f}}}\sum_{j=1}^{P_{\Gamma_{\mathbf{f}}}}\frac{3(\Gamma_{\mathbf{f}})_j}{\sum_{i=1}^{3}\left(u_{x\mathbf{f}i,j}-u_{x\infty}\right)}, \quad (54)$$

where: u_{y_1} and u_{y_2} – transverse displacements on RVE flanks. For coupled thermoelasticity problem:

$$\alpha_{eff}=\frac{1}{d}\frac{\Delta u_x}{\Delta T}=\frac{1}{d}\sum_{j=1}^{P_{\Gamma_{\mathbf{f}}}}\frac{\sum_{i=1}^{3}\frac{u_{x\mathbf{f}i,j}-u_{x\infty}}{T_{\mathbf{f}i,j}-T_\infty}}{3}. \quad (55)$$

Simulation Results

Described models were realized in applied software by C++11 algorithmic language with high-performance parallel and distributed computing technology OpenCL v.1.2, and Qt SDK v.5.4.1. Working OS was Windows 7 Ultimate. Executable was built under x64 by MinGW v.4.9.2. Simulations were done on an ordinary configured PC. On Fig.2 are shown the results of CM effective thermal characteristics synthesis.

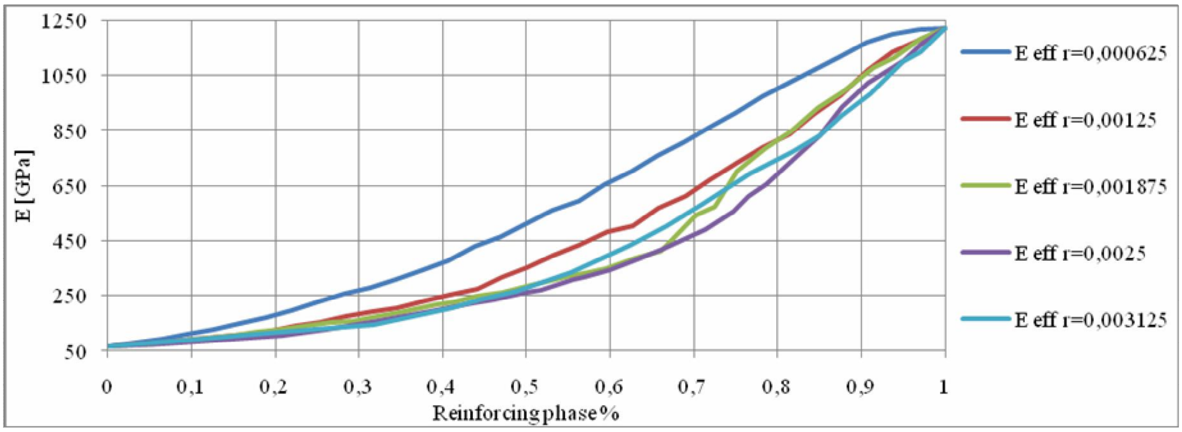


Fig.2.a. Composite materials effective thermal characteristics synthesis results

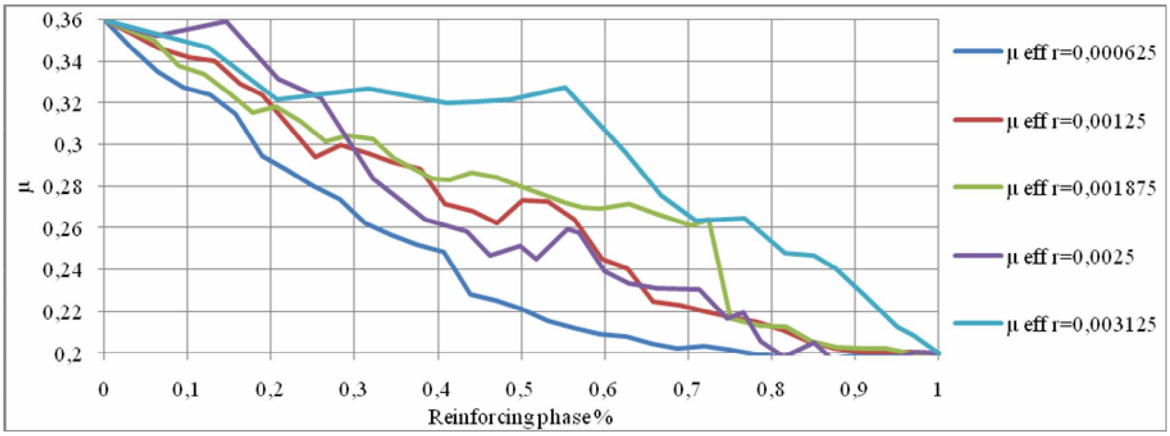


Fig.2.b. Composite materials effective thermal characteristics synthesis results

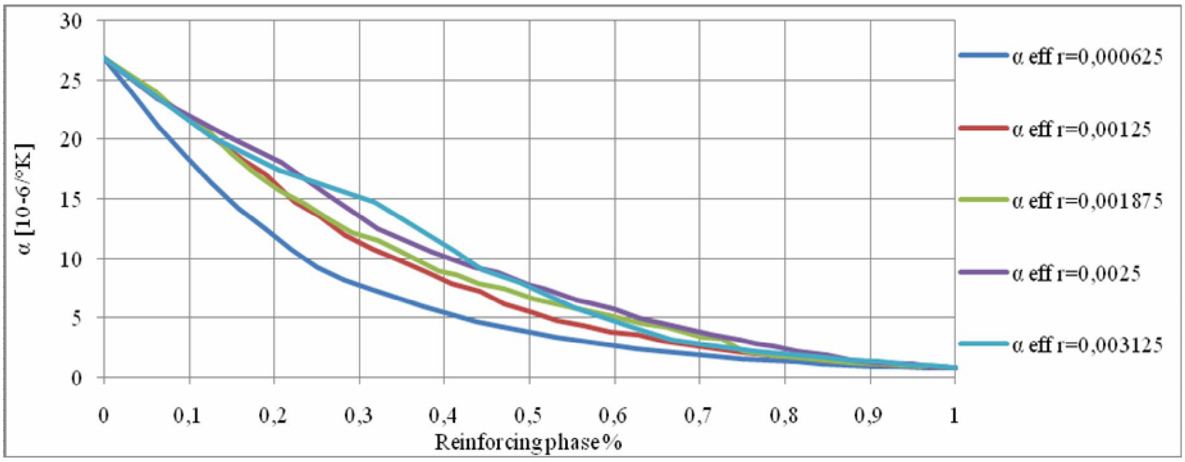


Fig.2.c. Composite materials effective thermal characteristics synthesis results

The CM model is Aluminum matrix with spherical Carbon inclusions with different sizes and concentration. Figure shows the phenomenon of synthesized characteristics percolation threshold appearing.

CONCLUSIONS

The numerical microlevel effective thermal characteristics synthesis models of composite materials with complex structure have gotten the further development:

- basing on the usage of finite element method for modeling coupled thermoelasticity problems and analogies method were developed microlevel composite materials models which allow one to synthesize thermal conduction coefficient, Young's modulus, Poisson's ratio and temperature coefficient of linear expansion;

2) the main difference is combined formalization of coupled multiphysics problems, which allows one to simultaneously take into account multiphysics boundary conditions;
3) this approach is especially useful when used in engineering applications which provide a high level of abstraction;
4) the models successfully implemented by technologies of high-performance parallel and distributed computing, which opens the possibility of directly effective usage in problems of composite materials optimal design;
5) the simulation results are shown.

REFERENCES

1. **Gorobets V. and Mendeleyev V. 2012.** Influence of pollutions on the thermal characteristics, heat efficiency and optimal dimensions of tubes with londitudinal fins. EconTechMod, 1(1):35-40.
2. **Balinski A. 2012.** Nanostructure of the soluble sodium silicate in the aspect of basic mechanical characteristic of the moulding sands. EconTechMod, 1(1):3-8
3. **Lubin G. 1982.** Handbook of Composites. New-York: Van Nostrand Reinhold Company Inc.
4. **Narusberh V. and Teters G. 1988.** Stability and optimization of composite shells. Riga: Zynatne. (in Russian).
5. **Jaworski N., et al. 2013.** Research of composite materials optimal design task based on numerical simulation. Proc. of CSIT’2013, 46-48, Lviv.
6. **Jaworski N., et al. 2013.** Architecture of the composite materials distributed heterogeneous computer-aided design system. Proc. of CADSM’ 2013, 440-442, Polyana.
7. **Matthews F., et al. 2000.** Finite element modelling of composite materials and structures. New-York: CRC Press LLC.
8. **Barbero E. 2008.** Finite element analysis of composite materials. New-York: CRC Press LLC.
9. **Torquato S. 2002.** Random Heterogeneous Materials. Microstructure and Macroscopic Properties. New-York: Springer.
10. **Kanit T., et al. 2003.** Determination of the size of the representative volume element for random composites: statistical and numerical approach. Int. Journal of Solids and Structures. 40:3647-3679.
11. **Smerdov A. 2007.** Development of design methods of composite materials and structures for rocket and space technique. Preprint. Moscow: Moscow State University Press. (in Russian).
12. **Jaworski N., et al. 2014.** Thermal Analysis Methods for Design of Composite Materials with Complex Structure. ECS Transactions. 59(1):513-523.
13. **Zienkiewicz O. and Morgan K.** 1983. Finite elements and approximation. New-York: Wiley.
14. **Farmaga I., et al. 2011.** Finite Element Meshing of Composites with Spherical Inclusions. Machine Dynamics Research, 35(3):13-21.
15. **Farmaga I., et al. 2012.** Regular and adaptive algorithms for modelling of spherical inclusions by finite element method. Proc. of TCSET’2012, 505-507, Lviv-Slavske.
16. **Jaworski N., et al. 2012.** Finding Effective Thermal Characteristics of Composite Materials Based on the Analysis of Thermal Conductivities. Bulletin LPNU "Computer Systems of Design: Theory and

Practice", 747:59-65, Lviv.
17. **Jaworski N., et al. 2012.** Development of the Discrete Model of Finding of the Effective Thermal Characteristics of Composite Materials with Complex Structure. Bulletin LPNU "Computer science and information technology ", 744:152-158, Lviv. (in Ukrainian).
18. **Hashin Z. 1962.** The elastic moduli of heteroheneous materials. Journal of Applied Mechanics, 29(1):143-150.
19. **ISO 8301:1991** Thermal insulation. Determination of steady-state thermal resistance and related properties. Heat flow meter apparatus.
20. **Government Standard of Ukraine B B.2.7-105-2000 (GOST 7076-99)** Building materials and products. Method of determination of steady-state thermal conductivity and thermal resistance. (in Ukrainian).
21. **Lurie A. 1970.** Theory of Elasticity. Moscow. (In Russian).
22. **Timoshenko S. and Goodier J. 1979.** Theory of Elasticity. Moscow: Nauka. (In Russian).
23. **Kovalenko A. 1970.** Fundamentals of Thermoelasticity. Kiev: Naukova Dumka. (In Russian).
24. **Jaworski N., et al. 2014.** Finding the Composite Materials Linear Temperature Expansion Coefficient Based on Thermoelasticity Problem Numerical Simulation. Proc. of CADMD'2014, 77-83, Lviv.
25. **Venikov V. 1976.** Theory of similarity and modelling. Moscow: Vysshaia shkola. (in Russian).
26. **Dulnev G. 1984.** Heat and Mass Transfer in Electronic Equipment. Moscow: Vysshaia shkola. (in Russian).
27. **Fedasuk D. 1999.** Methods and tools for thermal design of microelectronic devices. Lviv: LPNU. (in Ukrainian).
28. **Robertson A. and Gross D. 1958.** An Electrical-Analog Method for Transient Heat-Flow Analysis. Jour. of Res. of the Nat. Bureau of Standards, 61(2).
29. **Neumann L. and Demirchian K. 1981.** Theoretical Foundations of Electrical Engineering. Leningrad: Energoizdat. (in Russian).