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MULTI SCALE MODELING OF THERMOELASTIC PROPERTIES OF COMPOSITES WITH PERIODIC STRUCTURE OF HETEROGENEITIES

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Abstract. The majority of processes in composite materials involve a wide range of scales. Because of the scale disparity in multi scale problem, it's often impossible to resolve the effect of small scales directly. In this paper we perform multi scale modeling in order to analyze properties of composite materials with periodical structure under temperature and stresses influence. We consider a homogeneous matrix with periodic system of spherical particles separated from the matrix by an interphase. Each component has its own thermodynamic and mechanical (elastic) properties. We replace differential equations with rapidly varying coefficients by homogenized equations having effective parameters, which incorporate multi scale structure and properties of any component. We study, how effective properties of the system "matrix-interphase-inclusion" can depend on sizes of inclusions, thickness of interphase, mechanical and thermodynamic properties of components of a composite material.

1. Introduction

In this paper we derive and study effective properties of heterogeneous thermo elastic media formed by periodic variations of material properties of the components of nano- and micro-composite materials. According to experimental data [1] substantial variation in thermo mechanical properties of nanocomposites can be achieved by filling highly elastic polymeric matrix with high-strength dispersed particles (carbon, silicates, organic clay). Reinforcement effect is directly connected with peculiarities of interaction between hard phase filling (high modular material), polymeric matrix (low modular material) and formed interphase (medium modular material). A variety of theoretical treatments of elastic composites have been described in monographs [2, 3], while Bahvalov and Panasenko [4], Sanchez-Palencia [5] firstly introduced and employed the method of homogenization. In this paper we develop and imply analytical homogenization technique and numerical methods with the aim to study mechanical and thermodynamic characteristics of hyperelastic polymeric nano- and micro-composite materials. We start with a brief overview of used homogenization technique [4-8]. We use this technique in derivation of cell problems and homogenized equations. Homogenized equations need to be solved in order to find temperature distribution, displacements, stresses and strains within the material under study. Cell problems' solution allows us to determine effective properties of the medium, which was three-dimensional composite, consisting of homogeneous matrix with periodic system of spherical particles, separated from the matrix by an interphase. Effective properties, incorporating multi scale structure and properties of components of the composite are determined numerically. We present and discuss some computed results for elastomer composites, consisting of nano- or micro- particles of schungite, incorporated into butadiene-styrene rubber matrix. And then we make conclusions.

2. Problem statement

Let us consider a three-dimensional composite material, which is composed of periodically repeated elements, the so-called period cells. We denote by Ω the volume occupied by material and by $\partial\Omega$ the boundary of this volume.

The (thermo) elasticity equations for the composite are described by the equations

$$\frac{\partial \sigma_{ij}}{\partial x_i} + F_i = 0 \quad in\ \Omega\ , \tag{1}$$

where σ_{ij} denote the components of stress tensor, F_i – components of an external force, divided by volume, x_i (i=1,2,3) – coordinates.

Duhamel-Neumann's law, which is the generalization of Hooke's law in case of presence of thermotension, can be written as

$$\begin{aligned} \sigma_{ij} &= c_{ijkl}\frac{\partial u_i}{\partial x_l} - \beta_{ij}\theta, \\ \beta_{ij} &= c_{ijkl}\alpha_{kl}, \end{aligned} \tag{2}$$

where u_i are components of displacement vector; c_{ijkl} and α_{kl} are components of stiffness tensor and thermal expansion tensor respectively; T_0 is the temperature in unstrained state; $\theta = T - T_0$ is the drop of temperature.

Components q_i of heat flux vector are determined by the Fourier's law:

$$q_i = -k_{ij}\frac{\partial \theta}{\partial x_j}, \tag{3}$$

where k_{ij} are the components of thermal conductivity tensor.

Taking thermoelasticity into account, we can write heat conductivity equation as

$$-\frac{\partial q_i}{\partial x_i} - T_0\beta_{ij}\frac{\partial}{\partial x_j}\left(\frac{\partial u_i}{\partial t}\right) = \rho c_V \frac{\partial \theta}{\partial t} \quad in\ \Omega\ , \tag{4}$$

where ρ is density, c_V is the heat capacity at constant volume, t is time.

Considering boundary conditions, let us specify forces p_i^* on part $\partial\Omega_1$ of the boundary $\partial\Omega$ and displacements u_i^* on part $\partial\Omega_2$ of the boundary $\partial\Omega$ ($\partial\Omega = \partial\Omega_1 \cup \partial\Omega_2$):

$$\sigma_{ij}n_j\big|_{\partial\Omega_1} = p_i^*, \quad u_i\big|_{\partial\Omega_2} = u_i^*. \tag{5}$$

Suppose that heat exchange condition at the boundary $\partial\Omega$ looks like this:

$$q_n\big|_{\partial\Omega} = (q_j n_j)\big|_{\partial\Omega} = -\left(k_{ij}\frac{\partial\theta}{\partial x_i}\right)n_j\bigg|_{\partial\Omega} = \beta\left(\theta + T_0\right) - q_n^* , \tag{6}$$

where β is the heat transfer coefficient, q_n^* is the external heat flux along component n_j of a unit normal vector.

Let initial conditions be given by

$$u_i\big|_{t=0} = u_i^0, \quad \frac{\partial u_i}{\partial t}\bigg|_{t=0} = \frac{\partial u_i^0}{\partial t}, \quad \theta\big|_{t=0} = 0. \tag{7}$$

Now we need to add some conditions on the interfaces Σ between different components of the composite material. Let us consider the case of an ideal contact, which means that stresses and displacements are continuous on the interfaces Σ between the components:

$$\left[\sigma_{ij} n_j\right]\big|_{\Sigma} = 0, \quad \left[u_i\right]\big|_{\Sigma} = 0. \tag{8}$$

Let us also consider continuity conditions for the heat flux and temperature on the interfaces Σ between the components of the composite:

$$\left[q_n\right]\big|_{\Sigma} = \left[q_j n_j\right]\big|_{\Sigma} = 0, \quad \left[\theta\right]\big|_{\Sigma} = 0. \tag{9}$$

3. Asymptotic theory

Problem (1)-(4) with boundary, initial and interface conditions (5-9) can be solved in the framework of homogenization technique. We designate linear dimension of period cell in any direction by *l* and characteristic size of the region, within which the system is studied, by *L*. Suppose *l* to be small in comparison with *L*. In this case we can obtain an asymptotic expansion of the solution of our problem in terms of a small parameter ε, which is the ratio of period of the structure to a characteristic size within the region $\varepsilon = l/L << 1$. Hence, there are two natural spatial length scales. One of them (the fast scale) characterizes variations of properties of heterogeneous medium within one period cell, another (the slow scale) characterizes the variations within the region of interest. Equations, boundary, initial and interface conditions depend on both fast and slow variables. In addition to slow coordinates x_i we introduce fast coordinates $\xi_i = x_i/\varepsilon$ and seek the solution of the problem (1)-(4) as series of small parameter ε:

$$\begin{aligned} u_i\left(x,t\right) &= u_i^{(0)}\left(x,t\right) + \varepsilon u_i^{(1)}\left(x,\xi,t\right) + \varepsilon^2 u_i^{(2)}\left(x,\xi,t\right) + ..., \\ \theta\left(x,t\right) &= \theta^{(0)}\left(x,t\right) + \varepsilon\theta^{(1)}\left(x,\xi,t\right) + \varepsilon^2\theta^{(2)}\left(x,\xi,t\right) + ..., \end{aligned} \tag{10}$$

where $u_i^{(k)}\left(x,\xi,t\right)$ and $\theta^{(k)}\left(x,\xi,t\right)$ (k=1,2,..) are *l*-periodic functions of fast variable $\xi = x/\varepsilon$. Substitution of expansions (10) into Duhamel-Neumann's law (2) yields an expansion for the stress tensor of the form

$$\begin{aligned} \sigma_{ij} &= \sigma_{ij}^{(0)} + \varepsilon\sigma_{ij}^{(1)} + \varepsilon^2\sigma_{ij}^{(2)} + ..., \\ \sigma_{ij}^{(p)}\left(x,\xi,t\right) &= c_{ijkl}\left(\xi\right)\left(\frac{\partial u_k^{(p)}}{\partial x_l} + \frac{\partial u_k^{(p+1)}}{\partial \xi_l}\right) - \beta_{ij}\left(\xi\right)\theta^{(p)}, \quad p = 0,1,2,.. \end{aligned} \tag{11}$$

If ε tends to zero, the asymptotic expansion converges to the solution, satisfying the homogenized equation with effective coefficients.
By substituting expansions (10)-(11) into equations (1) and setting equal the factors at identical powers of ε, we get:
at ε^{-1}:

$$\frac{\partial \sigma_{ij}^{(0)}}{\partial \xi_j} = 0, \tag{12}$$

at ε^{0}:

$$\frac{\partial \sigma_{ij}^{(0)}}{\partial x_j} + \frac{\partial \sigma_{ij}^{(1)}}{\partial \xi_j} + F_i = 0. \tag{13}$$

Substitution of $\sigma_{ij}^{(0)}$ in the form (11) into equations (12) gives us:

$$\frac{\partial \sigma_{ij}^{(0)}}{\partial \xi_j} = \frac{\partial}{\partial \xi_j}\left(c_{ijkl}(\xi) \frac{\partial u_k^{(1)}(x,\xi,t)}{\partial \xi_l} \right) + \frac{\partial u_k^{(0)}(x,t)}{\partial x_l} \frac{\partial c_{ijkl}(\xi)}{\partial \xi_j} - \theta^{(0)}(x,t) \frac{\partial \beta_{ij}(\xi)}{\partial \xi_j} = 0. \tag{14}$$

We seek the second term in expansion (10) for components of displacement $u_m^{(1)}(x,\xi,t)$ in terms of

$$u_m^{(1)}(x,\xi,t) = N_m^{kl}(\xi) \frac{\partial u_k^{(0)}(x,t)}{\partial x_l} + V_m(\xi)\theta^{(0)}(x,t). \tag{15}$$

Substituting (15) into equations (14), we derive equations, which we need to solve in order to find periodic functions $N_m^{kl}(\xi)$ and $V_m(\xi)$:

$$\frac{\partial}{\partial \xi_j}\left(c_{ijmn}(\xi) \frac{\partial N_m^{kl}(\xi)}{\partial \xi_n} \right) = -\frac{\partial c_{ijkl}(\xi)}{\partial \xi_j}, \tag{16}$$

$$\frac{\partial}{\partial \xi_j}\left(c_{ijmn}(\xi) \frac{\partial V_m(\xi)}{\partial \xi_n} \right) = \frac{\partial \beta_{ij}(\xi)}{\partial \xi_j}. \tag{17}$$

By substituting expansions (10) into heat conductivity equation (4) and setting equal the factors at identical powers of ε, we get:
at ε^{-1}:

$$\frac{\partial}{\partial \xi_i}\left(k_{ij}(\xi)\left(\frac{\partial \theta^{(0)}(x,t)}{\partial x_j} + \frac{\partial \theta^{(1)}(x,\xi,t)}{\partial \xi_j} \right) \right) = 0, \tag{18}$$

at ε^0:

$$\frac{\partial}{\partial x_i}\left(k_{ij}(\xi)\left(\frac{\partial\theta^{(0)}}{\partial x_j}+\frac{\partial\theta^{(1)}}{\partial\xi_j}\right)\right)+\frac{\partial}{\partial\xi_i}k_{ij}(\xi)\left(\frac{\partial\theta^{(1)}}{\partial x_j}+\frac{\partial\theta^{(2)}}{\partial\xi_j}\right)- \\ -T_0\beta_{ij}\left(\frac{\partial}{\partial x_j}\left(\frac{\partial u_i^{(0)}(x,t)}{\partial t}\right)+\frac{\partial}{\partial\xi_j}\left(\frac{\partial u_i^{(1)}(x,\xi,t)}{\partial t}\right)\right)=\rho c_V\frac{\partial\theta^{(0)}}{\partial t} \tag{19}$$

In case of the solution of decoupled problem, equation (19) takes the form (19a):

$$\frac{\partial}{\partial x_i}\left(k_{ij}(\xi)\left(\frac{\partial\theta^{(0)}}{\partial x_j}+\frac{\partial\theta^{(1)}}{\partial\xi_j}\right)\right)+\frac{\partial}{\partial\xi_i}k_{ij}(\xi)\left(\frac{\partial\theta^{(1)}}{\partial x_j}+\frac{\partial\theta^{(2)}}{\partial\xi_j}\right)=\rho c_V\frac{\partial\theta^{(0)}}{\partial t}. \tag{19a}$$

We seek the second term in expansion (10) for the drop of temperature $\theta^{(1)}(x,\xi,t)$ in terms of

$$\theta^{(1)}(x,\xi,t)=W_j(\xi)\frac{\partial\theta^{(0)}(x,t)}{\partial x_j}. \tag{20}$$

Substituting relationship (20) into equation (19), we derive equations, which we need to solve in order to find periodic functions $W_j(\xi)$:

$$\frac{\partial}{\partial\xi_i}\left(k_{im}(\xi)\frac{\partial W_j(\xi)}{\partial\xi_m}\right)+\frac{\partial k_{ij}(\xi)}{\partial\xi_i}=0. \tag{21}$$

By substituting expansions (10) into boundary conditions (5)-(6) and initial conditions (7) and setting equal the factors at identical powers of ε, we get:

from boundary conditions:

$$\sigma_{ij}^{(0)}n_j\Big|_{\partial\Omega_1}=p_i^*,\quad \sigma_{ij}^{(1)}n_j\Big|_{\partial\Omega_1}=0,\quad \sigma_{ij}^{(2)}n_j\Big|_{\partial\Omega_1}=0, \\ u_i^{(0)}\Big|_{\partial\Omega_1}=u_i^*,\quad u_i^{(1)}\Big|_{\partial\Omega_1}=0,\quad u_i^{(2)}\Big|_{\partial\Omega_1}=0, \tag{22}$$

$$q_j^{(0)}n_j\Big|_{\partial\Omega_2}=\beta\left(\theta^{(0)}+T_0\right)-q_n^*,\quad q_j^{(1)}n_j\Big|_{\partial\Omega_2}=\theta^{(1)},\quad q_j^{(2)}n_j\Big|_{\partial\Omega_2}=\theta^{(2)},... \tag{23}$$

from initial conditions:

$$u_i^{(0)}(x,t)\Big|_{t=0}=u_i^0,\quad u_i^{(1)}(x,t)\Big|_{t=0}=0,\quad u_i^{(2)}(x,t)\Big|_{t=0}=0,... \\ \frac{\partial u_i^{(0)}(x,t)}{\partial t}\Big|_{t=0}=\frac{\partial u_i^0}{\partial t},\quad \frac{\partial u_i^{(1)}(x,t)}{\partial t}\Big|_{t=0}=0,\quad \frac{\partial u_i^{(2)}(x,t)}{\partial t}\Big|_{t=0}=0, \\ \theta^{(0)}(x,t)\Big|_{t=0}=0,\quad \theta^{(1)}(x,t)\Big|_{t=0}=0,\quad \theta^{(2)}(x,t)\Big|_{t=0}=0. \tag{24}$$

Let us substitute expansions (10) into conditions (8)-(9) on the interfaces Σ between the components. Requirement of continuity of displacements and continuity condition for temperature give us:

$$\left[u_i^{(0)}\right]\Big|_\Sigma = 0, \quad \left[u_i^{(1)}\right]\Big|_\Sigma = 0, \quad \left[u_i^{(2)}\right]\Big|_\Sigma = 0, \ldots \tag{25}$$

$$\left[\theta^{(0)}\right]\Big|_\Sigma = 0, \quad \left[\theta^{(1)}\right]\Big|_\Sigma = 0, \quad \left[\theta^{(2)}\right]\Big|_\Sigma = 0, \ldots \tag{26}$$

Condition of the absence of external loads on the interfaces Σ between the components (8), written with account of (11), gives us:

$$\left[\left(c_{ijkl}\frac{\partial u_k^{(0)}}{\partial x_l} + c_{ijkl}\frac{\partial u_k^{(1)}}{\partial \xi_l} - \beta_{ij}\theta^{(0)}\right)n_j\right] = 0, \quad \left[\left(c_{ijkl}\frac{\partial u_k^{(1)}}{\partial x_l} + c_{ijkl}\frac{\partial u_k^{(2)}}{\partial \xi_l} - \beta_{ij}\theta^{(1)}\right)n_j\right] = 0, \ldots \tag{27}$$

Using relationships

$$q_i = -k_{ij}\frac{\partial \theta}{\partial x_j} = -k_{ij}\left(\frac{\partial \theta^{(0)}}{\partial x_j} + \frac{\partial \theta^{(1)}}{\partial \xi_j}\right) - \varepsilon k_{ij}\left(\frac{\partial \theta^{(1)}}{\partial x_j} + \frac{\partial \theta^{(2)}}{\partial \xi_j}\right) - \varepsilon^2 k_{ij}\left(\frac{\partial \theta^{(2)}}{\partial x_j} + \frac{\partial \theta^{(3)}}{\partial \xi_j}\right) - \ldots$$

and the requirement of continuity of heat flux, we get the following conditions on the interfaces Σ between the components:

$$-\left[\left(k_{ij}\frac{\partial \theta^{(0)}}{\partial x_j} + k_{ij}\frac{\partial \theta^{(1)}}{\partial \xi_j}\right)n_i\right]\Bigg|_\Sigma = 0, \quad -\left[\left(k_{ij}\frac{\partial \theta^{(1)}}{\partial x_j} + k_{ij}\frac{\partial \theta^{(2)}}{\partial \xi_j}\right)n_i\right]\Bigg|_\Sigma = 0, \ldots \tag{28}$$

Substituting (15), (20) into (25)-(26), we have

$$\begin{aligned} &\left[u_i^{(0)}\right]\Big|_\Sigma = 0, \\ &\left[u_i^{(1)}\right]\Big|_\Sigma = \left[N_i^{kl}\right]\Big|_\Sigma \frac{\partial u_k^{(0)}}{\partial x_l} + \left[V_i\right]\Big|_\Sigma \theta^{(0)} = 0, \ldots \end{aligned} \tag{29}$$

$$\begin{aligned} &\left[\theta^{(0)}\right]\Big|_\Sigma = 0, \\ &\left[\theta^{(1)}\right]\Big|_\Sigma = \left[W_j\right]\Big|_\Sigma \frac{\partial \theta^{(0)}}{\partial x_j} = 0, \ldots \end{aligned} \tag{30}$$

Let us substitute (15), (20) into (27) and (28). Taking equations (29)-(30) into consideration, we obtain

$$\left[\left(c_{ijkl} + c_{ijmn}\frac{\partial N_m^{kl}(\xi)}{\partial \xi_n}\right)n_j\right]\Bigg|_\Sigma \frac{\partial u_k^{(0)}}{\partial x_l} + \left[\left(c_{ijmn}\frac{\partial V_m}{\partial \xi_n} - \beta_{ij}\right)n_j\right]\Bigg|_\Sigma \theta^{(0)} = 0, \tag{31}$$

$$\left[\left(k_{ij}+k_{ik}\frac{\partial W_j}{\partial \xi_k}\right)n_i\right]\Bigg|_{\Sigma}\frac{\partial \theta^{(0)}}{\partial x_j}=0 \tag{32}$$

Equations (31)-(32) should be valid for any arbitrary variations of $u_k^{(0)}$ and $\theta^{(0)}$. Consequently, coefficients at their derivatives should be identically zero, and we can write the following equations:

$$\begin{aligned}
&\left[N_m^{kl}\right]\Big|_{\Sigma}=0,\\
&\left[V_m\right]\Big|_{\Sigma}=0,\\
&\left[W_j\right]\Big|_{\Sigma}=0,\\
&\left[C_{ijkl}n_j\right]\Big|_{\Sigma}=0,\quad C_{ijkl}=c_{ijkl}+c_{ijmn}\frac{\partial N_m^{kl}(\xi)}{\partial \xi_n},\\
&\left[B_{ij}n_j\right]\Big|_{\Sigma}=0,\quad B_{ij}=\beta_{ij}-c_{ijmn}\frac{\partial V_m}{\partial \xi_n},\\
&\left[K_{ij}n_i\right]\Big|_{\Sigma}=0,\quad K_{ij}=k_{ij}+k_{ik}\frac{\partial W_j}{\partial \xi_k}.
\end{aligned} \tag{33}$$

As it was stated above, periodic functions $N_m^{kl}(\xi)$, $V_m(\xi)$ и $W_j(\xi)$ can be found as solutions of local problems (16)-(17), (21). Using (33), we rewrite these local problems (cell problems) in form of

$$\frac{\partial}{\partial \xi_j}\left(c_{ijkl}(\xi)+c_{ijmn}(\xi)\frac{\partial N_m^{kl}(\xi)}{\partial \xi_n}\right)=\frac{\partial C_{ijkl}(\xi)}{\partial \xi_j}=0, \tag{16a}$$

$$\frac{\partial}{\partial \xi_j}\left(\beta_{ij}(\xi)-c_{ijmn}(\xi)\frac{\partial V_m(\xi)}{\partial \xi_n}\right)=\frac{\partial B_{ij}}{\partial \xi_j}=0, \tag{17a}$$

$$\frac{\partial}{\partial \xi_i}\left(k_{ij}(\xi)+k_{im}(\xi)\frac{\partial W_j(\xi)}{\partial \xi_m}\right)=\frac{\partial K_{ij}(\xi)}{\partial \xi_i}=0. \tag{21a}$$

Homogenized macroscopic equations we get, averaging equations (13) and (19) (or (19a)) over periodic cell. Let us define the procedure of averaging over periodic cell as $\langle ...\rangle=\int\limits_{V_{cell}} ...dV_{cell}$ and perform averaging of equation (13). Due to periodicity of functions $\sigma_{ij}^{(1)}$ integrals on opposite faces of can be cancelled, and we have:

$$\int\limits_{V_{cell}}\frac{\partial \sigma_{ij}^{(1)}}{\partial \xi_j}dV_{cell}=\oiint\limits_{\partial V_{cell}}\sigma_{ij}^{(1)}n_j dS=0$$

Hence, as a result of averaging (13), we obtain

$$\frac{\partial\left\langle \sigma_{ij}^{(0)}\right\rangle}{\partial x_j}+F_i=0. \tag{34}$$

It follows from relationships (11) and (15) that the homogenized components of stress tensor can be written as

$$\begin{aligned}\left\langle \sigma_{ij}^{(0)}\left(x,\xi,t\right)\right\rangle &=\left\langle\left(c_{ijkl}+c_{ijmn}\frac{\partial N_m^{kl}\left(\xi\right)}{\partial \xi_n}\right)\right\rangle\frac{\partial u_k^{(0)}\left(x,t\right)}{\partial x_l}-\left\langle\left(\beta_{ij}-c_{ijmn}\frac{\partial V_m}{\partial \xi_n}\right)\right\rangle\theta^{(0)}\left(x,t\right)=\\&=\left\langle C_{ijkl}\right\rangle\frac{\partial u_k^{(0)}\left(x,t\right)}{\partial x_l}-\left\langle B_{ij}\right\rangle\theta^{(0)}\left(x,t\right).\end{aligned} \tag{35}$$

Equations (35) are analogous to equations (2) and can be considered as Duhamel-Neumann's law for the effective medium with averaged properties. It is important to note that the homogenized components of stiffness tensor $\left\langle C_{ijkl}\right\rangle$ and the homogenized components of thermoelasticity tensor $\left\langle B_{ij}\right\rangle$ keep track of the microstructure of a given composite material.
Substitution of (35) into (34) gives us the homogenized thermo elasticity equations:

$$\left\langle C_{ijkl}\right\rangle\frac{\partial^2 u_k^{(0)}\left(x,t\right)}{\partial x_j\partial x_l}-\left\langle B_{ij}\right\rangle\frac{\partial \theta^{(0)}\left(x,t\right)}{\partial x_j}+F_i=0. \tag{36}$$

Let us perform averaging of equation (19). Using (15), (20) and taking ξ–periodicity of functions $\theta^{(1)},\theta^{(2)}$ into account, we get the homogenized heat conductivity equation

$$\left\langle K_{ij}\right\rangle\frac{\partial^2\theta^{(0)}}{\partial x_i\partial x_j}-T_0\left\langle \tilde{B}_{ij}\right\rangle\frac{\partial}{\partial x_j}\left(\frac{\partial u_i^{(0)}}{\partial t}\right)=\left\langle C_V\right\rangle\frac{\partial\theta^{(0)}}{\partial t}, \tag{37}$$

where we have introduced the following notations:

$$C_V=\rho c_V+T_0\beta_{ij}\frac{\partial V_i\left(\xi\right)}{\partial \xi_j},\quad \left\langle C_V\right\rangle=\left\langle \rho c_V\right\rangle+T_0\left\langle \beta_{ij}\frac{\partial V_i\left(\xi\right)}{\partial \xi_j}\right\rangle, \tag{38}$$

$$\tilde{B}_{ij}=\beta_{ij}+\beta_{kl}\frac{\partial N_k^{ij}}{\partial \xi_l}=c_{ijmn}\alpha_{mn}+c_{klmn}\alpha_{mn}\frac{\partial N_k^{ij}}{\partial \xi_l}=\left(c_{ijmn}+c_{klmn}\frac{\partial N_k^{ij}}{\partial \xi_l}\right)\alpha_{mn}. \tag{39}$$

Finally the homogenized thermo elasticity problem can be written as system of macroscopic motion equations (36) and macroscopic heat conductivity equation (37).
Equations (36)-(37) should be supplemented with appropriate boundary and initial conditions. As a result of averaging and keeping only main terms of expansions in boundary and initial conditions (22)-(24), we obtain boundary conditions in the form of (see eq. (35))

$$\left\langle \sigma_{ij}^{(0)} \right\rangle n_j \Big|_{\partial\Omega_1} = \left(\left\langle C_{ijkl} \right\rangle \frac{\partial u_k^{(0)}(x,t)}{\partial x_l} - \left\langle B_{ij} \right\rangle \theta^{(0)}(x,t) \right) n_j \Big|_{\partial\Omega_1} = p_i^* , \qquad (40)$$
$$u_i^{(0)} \Big|_{\partial\Omega_1} = u_i^*,$$

$$\left\langle q_i^{(0)} \right\rangle n_i \Big|_{\partial\Omega_2} = \left\langle K_{ij} \right\rangle \frac{\partial \theta^{(0)}}{\partial x_j} n_i \Bigg|_{\partial\Omega_2} = \beta\left(\theta^{(0)} + T_0\right) - q_n^* \qquad (41)$$

and initial conditions

$$u_i^{(0)}(x,t)\Big|_{t=0} = u_i^0, \quad \frac{\partial u_i^{(0)}(x,t)}{\partial t}\Bigg|_{t=0} = \frac{\partial u_i^0}{\partial t}, \quad \theta^{(0)}(x,t)\Big|_{t=0} = 0. \qquad (42)$$

Solution of homogenized thermo elasticity problem (36)-(42) allows us to determine $u_i^{(0)}(x,t)$ and $\theta^{(0)}(x,t)$.
In case of decoupled problem, equation (19) takes the form (19a) and homogenized equation (37) acquires the form

$$\left\langle K_{ij} \right\rangle \frac{\partial^2 \theta^{(0)}}{\partial x_i \partial x_j} = \left\langle \rho c_V \right\rangle \frac{\partial \theta^{(0)}}{\partial t}. \qquad (37a)$$

All effective characteristics of the medium can be found as a result of solution of cell problems (16a), (17a) и (21a). Having solved cell problems, we determine functions $N_m^{kl}(\xi)$, $V_m(\xi)$ and $W_j(\xi)$. Local problems' solutions are ξ–periodic over period cell. To render solutions for $N_m^{kl}(\xi)$, $V_m(\xi)$ and $W_j(\xi)$ unique, we impose further normalization conditions

$$\left\langle N_m^{kl} \right\rangle = 0, \quad \left\langle V_m \right\rangle = 0, \quad \left\langle W_j \right\rangle = 0. \qquad (43)$$

Having solved homogenized problem (36)-(42) and cell problems (16a)-(17a), (21a), (43), we are in a position to determine temperature and displacements' distributions, considering two first terms of expansions (10)-(11) (accurate within ε^2). These solutions will look like

$$u_i(x,t) = u_i^{(0)}(x,t) + \varepsilon\left(N_m^{kl}(\xi) \frac{\partial u_k^{(0)}(x,t)}{\partial x_l} + V_m(\xi)\theta^{(0)}(x,t) \right)..., \qquad (44)$$
$$\theta(x,t) = \theta^{(0)}(x,t) + \varepsilon\left(W_j(\xi) \frac{\partial \theta^{(0)}(x,t)}{\partial x_j} \right) + ...$$

As a result of averaging of relationships (44) we have

$$\left\langle u_i(x,t) \right\rangle = u_i^{(0)}(x,t), \quad \left\langle \theta(x,t) \right\rangle = \theta^{(0)}(x,t) \qquad (45)$$

This means that the main terms of temperature (and displacements’) expansions are equal to average (over periodic cell) meanings. Next terms of expansions can be considered as local corrections, whose average (over periodic cell) values are zeros.

4. Illustrative examples

In order to solve cell problems (16a), (17a), (21a), complemented by normalization condition (43) we developed program complex, based on the object-oriented approach [8, 9]. This program complex implements algorithm of analytic-numerical method of blocks, which can be considered as a modification of finite element method. The idea is to use relatively complex curvilinear parts of the domain as elements. These elements (named blocks) coincide with different phases of the material (spherical inclusion, interphase and matrix). In each element we use special system of analytical functions with appropriate approximation properties, which rigorously satisfy initial equations. On the base of these functions one can construct local solution in element (block) with definite boundary conditions and shape functions for finite element method. Then local solutions for elements are consolidated into a global solution for the whole region of interest [9].

As an illustrative example we consider three-dimensional composite, consisting of homogeneous matrix with periodic system of spherical particles separated from the matrix by an interphase. Figure 1 represents the overall view of a periodic cell of this composite. For elastomeric composites, consisting of nano- or micro- particles of schungite, incorporated into butadiene-styrene rubber matrix, 3D cell problems (16a), (21a) were solved numerically. It allowed us to determine components of effective heat conductivity and stiffness tensors as well as effective Young modulus and bulk modulus. Volume concentration of inclusions (schungite) was equal to 2 %.

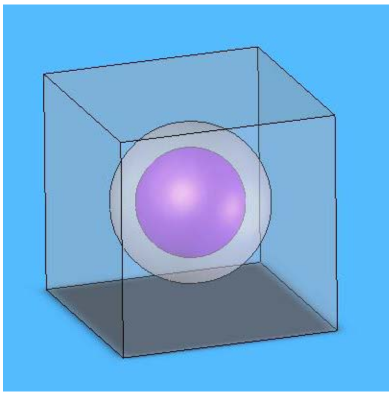

Fig. 1. Periodic cell.

In Fig. 2 we plot the solution of cell problem (21a). Interphase had thickness 25 nm. Heat conductivity coefficients of matrix, inclusion and interphase were equal to $k_m = 0.04\ W/(m \cdot K)$, $k_i = 3.81\ W/(m \cdot K)$ and $k_l = 1.97\ W/(m \cdot K)$ respectively. In case, when inclusions had radius R=25 nm, effective heat conductivity coefficient was equal to $k = 0.056\ W/(m \cdot K)$.

The dependence of effective heat conductivity coefficient k on the size of inclusions R. is shown in Fig. 3. It can be seen that at $R \sim 25$ nm the ratio of effective heat conductivity coefficient of homogenized material to heat conductivity coefficient of matrix is ~1.4. With increasing of radii of inclusions R the value of effective heat conductivity coefficient k decreases; it is nearly approaching the heat conductivity of matrix k_m, when R becomes ~200-250 nm and bigger.

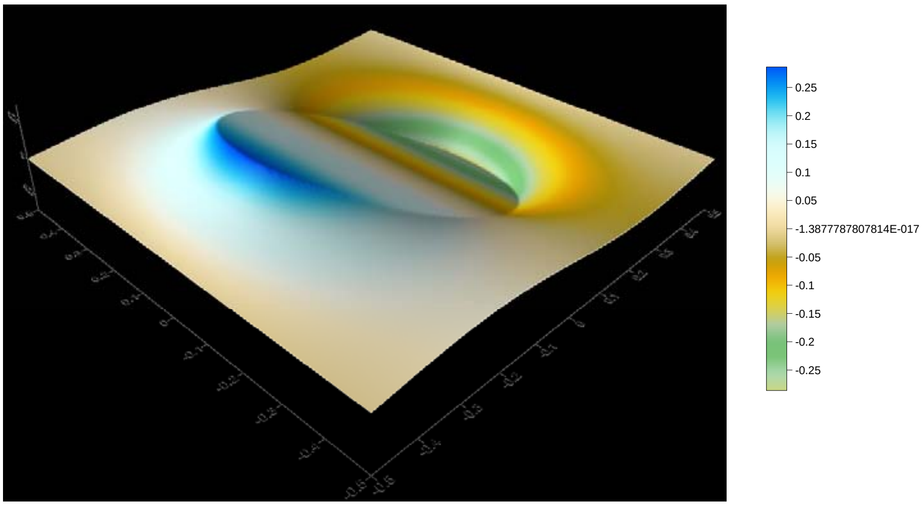

Fig. 2. Solution of cell problem.

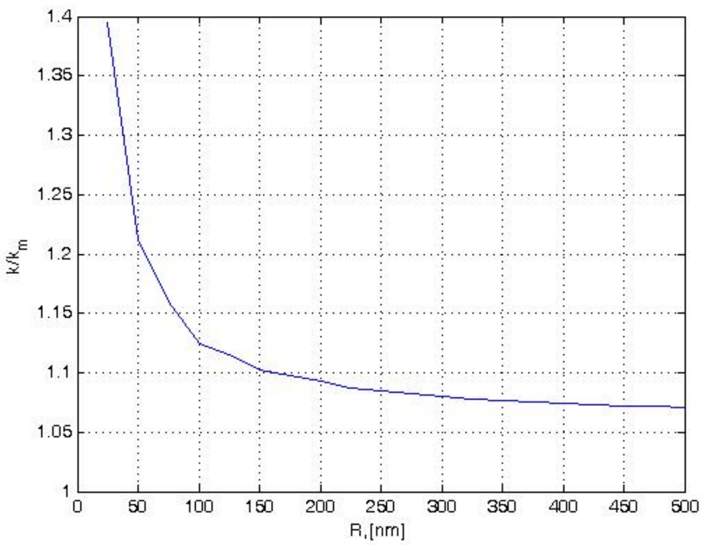

Fig. 3. Dependence of effective heat conductivity coefficient on the size of inclusions *R*.

According to experiments [1], Young modulus of butadiene-styrene rubber matrix was taken to be equal to E_m=135 Mpa. Poison ratio of butadiene-styrene rubber matrix was equal to v_m=0.4999. Young modulus and Poisson ratio of schungite were considered to be E_i=1.5 GPa and v_i=0.3 respectively. The thickness of interphase was determined in accordance with expression, see [10]

$$l = l_0 C_\infty \left(\frac{R}{l_0 C_\infty} \right)^{2(d-d_f)/d}, \qquad (46)$$

where l_0=1.54 nm is the length of skeletal bond of main chain , C_∞=12.5 is the kinetic flexibility of a polymeric molecular chain, d=3 is the spatial dimension, d_f = 2.568 is the fractal dimension of the filling compound surface.

Young modulus of the interphase was calculated using expression [10]

$$E_l = 0.44 + 0.94 \cdot (C_\infty^l - 3), \qquad (47)$$

where C_∞^l =3.58 is the kinetic flexibility of polymeric molecular chain in the layer. Poison ratio of the interphase was varied, and in computations we set it to be $\nu_l = \{0.4999, 0.3\}$.

Computation results for effective Young modulus E and bulk modulus K are shown in Fig. 4. As it can be seen from Fig. 4a, the decrease of radii of inclusions R at first can cause essential growth of Young modulus, but then Young modulus abruptly declines. In the range 15 nm<R<985 nm the maximum value of Young modulus was attained at R~25 nm.

At the same time, mechanical properties of elastomeric composites with small volume fraction of inclusions depend on size of nanoparticles as well as on mechanical properties of interphase. Fig. 4b indicates that the dependence of effective bulk modulus on Poison ratio of interphase can be very essential.

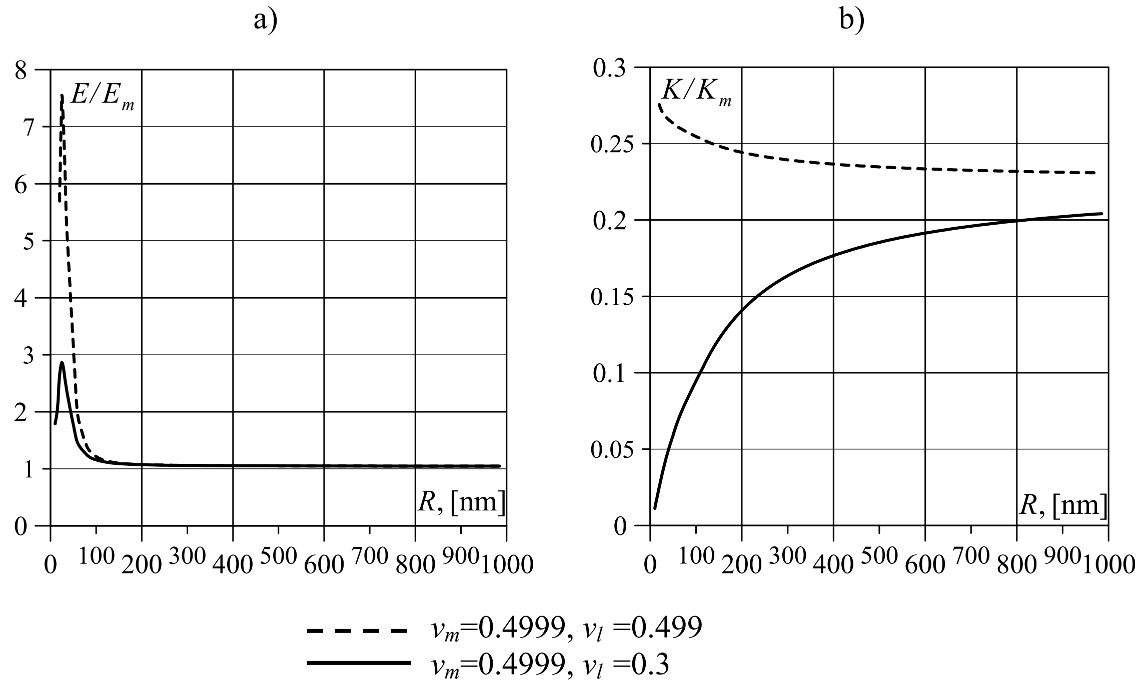

Fig. 4. a) Young modulus depending on radius R of inclusion, b) bulk modulus depending on radius R of inclusion.

Comparison of our numerical results with experiments [1] was made for values of Young modulus. Results of this comparison are represented in Table 1. According to [1], experimental results for Young modulus corresponded to displacements ~105 nm. Experimental thickness of interphase was 25 nm, its Young modulus was E_l=0.987 GPa. Size of nanoparticle was ~40 nm, size of microparticle was ~200 nm. As it can be seen from Table 1, numerical values for Young modulus are in a good agreement with experimental ones.

Table 1. Comparison of numerical and experimental [1] results for Young modulus.

	Numerical results, MPa	Experimental results, MPa	Spread of experimental values, MPa
Nanoparticles	167	~193	[170, 216]
Microparticles	153	~140	[126, 154]

5. Conclusions

In this paper we performed multi scale modeling of thermo elastic properties of composites with periodic structure of heterogeneities. We considered homogeneous matrix with periodic system of spherical particles, separated from the matrix by an interphase. Asymptotic averaging was applied in order to derive homogenized motion and heat conductivity equations for effective medium with averaged properties. In frames of homogenization technique we derived local cell problems. Cell problems' solution made it possible to determine effective properties of the medium as averaged coefficients, which incorporate peculiarities of spatial structure, mechanical and thermodynamic properties of composite components. 3D cell problems were solved numerically for the case of elastomeric composites, consisting of nano- or micro- particles of schungite, incorporated into butadiene-styrene rubber matrix. As a result of computations we came to the conclusion that for radii of inclusions, which belong to nano region (~25 nm), effective heat conductivity coefficient of homogenized composite material can be half as much as heat conductivity coefficient of the matrix. When radii of inclusions become ~200-250 nm and bigger (micro region), effective heat conductivity coefficient becomes close to the heat conductivity coefficient of matrix. Mechanical properties of elastomeric composites with small volume fraction of inclusions depend on the size of nanoparticles as well as on the mechanical properties of interphase. Reduction in size of particles from micro to nanosizes resulted in the effect of reinforcement of Young modulus at some values of particle size in the nano region. But posterior reduction of nanoparticle sizes led to an abrupt decrease of Young modulus. The effective values of Young modulus, calculated in the frames of our approach, were in a good agreement with analogous results, obtained experimentally.

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