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► **To cite this version:**

Anna Nasedkina, Andrey Nasedkin, Vladimir Remizov. Some approaches to modeling of the effective properties for thermoelastic composites. 2nd ECCOMAS Young Investigators Conference (YIC 2013), Sep 2013, Bordeaux, France. hal-00855866

HAL Id: hal-00855866

<https://hal.science/hal-00855866v1>

Submitted on 30 Aug 2013

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Some approaches to modeling of the effective properties for thermoelastic composites

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Abstract. *The work deals with the modeling of thermoelastic composites with regular and irregular structures. The approaches to the modeling of the effective properties include the construction of the representative volumes with account for microstructure, the effective moduli method for the mechanics of composites, and the finite element technologies for solving the problems for the representative volumes.*

Keywords: Composite, Thermoelasticity, Multiscale Modeling, Finite Element Method, Effective Moduli Method.

1 INTRODUCTION

The determination of the effective properties for the composite materials with field coupling, such as thermoelastic porous materials, is very important in the case of account for their microstructure. The paper develops the approaches to the modeling of composite materials based on the effective moduli method for the mechanics of composites, computer modeling of the representative volumes with account for their microstructure and application of the finite element technologies for solving coupled problems for the representative volumes of composites under special boundary conditions.

The methodology of the modeling of composite materials consists in the following steps. At microlevel the models of elastic skeleton of the representative volumes are built so that they take into account some characteristics of porous isotropic or anisotropic heterogeneous composite structures. These mathematical models are then transformed into finite element models. The effective properties of these composites are determined with the help of the effective moduli method and by finite element solving of several thermoelasticity problems for representative volume with special boundary conditions. At macrolevel the compound structure is considered to be an elastic or thermoelastic material with effective properties.

The main ideas for the approaches presented in the paper can be illustrated by examples of composite poroelastic and thermoelastic materials which are of interest for the problems of bio- and geomechanics.

2 THERMOELASTIC MATERIAL MODEL

Let us consider heterogeneous thermoelastic material in a volume Ω . Then the thermoelastic static problem is described by the equations

$$\nabla \cdot \boldsymbol{\sigma} = 0, \quad \boldsymbol{\sigma} = \mathbf{c} \cdot \boldsymbol{\varepsilon} - \boldsymbol{\beta} \theta, \quad \boldsymbol{\varepsilon} = \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^*) \quad (1)$$

$$\nabla \cdot \mathbf{q} = 0, \quad \mathbf{q} = -\mathbf{k} \cdot \nabla \theta \quad (2)$$

where $\boldsymbol{\sigma}$ is the stress tensor, \mathbf{c} is the tensor of elastic stiffness, $\boldsymbol{\varepsilon}$ is the strain tensor, $\boldsymbol{\beta}$ is the tensor of thermal stress coefficients, θ is the temperature increment from natural state, \mathbf{u} is the displacement vector, \mathbf{q} is the vector of the heat flux, \mathbf{k} is the tensor of thermal conductivities.

As is known, according to the porothermoelastic analogy the problems of thermoelasticity (1), (2) can be considered as the problems of poroelasticity and vice versa. Indeed, in the framework of static Biot's theory of poroelasticity the poroelastic static problem is described by the equations

$$\nabla \cdot \boldsymbol{\sigma} = 0, \quad \boldsymbol{\sigma} = \mathbf{c} \cdot \boldsymbol{\varepsilon} - \mathbf{b} p, \quad \boldsymbol{\varepsilon} = \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^*) \quad (3)$$

$$\nabla \cdot \mathbf{v}_f = 0, \quad \mathbf{v}_f = -\tilde{\mathbf{k}}_f \quad (4)$$

Here \mathbf{b} is the Biot's tensor, p is the pore pressure, \mathbf{v}_f is the filtration velocity vector, $\tilde{\mathbf{k}}_f = \mathbf{k}_f / \mu_f$, \mathbf{k}_f is the tensor of permeability coefficients, μ_f is the fluid viscosity.

It is obvious that poroelastic and thermoelastic composites in the framework of the models (1), (2) and (3), (4) can be considered as identical materials as the following substitutions can be made $p \leftrightarrow \theta$, $\mathbf{b} \leftrightarrow \boldsymbol{\beta}$, $\tilde{\mathbf{k}}_f \leftrightarrow \mathbf{k}$. We note that the thermal problem (2) and the filtration problem (4) in the stationary case are not coupled with the mechanical fields.

3 MODELS OF REPRESENTATIVE VOLUMES FOR BINARY COMPOSITES

At microlevel we consider the models of elastic 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. Newnam corresponds to 3-0 connectivity and the second case corresponds to 3-3 connectivity (closed and open inclusions or pores, respectively).

The model of 3-3 connectivity type is constructed by the following manner. The cube constructed by translation of equal structured cells along three directions is considered as a representative volume. Each cell in its turn also represents a cube consisting of $10 \times 10 \times 10$ cubic elements. The connected skeleton with the elements in the cube corners always exist in the cell. The skeleton consist of parallelepiped represented by own edges (linear dimensions are pointed out by the randomizer) as well as the chains of elements connecting its corners with the corners of the main cell. The connecting element chains are generated by the randomizer as well. When the skeleton occupies 10 % of cells volume, the maximum possible porosity that can be achieved in this model is up to 90%.

We would like to note that such models for porous composite can lose the coherence of the skeleton in the case of the large amount of pores and also does not support the structure of the composite connectivity (3-0 or 3-3). In order to built connected structures in the cubic lattice the algorithms of the percolation theory can be used that allow obtaining flowing clusters. The generation of the structures for representative volumes are carried out using separate programs in C and are then subsequently transferred to ANSYS.

4 EFFECTIVE MODULI METHOD FOR THERMOELASTIC COMPOSITES

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. The choice of the representative volume and boundary problems for the heterogeneous medium and the comparison medium is very important, as well as the technologies for solving the problems for heterogeneous media.

For poroelastic homogeneous comparison medium we adopt that the same equations (1), (2) are satisfied with constant modules \mathbf{c}^{eff} , $\boldsymbol{\beta}^{eff}$, \mathbf{k}^{eff} , which are to be determined.

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

$$\mathbf{u} = \mathbf{x} \cdot \boldsymbol{\varepsilon}_0, \quad \theta = \theta_0, \quad \mathbf{x} \in \Gamma \quad (5)$$

where $\boldsymbol{\varepsilon}_0 = \boldsymbol{\varepsilon}_0^*$, θ_0 are some values that do not depend on \mathbf{x} . Then $\mathbf{u} = \mathbf{x} \cdot \boldsymbol{\varepsilon}_0$, $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_0$, $\theta = \theta_0$, $\boldsymbol{\sigma} = \boldsymbol{\sigma}_0 = \mathbf{c}^{eff} \cdot \boldsymbol{\varepsilon}_0 - \boldsymbol{\beta}^{eff} \theta_0$ will give the solution for the problem (1), (2), (5) in the volume Ω for the homogeneous comparison medium.

Let us solve now the same problem (1), (2), (5) for heterogeneous medium and assume that for this medium and for the comparison medium the averaged stresses are equal $\langle \boldsymbol{\sigma} \rangle = \langle \boldsymbol{\sigma}_0 \rangle$, where hereinafter the angle brackets denote the averaged by the volume value $\langle \dots \rangle = (1/\Omega) \int_{\Omega} (\dots) d\Omega$. Therefore we obtain that for the effective moduli of the composite the equation $\langle \boldsymbol{\sigma} \rangle = \mathbf{c}^{eff} \cdot \boldsymbol{\varepsilon}_0 - \boldsymbol{\beta}^{eff} \theta_0$ is satisfied, where $\boldsymbol{\varepsilon}_0$ and θ_0 are the given values from the boundary conditions (5). Hence, even in the assumption of the anisotropy of the general form for the comparison medium, all the stiffness modules c_{ijkl}^{eff} and thermal stress coefficients β_{ij}^{eff} can be computed. Indeed, setting in (8) $\boldsymbol{\varepsilon}_0 = \varepsilon_0(\mathbf{e}_l \mathbf{e}_m + \mathbf{e}_m \mathbf{e}_l)/2$, $\varepsilon_0 = \text{const}$, $\theta_0 = 0$ for fixed indexes l and m ($\mathbf{e}_l, \mathbf{e}_m$ are the orts of the Cartesian coordinate system), we get the computation formulas for the elastic modules c_{ijlm}^{eff} : $c_{ijlm}^{eff} = \langle \sigma_{ij} \rangle / \varepsilon_0$. If in (8) we set $\boldsymbol{\varepsilon}_0 = 0$, $\theta_0 \neq 0$, than from the boundary problem (1), (2), (5) the thermal stress effective modules can be obtained: $\beta_{ij}^{eff} = \langle \sigma_{ij} \rangle / \theta_0$. An important justification of the choice of the boundary condition $\mathbf{u} = \mathbf{x} \cdot \boldsymbol{\varepsilon}_0$ 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 $\langle \boldsymbol{\varepsilon} \rangle = \langle \boldsymbol{\varepsilon}_0 \rangle$, $\langle \boldsymbol{\sigma} \cdot \boldsymbol{\varepsilon} \rangle = \langle \boldsymbol{\sigma}_0 \cdot \boldsymbol{\varepsilon}_0 \rangle$ also take place. Therefore with such boundary condition for two media under consideration their mechanical potential energies appear to be equal.

In order to determine the effective coefficients of the tensor \mathbf{k} it is sufficient to consider the thermal conductivity equation (2). For the formulation of the corresponding boundary-value problem we adopt the boundary conditions in the form

$$\theta = \mathbf{x} \cdot \mathbf{G}_0, \quad \mathbf{x} \in \Gamma \quad (6)$$

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 (2), (6) in the volume Ω for the homogeneous comparison medium. Then having solved the problem (2), (6) 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 (6). Then for the comparison medium with anisotropy of general form it is not difficult to obtain computation formulas for thermal conductivity modules k_{il}^{eff} . Indeed, setting in (6) $\mathbf{G}_0 = G_0 \mathbf{e}_l$, $G_0 = \text{const}$ for fixed index l , we get computation formulas for the modules k_{il}^{eff} : $k_{il}^{eff} = -\langle q_i \rangle / G_0$. The choice of the boundary condition $\theta = \mathbf{x} \cdot \mathbf{G}_0$ in (6) 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 $\langle \mathbf{G} \rangle = \langle \mathbf{G}_0 \rangle$, $\langle \mathbf{q} \cdot \mathbf{G} \rangle = \langle \mathbf{q}_0 \cdot \mathbf{G}_0 \rangle$. Thus, with the boundary condition (6) for two media their potential energies appear to be equal.

The approaches described above are associated with the averaging of the modules \mathbf{c} , $\boldsymbol{\beta}$, \mathbf{k} . Therefore in analogy with classical composite mechanics we will call this method as Voight averaging analogue and will mark the effective moduli obtained with the superscript "V" $\mathbf{c}^{eff} = \mathbf{c}^{Veff}$, $\boldsymbol{\beta}^{eff} = \boldsymbol{\beta}^{Veff}$, $\mathbf{k}^{eff} = \mathbf{k}^{Veff}$.

The second way of determination of the effective moduli is related to another type of the boundary conditions. In this case the boundary conditions are set for the stress vector and normal component of thermal flux analogously to the second type of the boundary conditions described for the poroelastic problems in [2]. This method is known as Reuss averaging analogue.

We also note that using the analogy between thermo- and poroelasticity problems, it is possible to calculate the effective moduli for anisotropic poroelastic composites of analogous structures [2].

5 RESULTS AND CONCLUSIONS

During the finite element computations of the heterogeneous thermoelasticity problems for representative volumes anisotropic thermoelastic materials and different boundary conditions for displacements, temperatures, stresses and heat fluxes were considered. The set of problems can be considered as analogues to Voight and Reuss approaches for heterogeneous anisotropic structure. The effective modules obtained from the computations of different boundary problems were compared [2]. Using the analogy between thermo- and poroelasticity problems, the possibilities of the effective moduli determination are discussed for anisotropic poroelastic composites of analogous structures.

The finite element computations were made with the help of the computation complex ANSYS and special set of computer programs written in marcolanguage APDL ANSYS. At that the generation of the range of the structures for representative volumes were carried out using separate programs in C and subsequent transfer of solid and finite element models to ANSYS.

The technologies developed enable to analyze multiphase anisotropic thermoelastic and poroelastic composites with regard to its microstructure and study the problems for macrovolumes of these composites.

ACKNOWLEDGEMENT

The work was partially supported by RFBR, research projects No. 12-01-00829, 13-01-00943 a and No. 12-01-31411 mol_a.

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