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CROSS-PROPERTY CONNECTIONS BETWEEN YOUNG'S MODULUS AND DIFFUSION COEFFICIENT OF TWO-PHASE COMPOSITE

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The paper interrelates changes in the effective elastic and diffusion properties of a two-phase composite using microstructural parameters. It is suggested that there are some inhomogeneities identical in shape in the material. The development of the cross-property connections in the explicit tensor form has been presented. The segregation effect, being a constant jump in concentration of particles of the solute flux at the matrix/inhomogeneity interface, was taken into account. It is a good practice to apply the derived cross-property relations to finding some effective properties of material using others when the material's microstructure is unknown. The obtained expressions were put to the test for isotropic material with pores; the approximate correlations were compared with exact ones found for the specific microstructure.

Keywords: effective Young's modulus, effective diffusion coefficient, cross-property connection, segregation effect

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СООТНОШЕНИЯ МЕЖДУ МОДУЛЕМ ЮНГА И КОЭФФИЦИЕНТОМ ДИФФУЗИИ ДВУХФАЗНОГО МАТЕРИАЛА

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В работе устанавливается взаимосвязь между изменениями эффективных упругих и диффузионных свойств двухфазного композита через микроструктурные параметры. Предполагается, что в материале присутствуют одинаковые по форме неоднородности. Представлен вывод соотношений в явном тензорном виде. При установлении взаимосвязи между эффективными свойствами учитывается эффект сегрегации, заключающийся в скачке концентрации растворенного вещества на границе раздела матрица/неоднородность. Полученные соотношения целесообразно использовать для определения одних эффективных свойств через другие, когда микроструктура материала неизвестна. Установленная взаимосвязь проверена для изотропного материала с порами. Найденные приближенные соотношения сравниваются с точными, полученными для конкретной микроструктуры.

Ключевые слова: эффективный модуль Юнга, эффективный коэффициент диффузии, взаимосвязь между свойствами композита

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Introduction

Finding connections between various effective properties of heterogeneous materials is a fundamental problem of mechanics [1, 2]. These mathematical expressions interrelate the changes in different physical properties caused by a certain microstructure. The significance of this problem is defined by the fact that it allows one to determine certain effective properties by means of others in the absence of exhaustive information on the composite microstructure.

The search for various cross-property connections have been a topic for studies in literature since 1960s. An in-depth review of this problem is presented in [3]; according to the data presented the published studies may be conditionally divided into four directions:

qualitative research;

establishment of empirical dependencies;

determination of the ranges of material characteristic changes;

finding connections for materials with isolated inhomogeneities in explicit form.

There are currently a limited number of the published works devoted to the fourth direction. Explicit connections between effective elastic and conductive properties of materials were established in [4, 5]. These expressions describe anisotropic material with an isotropic matrix; the accuracy of the proposed connections depends on the shape of the inhomogeneities and the difference in the elastic properties of the constituents. Equations connecting strength characteristics of metal composite with graphite flakes to its thermal conductivity were obtained in [6]. Connections between effective thermal expansion and effective thermal conductivity were presented in [7, 8]. The accuracy of these correlations depends on the shape of inhomogeneities and the difference in the thermal conductivity of the constituents. Mutual dependencies between effective diffusion coefficient and thermal conductivity of a metal-diamond composite were presented in [7, 8]. Explicit connections between thermal and electrical properties of a composite were obtained in [11].

A significant difference between the problems of diffusion and thermal conductivity considered in [4, 5] is that temperature is a continuous function across the interface of two phases (matrix/inhomogeneity) while concentration is usually not [12]. This phenomenon of the diffusing particles accumulating at the phase interface or inside inhomogeneities is known as the segregation effect [13].

This work is devoted to establishing explicit connections between effective elastic and diffusion properties of a two-phase composite with inhomogeneities identical in shape while taking the segregation effect into account.

The obtained connections are tested for a case of isotropic porous material while interrelating the changes in Young's modulus and diffusion coefficient.

Connections between effective elastic and diffusion properties of a two-phase composite

The connections between effective elastic and conductive properties obtained in papers [4, 5] are based on the fact that the changes in these properties different in nature are under control of the same microstructural parameters. Two main assumptions were used in the course of deriving the connections:

inhomogeneities are spheroidal;

effective properties are determined in the framework of the non-interaction approximation (NIA).

However, papers [4, 5] show that the obtained connections are valid for materials with differently shaped inhomogeneities and at greater concentrations than the NIA permits. This is due to the fact that the shape and concentration of inhomogeneities influence the elastic and conductive properties to the same extent.

Based on an analogy between diffusion and conductivity equations, let us use a methodology described in papers [4, 5] to establish connections between effective elastic and diffusion properties. According to this methodology, property contribution tensors are introduced to describe the effect of an inhomogeneity on the properties of interest, they act as primary microstructural parameters [3].

We introduce the fourth-rank compliance contribution tensor **H** describing extra strain occurring over a reference volume due to the presence of the isolated inhomogeneity. The indicated tensor depends on the shape of the inhomogeneity and the difference in the elastic properties of the matrix and the inhomogeneity. In case the inclusion is spheroidal, tensor **H** is transversely-isotropic (the symmetry axis coincides with the symmetry axis of the spheroid) and can be presented as a linear combination of $\mathbf{T}_1$, $\mathbf{T}_2$, ..., $\mathbf{T}_6$ tensor basis elements:

$$\mathbf{H} = \sum_{k=1}^{6} h_k \mathbf{T}_k, \tag{1}$$

where

$$\mathbf{T}_1 = \boldsymbol{\theta\theta},$$
$$\mathbf{T}_2 = \frac{1}{2}\left((\boldsymbol{\theta\theta})^T_{(1,4)} + (\boldsymbol{\theta\theta})^T_{(2,4)} - \boldsymbol{\theta\theta} \right),$$
$$\mathbf{T}_3 = \boldsymbol{\theta}\mathbf{nn}, \ \mathbf{T}_4 = \mathbf{nn}\boldsymbol{\theta},$$
$$\mathbf{T}_5 = \frac{1}{4}\left(\mathbf{n}\boldsymbol{\theta}\mathbf{n} + (\mathbf{n}\boldsymbol{\theta}\mathbf{n})^T_{(1,2)(3,4)} + (\boldsymbol{\theta}\mathbf{nn})^T_{(1,4)} + (\boldsymbol{\theta}\mathbf{nn})^T_{(2,3)} \right),$$
$$\mathbf{T}_6 = \mathbf{nnnn},$$

$\boldsymbol{\theta}$ is a projection tensor; $\boldsymbol{\theta} = \mathbf{I} - \mathbf{nn}$ (**I** is the second-rank unit tensor).

Effective compliance tensor can be determined in the frame of the NIA in the following way:

$$\mathbf{S}^{eff} = \mathbf{S}^0 + \frac{1}{V}\sum_k V_k \mathbf{H}_k, \tag{2}$$

where $\mathbf{S}^0$ is a matrix compliance tensor, V is a reference volume, V_k is the volume of the k^{th} inhomogeneity.

When calculating effective elastic properties of the materials with inhomogeneities identical in shape, expression (2) can be rewritten in a form:

$$\mathbf{S}^{eff} = \mathbf{S}^0 + \rho\left(W_1\mathbf{II} + W_2\mathbf{J}\right) + W_3\left(\mathbf{I}\boldsymbol{\omega} + \boldsymbol{\omega}\mathbf{I}\right) + W_4\left(\mathbf{J}\cdot\boldsymbol{\omega} + \boldsymbol{\omega}\cdot\mathbf{J}\right) + W_5\boldsymbol{\Omega}, \tag{3}$$

where

$$\mathbf{J} = \frac{1}{2}\left((\mathbf{II})^T_{(1,4)} + (\mathbf{II})^T_{(2,4)} \right)$$

is the fourth-rank unit tensor; parameters $W_i (i = 1, 2, ..., 5)$ are expressed by means of h_i coefficients as

$$W_1 = h_1 - h_2/2, \ W_2 = h_2,$$
$$W_3 = -2h_1 + h_2 + 2h_3,$$
$$W_4 = -2h_2 + h_5,$$
$$W_5 = h_1 + \frac{h_2}{2} - 2h_3 - h_5 + h_6,$$

while

$$\boldsymbol{\Omega} = \frac{1}{V}\sum_k V_k (\mathbf{nnnn})^{(k)},$$
$$\boldsymbol{\omega} = \frac{1}{V}\sum_k V_k (\mathbf{nn})^{(k)}, \tag{4}$$
$$\rho = \mathrm{tr}\boldsymbol{\omega} = \frac{1}{V}\sum_k V_k;$$

ρ is a volume fraction of the inhomogeneities.

One can determine the effective diffusion properties of the material consisting of a matrix with an isotropic diffusivity tensor $\mathbf{D}_0 = D_0\mathbf{I}$ and inhomogeneities with $\mathbf{D}_1 = D_1\mathbf{I}$ in a similar way [14]. Either a second-rank diffusivity contribution tensor $\mathbf{H}^D$ which determines additional mass flux caused by the presence of the inhomogeneity in the material, or a second-rank diffusion resistivity contribution tensor $\mathbf{H}^{DR}$ $\left(\mathbf{H}^{DR} = -\mathbf{H}^D / D_0^2\right)$, is introduced.

Both the matrix and the inhomogeneity obey linear Fick's law. The normal component of the flux is deemed to be continuous at the interface of the matrix (denoted by "+") and the inhomogeneity (denoted by "–"), while the concentration is subject to a jump

$$c(x)\Big|_{x\to\partial V+} = sc(x)\Big|_{x\to\partial V-}, \tag{5}$$

where s is the segregation factor.

The presence of the segregation effect leads to a fundamental distinction of the diffusion process from that of thermal conductivity considered in papers [4, 5]. The segregation factor shows a ratio of the concentrations at the inhomogeneity's interface and inside of it; it equals one in case of a continuous concentration function at the matrix/inhomogeneity interface. A case of $s > 1$ corresponds to a material in which the diffusing particles accumulate at the interface of two phases, while the $s < 1$ case corresponds to trapping of particles inside the inhomogeneities [14]. In studies of matrices with pores, only the $s \le 1$ case is of interest from the physical point of view.

In case of the spheroidal inhomogeneity, the contribution tensors are determined in the following matter:

$$\begin{gathered}\mathbf{H}^D = D_0\left[B_1(\mathbf{I}-\mathbf{nn}) + B_2\mathbf{nn}\right],\\ \mathbf{H}^{DR} = -\frac{1}{D_0}\left[B_1(\mathbf{I}-\mathbf{nn}) + B_2\mathbf{nn}\right],\end{gathered} \tag{6}$$

while the B_1 and B_2 coefficients depend on the shape of the inhomogeneities, the difference in the diffusion coefficients of the matrix and the inhomogeneity, as well as the segregation factor.

The effective diffusivity tensor is introduced in the frame of the NIA as

$$\mathbf{D}^{eff} = D_0\mathbf{I} + \frac{1}{V}\sum_k V_k \mathbf{H}_k^D, \tag{7}$$

while the effective resistivity tensor has a form

$$\left(\mathbf{D}^{eff}\right)^{-1} = \frac{1}{D_0}\mathbf{I} + \frac{1}{V}\sum_k V_k \mathbf{H}_k^{DR}. \tag{8}$$

Effective diffusion properties of the material with the inhomogeneities identical in shape can be expressed using the ρ volume fraction of the inhomogeneities and the second-rank tensor $\boldsymbol{\omega}$ determined by expressions (4) in the following manner:

$$\begin{gathered}\frac{1}{D_0}\mathbf{D}^{eff} - \mathbf{I} = \mathbf{I} - D_0\left(\mathbf{D}^{eff}\right)^{-1} = \\ = B_1\rho\mathbf{I} + (B_2 - B_1)\boldsymbol{\omega}.\end{gathered} \tag{9}$$

Establishing explicit connections between the effective elastic and diffusion properties is possible if they are expressed in terms of the same microstructural parameters, i.e. the ρ scalar parameter and $\boldsymbol{\omega}$ tensor parameter. Therefore, to obtain the cross-property connections, we need to eliminate the summand containing the fourth-rank $\boldsymbol{\Omega}$ tensor in effective compliance tensor expression (3). According to statements in papers [4, 5], this is possible by means of correcting W_1, W_2, W_3, W_4 coefficients:

$$\begin{gathered}\mathbf{S}^{eff} = \mathbf{S}^0 + \frac{1}{E_0}\Big[\rho\left(s_1\mathbf{I}\cdot\mathbf{I} + s_2\mathbf{J}\right) + \\ + \frac{s_3}{2}\left(\mathbf{I}\cdot\boldsymbol{\omega} + \boldsymbol{\omega}\cdot\mathbf{I}\right) + \frac{s_4}{2}\left(\mathbf{J}\cdot\boldsymbol{\omega} + \boldsymbol{\omega}\cdot\mathbf{J}\right)\Big],\end{gathered} \tag{10}$$

where E_0 is Young's modulus of the matrix, s_i (i = = 1, 2, 3, 4) coefficients are determined as

$$\begin{gathered}s_1 = E_0\left(\hat{h}_1 - \hat{h}_2/2\right),\\ s_2 = E_0\hat{h}_2,\\ s_3 = E_0\left(-2\hat{h}_1 + \hat{h}_2 + 2\hat{h}_3\right),\\ s_4 = E_0\left(-2\hat{h}_2 + \hat{h}_5\right),\end{gathered}$$

and $\hat{h}_i$ (i = 1, 2, ..., 5) coefficients are expressed through hi as follows:

$$\hat{h}_i = h_i\left(1-\delta\ \mathrm{sign}h_i\right)$$
$$\text{at } i = 1, 2, 6;$$
$$\hat{h}_i = h_i\left(1+\delta\ \mathrm{sign}h_i\right)$$
$$\text{at } i = 3, 5;$$
$$\delta = \\ = \frac{h_1 + h_2/2 - 2h_3 - h_5 + h_6}{|h_1| + |h_2|/2 + 2|h_3| + |h_5| + |h_6|}.$$

To derive the connections between the effective elastic and diffusion properties of the material for a general case of orientation distribution of inhomogeneities, let us express the $\boldsymbol{\omega}$ tensor and the ρ parameter using the $\mathbf{D}^{eff}$ and $\left(\mathbf{D}^{eff}\right)^{-1}$ tensors, respectively:

$$\boldsymbol{\omega} = \\ = \frac{1}{\left(B_2 - B_1\right)}\left(\frac{1}{D_0}\mathbf{D}^{eff} - \mathbf{I}\right) - \\ - \frac{B_1}{\left(B_2 - B_1\right)}\rho\mathbf{I}, \tag{11}$$
$$\rho = \frac{\mathrm{tr}\mathbf{D}^{eff} - 3D_0}{D_0\left(2B_1 + B_2\right)};$$

$$\boldsymbol{\omega} = \\ = \frac{1}{\left(B_2 - B_1\right)}\left(\mathbf{I} - D_0\left(\mathbf{D}^{eff}\right)^{-1}\right) - \\ - \frac{B_1}{\left(B_2 - B_1\right)}\rho\mathbf{I}, \tag{12}$$
$$\rho = \frac{3 - D_0\mathrm{tr}\left(\mathbf{D}^{eff}\right)^{-1}}{2B_1 + B_2}.$$

As a result of substituting these expressions in Eq. (10), we can obtain two correlations establishing an explicit connection between the effective compliance and the effective diffusion properties:

$$E_0\left(\mathbf{S}^{eff} - \mathbf{S}^0\right) = \\ = \left(\alpha_1\mathbf{I}\cdot\mathbf{I} + \alpha_2\mathbf{J}\right)\times \\ \times\left(\mathrm{tr}\mathbf{D}^{eff}/D_0 - 3\right) + \\ + \alpha_3\left[\left(\mathbf{D}^{eff}/D_0 - \mathbf{I}\right)\mathbf{I} + \\ + \mathbf{I}\left(\mathbf{D}^{eff}/D_0 - \mathbf{I}\right)\right] + \\ + \alpha_4\left[\left(\mathbf{D}^{eff}/D_0 - \mathbf{I}\right)\cdot\mathbf{J} + \\ + \mathbf{J}\cdot\left(\mathbf{D}^{eff}/D_0 - \mathbf{I}\right)\right] \tag{13}$$

while using relations (11) and

$$E_0\left(\mathbf{S}^{eff} - \mathbf{S}^0\right) = \\ = \left(\alpha_1\mathbf{II} + á_2\mathbf{J}\right)\times \\ \times\left(3 - D_0\mathrm{tr}\left(\mathbf{D}^{eff}\right)^{-1}\right) + \\ + \alpha_3\left[\left(\mathbf{I} - D_0\left(\mathbf{D}^{eff}\right)^{-1}\right)\mathbf{I} + \\ + \mathbf{I}\left(\mathbf{I} - D_0\left(\mathbf{D}^{eff}\right)^{-1}\right)\right] + \\ + \alpha_4\left[\left(\mathbf{I} - D_0\left(\mathbf{D}^{eff}\right)^{-1}\right)\cdot\mathbf{J} + \\ + \mathbf{J}\cdot\left(\mathbf{I} - D_0\left(\mathbf{D}^{eff}\right)^{-1}\right)\right] \tag{14}$$

while using relations (12);
here

$$\alpha_1 = \frac{s_1\left(B_2 - B_1\right) - s_3B_1}{\left(B_2 - B_1\right)\left(2B_1 + B_2\right)},$$
$$\alpha_2 = \frac{s_2\left(B_2 - B_1\right) - s_4B_1}{\left(B_2 - B_1\right)\left(2B_1 + B_2\right)},$$
$$\alpha_3 = \frac{s_3}{2\left(B_2 - B_1\right)},$$
$$\alpha_4 = \frac{s_4}{2\left(B_2 - B_1\right)}.$$

Cross-property connections between effective Young's modulus and effective diffusion coefficient of a porous material

To derive connections between effective elastic moduli and effective diffusion coefficients, we need to use a component representation of Eqs. (13) and (14). In case of isotropic material, the following connections are in effect:

$$\frac{E^{eff}}{E_0} = \left[1 + \left(3\alpha_1 + 3\alpha_2 + 2\alpha_3 + 2\alpha_4\right)\left(\frac{D^{eff}}{D_0} - 1\right)\right]^{-1} \quad (15)$$

while using tensor expression (13) and

$$\frac{E^{eff}}{E_0} = \left[1 + \left(3\alpha_1 + 3\alpha_2 + 2\alpha_3 + 2\alpha_4\right)\left(1 - \frac{D_0}{D^{eff}}\right)\right]^{-1} \quad (16)$$

while using tensor expression (14).

Connections (15) and (16) express a dependence of one effective modulus on the other at the macro level. The necessary information on the microstructure is reduced to determining the shape of an individual inhomogeneity as α_i coefficients depend on it; in addition, there is no need to analyze the orientation distribution of inhomogeneities. In the general case, connections (15) and (16) are approximate, since they are obtained based on the approximate expression for effective compliance tensor (10).

Two cases correspond to the isotropic material containing inhomogeneities:

they have spherical shape,

they have arbitrary orientation distribution.

Connections (15) and (16) are exact in the first case as $\delta = 0$ and consequently the approximate expression for effective compliance tensor (10) coincides with the exact one. In the second case, $\delta \neq 0$ and expressions (15), (16) are approximate.

Let us investigate two these cases and evaluate the accuracy of the obtained approximate connections.

Using Eqs. (15), (16), let us determine the connection between effective Young's modulus and the effective diffusion coefficient of the material with spherical pores and compare the obtained expression and a direct calculation.

In case of the matrix with pores, the components of inhomogeneity's compliance contribution tensor h_i have the form

$$h_1 = \frac{q_6}{2\Delta},\ h_2 = \frac{1}{q_2},\ h_3 = -\frac{q_3}{\Delta},\quad h_4 = -\frac{q_4}{\Delta},\ h_5 = \frac{4}{q_5},\ h_6 = \frac{2q_1}{\Delta}, \quad (17)$$

where $\Delta = 2(q_1 q_6 - q_3 q_4)$ and

$$q_1 = \mu\left[4\kappa - 1 - 2(3\kappa - 1) f_0 - 2\kappa f_1\right],$$
$$q_2 = 2\mu\left[1 - (2 - \kappa) f_0 - \kappa f_1\right],$$
$$q_3 = q_4 = 2\mu\left[(2\kappa - 1) f_0 + 2\kappa f_1\right],$$
$$q_5 = 4\mu\left[f_0 + 4\kappa f_1\right],$$
$$q_6 = 8\mu\kappa\left[f_0 - f_1\right],$$
$$\kappa = (1 - \nu)/2;$$

μ – shear modulus of the matrix; ν – Poisson's ratio of the matrix; f_0, f_1 – functions depending on the shape of the spheroidal inhomogeneity, i.e. on the aspect ratio $\gamma = a_3/a$ (a_3 – semiaxis of rotation) as

$$f_0 = \frac{1 - g}{2\left(1 - \gamma^{-2}\right)},$$
$$f_1 = \frac{1}{4\left(1 - \gamma^{-2}\right)^2}\left[\left(2 + \gamma^{-2}\right) g - 3\gamma^{-2}\right],$$

where

$$g = \begin{cases} \dfrac{1}{\gamma\sqrt{1 - \gamma^2}} \arctan\dfrac{\sqrt{1 - \gamma^2}}{\gamma}, \gamma \le 1 \\ \dfrac{1}{2\gamma\sqrt{\gamma^2 - 1}} \ln\left(\dfrac{\gamma + \sqrt{\gamma^2 - 1}}{\gamma - \sqrt{\gamma^2 - 1}}\right), \gamma \ge 1. \end{cases}$$

Diffusivity tensor coefficients have the form

$$B_1 = \frac{1-\lambda}{s\lambda + (1-s\lambda) f_0},$$
$$B_2 = \frac{1-\lambda}{1-2(1-s\lambda) f_0}, \qquad (18)$$

where $\lambda = D_0/D_1$.

Then Eqs. (15) and (16) are reduced respectively to equalities

$$\frac{E^{eff}}{E_0} = \left[1 + \frac{(1-\nu)(9+5\nu)}{2(7-5\nu)} \times \frac{1+2s\lambda}{1-\lambda}\left(\frac{D}{D_0} - 1\right)\right]^{-1},$$
$$\frac{E^{eff}}{E_0} = \left[1 + \frac{(1-\nu)(9+5\nu)}{2(7-5\nu)} \times \frac{1+2s\lambda}{1-\lambda}\left(1 - \frac{D_0}{D}\right)\right]^{-1}. \qquad (19)$$

To obtain explicit cross-property connections, let us express the volume fraction of the inhomogeneities directly through the effective diffusion coefficient determined within the framework of the NIA and substitute it into the exact expression for the effective compliance tensor determined within the NIA as well.

Thus, the diffusivity and resistivity contribution tensors of the inhomogeneity are determined by expressions

$$\mathbf{H}_p^D = \frac{3(1-\lambda)}{2s\lambda + 1} D_0 \mathbf{I},$$
$$\mathbf{H}_p^{DR} = -\frac{3(1-\lambda)}{(2s\lambda + 1) D_0} \mathbf{I}. \qquad (20)$$

Substitution of first and second Eqs. (20) respectively into Eq. (7) for the effective diffusivity tensor and Eq. (8) for the effective resistivity tensor allows expressing the volume fraction of the inhomogeneities through effective diffusion properties.

Subsequent substitution of the obtained expression for ρ in effective compliance tensor given by Eq. (2) taking into account the formula for isotropic compliance contribution tensor of the spherical pore

$$\mathbf{H}_p = \frac{15(1-\nu)}{2\mu}\left[\frac{1}{10(1+\nu)}\frac{1}{3}\mathbf{I}\cdot\mathbf{I} + \frac{1}{7-5\nu}\left(\mathbf{J} - \frac{1}{3}\mathbf{I}\cdot\mathbf{I}\right)\right], \qquad (21)$$

leads to a result that completely coincides with expressions (19).

Thus, we tested the obtained approximate connections for a case of microstructure in which they are exact.

In the second case corresponding to the isotropic material (the arbitrary orientation distribution of the inhomogeneities), connections (15) and (16) are approximate. At the same time, we can establish connections between the effective elastic and diffusion properties for the case of arbitrary orientation distribution of spheroids independently by analogy with the method used above for the case of the spherical inhomogeneities.

For a quantitative and qualitative evaluations of the obtained approximate connections, let us compare them with the exact ones determined for this exact microstructure.

To establish exact connections, let us determine the volume fraction of the inhomogeneities using the effective diffusion coefficient of the isotropic material and then substitute the obtained expression in the equation determining effective Young's modulus. This approach is adequate due to the isotropy of the effective tensors. Therefore, the scalar parameter ρ is the only common microstructural parameter determining the effective properties of the material. When we use the NIA in terms of diffusivity contribution tensors, we obtain the following expression, which connects effective Young's modulus to the effective diffusion coefficient:

$$\frac{E^{eff}}{E_0} = \left[1 + \frac{E_0 h_\Sigma}{15\eta}\left(\frac{D^{eff}}{D_0} - 1\right)\right]^{-1}, \qquad (22)$$

and when we use the same method in terms

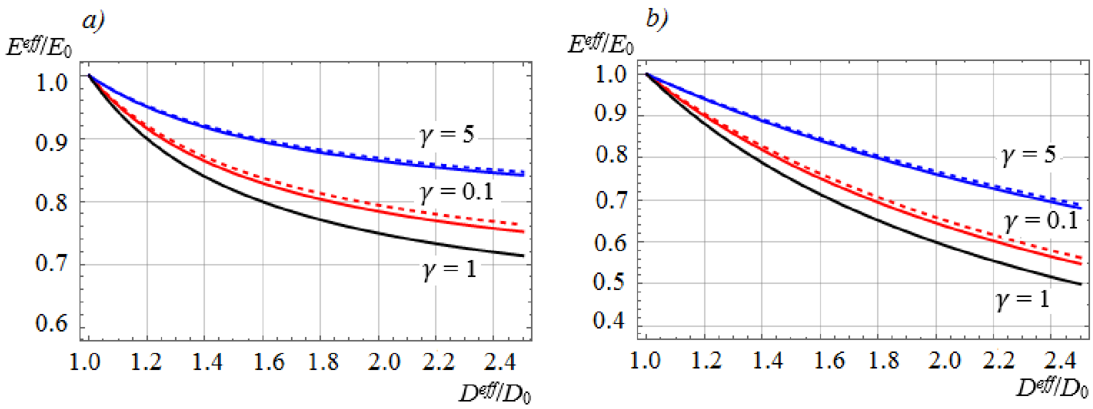

Fig. 1. Dependencies of relative effective Young's modulus on the relative effective diffusion coefficient while using compliance/resistivity (*a*) and compliance/diffusivity (*b*) cross-property connections for various values of the γ aspect ratios.
Approximate connections (solid lines) are compared to exact ones (dashed lines)

of resistivity contribution tensors the expression has a form:

$$\frac{E^{eff}}{E_0} = \left[1 + \frac{E_0 h_\Sigma}{15\eta}\left(1 - \frac{D_0}{D^{eff}}\right)\right]^{-1}, \qquad (23)$$

where $h_\Sigma = 8h_1 + 4h_2 + 4h_3 + 2h_5 + 3h_6$, $\eta = 2B_1/3 + B_2/3$.

Fig. 1 presents a comparison of the results obtained on the basis of approximate connections (15), (16) with the results obtained based on exact connections (22) and (23) respectively for the case of $\lambda = 0$, which corresponds to $D_1 \to \infty$ (in this case the segregation factor, as it follows from connection (18), is of no importance), $E_0 = 208$ GPa.

It is clear that connections (15) and (16) describe the relation between the effective properties at the macro level with sufficient accuracy. However, the effective values obtained using the resistivity tensors (Fig. 1, *a*) and the diffusivity tensors (Fig. 1, *b*) are different. This is due to the fact that the interaction of the inhomogeneities was neglected.

To obtain exact connection taking into account this interaction, let us employ Maxwell's homogenization scheme [3]. A result obtained using this scheme in terms of the diffusivity contribution tensors coincides with the result obtained in terms of the resistivity contribution tensors, and therefore the result is unambiguous as opposed to the NIA.

The author has already determined Young's modulus of the material with spheroidal pores in paper [15], and the effective diffusion coefficient of such material in paper [16]. To obtain exact connections, we need to substitute the expression of the volume fraction of the inhomogeneities

$$\rho = 3\frac{D^{eff} - D_0}{\left(D^{eff} + 2D_0\right)\eta}$$

into the expression for effective Young's modulus.

Fig. 2 presents a comparison of the approximate connections established in this work with the exact ones obtained using Maxwell's scheme for $\lambda = 0$, $E_0 = 208$ GPa.

An analysis of plots shown in Fig. 2 allows us to conclude that it is a good practice to use the connections obtained in terms of the diffusivity contribution tensors as they display better coincidence with the exact connections obtained within the Maxwell's scheme.

While studying the influence of segregation on the material cross-property connections, let us take into account that the diffusion coefficient of the pores is much greater than that of the matrix ($D_1 >> D_0$), but at the same time it is finite; such an assumption corresponds to a real material. To be specific, let us assume that $\lambda = 0.01$, $E_0 = 208$ GPa. A dependence on the segregation

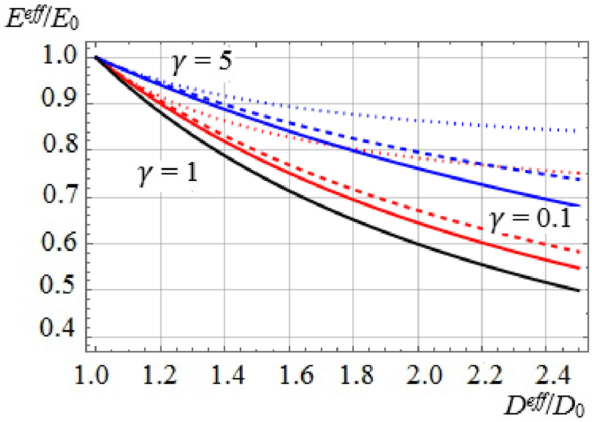

Fig. 2. Comparison of approximate compliance/diffusivity (solid lines) and compliance/resistivity (dashed lines) cross-property connections with exact connections (Maxwell's scheme, dashed lines)

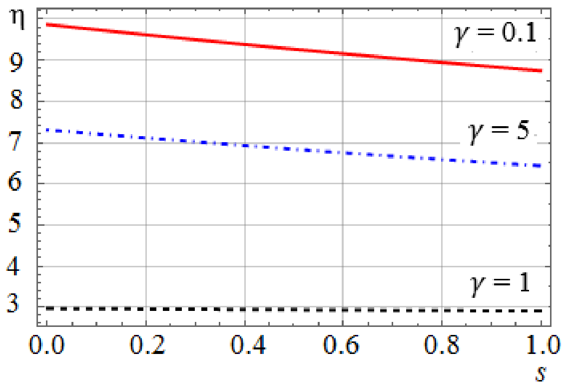

Fig. 3. Dependence of the η coefficient on the segregation factor at various aspect ratios γ

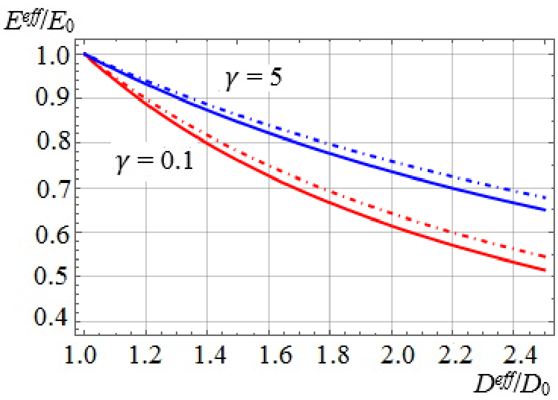

Fig. 4. Dependence of effective Young's modulus on the effective duffusion coefficient at two aspect ratios γ and the segregation parameter: $s = 1.00$ (solid line) and $s = 0.01$ (dash and dot line)

factor is implicitly present in expressions (15), (16) only in the η coefficient, since

$$3\alpha_1 + 3\alpha_2 + 2\alpha_3 + 2\alpha_4 = \\ = \frac{3(s_1 + s_2) + s_3 + s_4}{3\eta};$$

the same coefficient can be derived in the effective diffusivity tensor.

The dependence of the η coefficient on the segregation factor at various aspect ratios of the spheroid is presented in Fig. 3.

We can see that the segregation has no significant influence in the presence of spherical pores. In case of oblate and prolate spheroidal pores, the segregation influence is stronger, which affects the effective diffusion coefficients as well [14, 16]. However, according to the dependencies shown in Fig. 4, the segregation has no significant impact directly on the cross-property relations (the dependencies are based on compliance/diffusivity cross-property connection). Thus, another advantage of using the established cross-property connections in the explicit form consists in no dependence on whether or not the diffusing particles are trapped inside the pores: all we need is the information on the effective material properties (elastic or diffusion).

Conclusion

The paper provides explicit cross-property connections between effective elastic and diffusion properties of the material. The obtained dependencies can be applied to determine changes in certain effective properties by means of others in the absence of exhaustive information on the composite microstructure.

The cross-property connections were derived on the basis of a known (from literature) methodology described in terms of contribution tensors to determine a correlation between effective elastic and thermal conductivity properties. The dependencies take the segregation effect into account, which makes the diffusion problem fundamentally different from the thermal conductivity problem.

The case of isotropic material with containing trapped particles was detailed. The established cross-property connections describe the dependence of the effective Young's modulus of such material on the effective diffusion coefficient with sufficient accuracy.

Comparison of the results with the ones obtained within the Maxwell's scheme accounting for interaction between inhomogeneities shows that compliance/diffusivity connections are more preferable.

The paper analyzed the influence of segregation on the effective cross-property connections. It is shown, that accounting for segregation has no significant impact. This proves the advantage of applying the obtained connections when determining certain properties using the others at the macro level, since there is no need to estimate the segregation factor.

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