

On micromechanical modeling of particulate composites with inclusions of various shapes

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Abstract

The effective elastic properties of statistically homogeneous two-phase particulate composites are considered. Several first-order micromechanical models are re-written in terms of the inclusion compliance contribution tensor (**H**-tensor). This tensor is a convenient tool to evaluate contribution of arbitrarily shaped inclusions and cavities to the overall composite properties.

For any inclusion shape, the procedure starts with calculation of the **H**-tensor for a single inclusion. The non-interaction approximation is obtained by direct summation. More advanced micromechanical schemes are derived by substituting the non-interaction inclusion compliance contribution tensor into the formulae provided in the paper. The proposed procedure is illustrated by considering several two-dimensional and three-dimensional examples.

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1. Introduction

It is assumed that composite is statistically homogeneous so that a certain representative volume element (RVE) can be chosen. Then, the mechanical properties of the entire composite material are the same as those of the RVE. Discussion of the concept of representative volume element and information on how to choose the appropriate RVEs for composites of various microstructures can be found in Hill (1963), Markov (2000), and Nemat-Nasser and Hori (1993).

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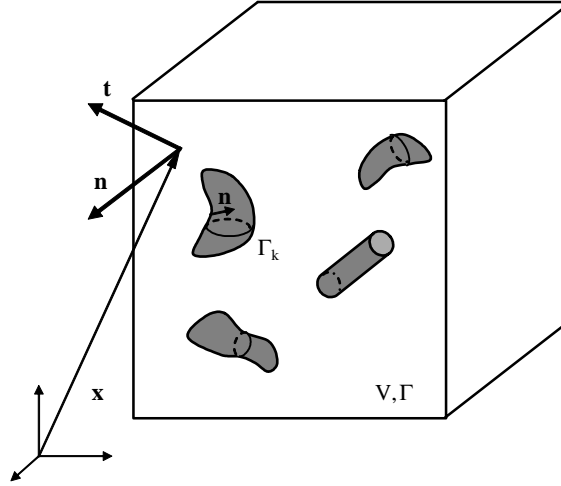


Fig. 1. Representative volume element.

We define macroscopic strain and stress in terms of the values of displacement \mathbf{u} and traction \mathbf{t} on the boundary Γ of the RVE of volume V (Fig. 1)

$$\boldsymbol{\varepsilon} = \frac{1}{2V} \int_{\Gamma} (\mathbf{u}\mathbf{n} + \mathbf{n}\mathbf{u}) d\Gamma, \quad \boldsymbol{\sigma} = \frac{1}{V} \int_{\Gamma} \mathbf{t}\mathbf{x} d\Gamma \quad (1)$$

where \mathbf{n} is the outward unit normal to Γ , \mathbf{x} is the position-vector of a point of the RVE boundary, and $\mathbf{u}\mathbf{n}$, $\mathbf{n}\mathbf{u}$, $\mathbf{t}\mathbf{x}$ are dyadic products of two vectors. In the literature, macroscopic strain and stress are often defined as averages of the corresponding fields over the RVE. It can be shown (using the divergence theorem) that definitions in terms of boundary values and in terms of volume averages are equivalent. We prefer definition (1) because no ambiguity arises when one of the phases consists of rigid inclusions or cavities. The fourth order effective elastic compliance and stiffness tensors (\mathbf{S} and \mathbf{C} , respectively) are defined as

$$\boldsymbol{\varepsilon} = \mathbf{S} : \boldsymbol{\sigma}, \quad \boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon} \quad (2)$$

where a colon denotes contraction over two indices.

Let us consider a composite with two phases, matrix and inclusions, having compliance tensors \mathbf{S}_M and \mathbf{S}_I , correspondingly. Inclusions are perfectly bonded to the matrix. Note that our terminology is different from that of Mura (1987)—we designate term “inclusion” instead of “inhomogeneity” to the dispersed second phase of the composite. To determine the effective elastic moduli, we use the *prescribed stress* procedure. Boundary of the RVE is subjected to traction $\mathbf{t} = \boldsymbol{\sigma}^0 \cdot \mathbf{n}$ corresponding to a uniform stress field $\boldsymbol{\sigma}^0$. To find the effective compliance, macroscopic strain has to be evaluated. We represent this strain as a sum of two terms:

$$\boldsymbol{\varepsilon} = \mathbf{S}_M : \boldsymbol{\sigma}^0 + \Delta\boldsymbol{\varepsilon} \quad (3)$$

where $\Delta\boldsymbol{\varepsilon}$ is the additional strain due to inclusions. This additional strain can be expressed in terms of displacement and tractions on the inclusion boundaries Γ_k :

$$\Delta\boldsymbol{\varepsilon} = - \sum_k \frac{1}{V} \left(\frac{1}{2} \int_{\Gamma_k} (\mathbf{u}\mathbf{n} + \mathbf{n}\mathbf{u}) d\Gamma + \mathbf{S}_M : \int_{\Gamma_k} \mathbf{t}\mathbf{x} d\Gamma \right) \quad (4)$$

When the inclusions are cavities, the boundary tractions are zeroes and

$$\Delta \varepsilon = - \sum_k \frac{1}{2V} \int_{\Gamma_k} (\mathbf{un} + \mathbf{nu}) d\Gamma \quad (5)$$

This definition of $\Delta \varepsilon$ was used by Kachanov et al. (1994) to analyze materials with holes of various shapes.

In linear elasticity, the additional strain in the RVE as defined by Eq. (3) must be proportional to the applied stress σ^0 :

$$\Delta \varepsilon = \mathbf{H}^{\text{RVE}} : \sigma^0 \quad (6)$$

where the forth-rank proportionality tensor \mathbf{H}^{RVE} is called the *inclusion compliance contribution tensor*. Since both $\Delta \varepsilon$ and σ^0 tensors are symmetric and deformation is elastic, tensor \mathbf{H}^{RVE} has the same symmetry as the elastic compliance tensor:

$$\mathbf{H}_{ijkl}^{\text{RVE}} = \mathbf{H}_{jilk}^{\text{RVE}} = \mathbf{H}_{klij}^{\text{RVE}} \quad (7)$$

The effective compliance is expressed in terms of the \mathbf{H} -tensor as

$$\mathbf{S} = \mathbf{S}_M + \mathbf{H}^{\text{RVE}} \quad (8)$$

Tensor \mathbf{H} was first introduced for 2D and 3D holes by Kachanov et al. (1994). The expressions for \mathbf{H}^{RVE} in the case of solids with non-interacting ellipsoidal inclusions were provided in Sevostianov and Kachanov, 1999, 2002. The goal of current publication is to obtain the explicit formulae for *interacting* ellipsoidal and non-ellipsoidal inclusions using various approximate micromechanical schemes.

Micromechanical models of composite materials are often formulated in terms of the strain and stress concentration factors \mathbf{A}_I and \mathbf{B}_I (Hill, 1963; Walpole, 1966; Wu, 1966 and later publications). These forth-rank tensors are defined by

$$\varepsilon_I = \mathbf{A}_I : \varepsilon, \quad \sigma_I = \mathbf{B}_I : \sigma \quad (9)$$

where ε_I and σ_I are the average strain and stress in the inclusion phase. From the analysis of the average strain in the RVE, it follows that the inclusion compliance contribution tensor satisfies

$$\mathbf{H}^{\text{RVE}} : \sigma = f_I (\mathbf{S}_I - \mathbf{S}_M) : \sigma_I \quad (10)$$

and is related to the stress concentration factor \mathbf{B}_I :

$$\mathbf{H}^{\text{RVE}} = f_I (\mathbf{S}_I - \mathbf{S}_M) : \mathbf{B}_I \quad (11)$$

where f_I is the volume fraction of inclusions (this result is consistent with formula (12.10) of Hill, 1963). Note that tensors \mathbf{A}_I and \mathbf{B}_I are defined for *elastic* inclusions only—they are not easily generalized to the cases of cavities or perfectly rigid inclusions. Moreover, in the latter cases, the expressions for the effective properties in terms of these tensors become indeterminate so that special limiting procedures are needed. However, if tensor \mathbf{H} is chosen to quantify contribution of heterogeneities to the overall elastic properties, both cavities and perfectly rigid inclusions can be modeled in a straightforward way. Tensor \mathbf{H} is also a convenient tool to analyze solids with the fluid-filled cavities, see Kachanov et al. (1995) and Shafiro and Kachanov (1997).

Direct calculation of \mathbf{H}^{RVE} requires solution of the appropriate boundary value problem for RVE. Analytical solutions of such problems are known for very few microgeometries (for instance, laminated structures or coated ellipsoid assemblages, see Milton, 2002). More universal approaches to calculation of the effective elastic properties include advanced numerical simulations (for example, Gusev, 1997; Roberts and Garboczi, 1999), and development of the approximate micromechanical schemes. We focus on the latter approach. To model composites with ellipsoidal or irregularly shaped inclusions we propose to calculate (analytically or numerically) the inclusion compliance contribution tensor of a single inclusion in the

infinite medium, and then use it in one of the well-established micromechanical schemes. Definition of \mathbf{H} -tensor for a single inclusion and predictions of effective elastic properties in terms of this tensor are provided below.

2. Single inclusion problem

To evaluate the contribution of an inclusion into the overall response of a composite, the single inclusion compliance contribution tensor is introduced. We consider an inclusion of volume V_I placed in the infinite elastic space (matrix) with remotely applied stress σ^∞ , and choose a certain reference volume \tilde{V} containing the inclusion (Fig. 2). The resulting strain and stress fields are disturbed by the presence of the inclusion. The average strain in the reference volume can be represented as

$$\varepsilon = \mathbf{S}_M : \sigma + \mathbf{H} : \sigma^\infty \quad (12)$$

where σ is the average stress in \tilde{V} , and \mathbf{H} is the inclusion compliance contribution tensor (note that this tensor is independent of the shape of the reference volume). Analysis of the average strains and stresses in each phase shows that \mathbf{H} -tensor must satisfy

$$\mathbf{H} : \sigma^\infty = \frac{V_I}{\tilde{V}} (\mathbf{S}_I - \mathbf{S}_M) : \sigma_I \quad (13)$$

Thus, \mathbf{H} is related to the stress concentration factor of a single inclusion \mathbf{B}_I by relationship $\mathbf{H} = \frac{V_I}{\tilde{V}} (\mathbf{S}_I - \mathbf{S}_M) : \mathbf{B}_I$ analogous to formula (11).

Note that definition (12) of tensor \mathbf{H} is slightly different from formula (2.1) of Sevostianov and Kachanov (2002). Their definition neglects the difference between remotely applied stress σ^∞ and average stress σ , and is inconsistent with their result (2.6). This inconsistency is removed if definition (12) of tensor \mathbf{H} is used.

Practically all developed micromechanical models are based on the solution for the *ellipsoidal* inclusion provided by Eshelby (1957). According to this solution, the strain and stress fields in the ellipsoid subjected to a remotely applied uniform strain or stress are constant, and the concentration factors are given by (see, for example, Benveniste, 1987)

$$\begin{aligned} \mathbf{A}_I &= [\mathbf{I} - \mathbf{s} : (\mathbf{S}_M - \mathbf{S}_I) : \mathbf{S}_I^{-1}]^{-1} \\ \mathbf{B}_I &= [\mathbf{I} + \mathbf{Q} : (\mathbf{S}_I - \mathbf{S}_M)]^{-1} \end{aligned} \quad (14)$$

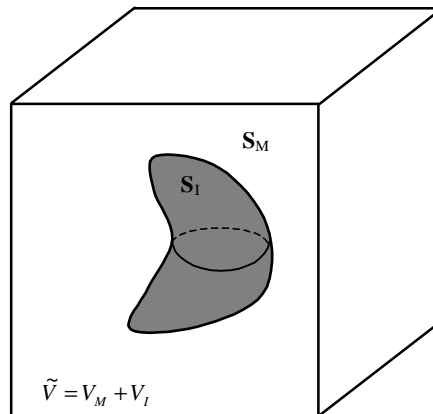


Fig. 2. Reference volume with an inclusion.

where $\mathbf{Q} = \mathbf{S}_M^{-1} : (\mathbf{I} - \mathbf{s})$, tensor \mathbf{s} is the forth-rank Eshelby tensor, and \mathbf{I} is the forth-rank unit tensor ($2\mathbf{I}_{ijkl} = \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}$). The components of \mathbf{s} are expressed in terms of elliptical integrals; in the special case of spheroidal inclusions, representation in elementary functions is available. The inclusion compliance contribution tensor is related to the Eshelby tensor (Sevostianov and Kachanov, 2002):

$$\mathbf{H} = \frac{V_I}{\tilde{V}} [(\mathbf{S}_I - \mathbf{S}_M)^{-1} + \mathbf{Q}]^{-1} \quad (15)$$

For *non-ellipsoidal inclusions*, the \mathbf{H} -tensor can be evaluated by either using analytical solutions when available, or numerical calculations for a single inclusion in the relatively large volume. Most of the analytical solutions in two-dimensional elasticity are based on the complex variable approach (Muskhelishvili, 1963; Savin, 1961). The examples of how these solutions can be used to derive the \mathbf{H} -tensors for holes of various shapes can be found in Tsukrov and Kachanov (1993), Kachanov et al. (1994), and Tsukrov and Novak (2002). In the three-dimensional elasticity, to the authors' knowledge, the "menu" of available solutions is very limited. Besides ellipsoidal inclusions (Eshelby's problem), some regular shapes have been analyzed by Wu and Du (1995), Rodin (1996), Markenscoff (1998), and Nozaki and Taya (2001).

3. Micromechanical modeling schemes

3.1. Non-interaction approximation

This approximation is reasonably accurate at low inclusion volume fractions ("dilute limit"). If interaction between inclusions in the composite is neglected, each inclusion can be assumed to be loaded by the same remotely applied stress σ^0 . Then, contributions of each inclusion into the additional strain, as defined by Eq. (4), can be treated separately, and the total inclusion compliance contribution tensor is a sum of individual \mathbf{H} -tensors:

$$\mathbf{H}^{\text{NI}} = \sum \mathbf{H}, \quad \mathbf{S} = \mathbf{S}_M + \mathbf{H}^{\text{NI}} \quad (16)$$

where the non-interaction approximation of \mathbf{H}^{RVE} is denoted as \mathbf{H}^{NI} , and the representative volume V is chosen as a reference volume \tilde{V} for all inclusions. Formula (16) is used in Tsukrov and Kachanov (1993), Kachanov et al. (1994), Shafiro and Kachanov (1997), and Sevostianov and Kachanov (1999) to find the non-interaction approximation of the mechanical properties of solids with 2D and 3D dry and fluid-filled cavities and 3D ellipsoidal inclusions. These non-interaction results can be utilized in the approximate micromechanical schemes developed for *interacting* inclusions. The corresponding procedures are provided below.

Note that all of the considered schemes have been extensively used and applied to various problems of micromechanical modeling. In our choice of references, we have limited ourselves to the original presentations of the methods. A comprehensive review of further advances in the development of first order micromechanical schemes can be found in Nemat-Nasser and Hori (1993) and Markov (2000). Also, the predictions of various schemes can differ significantly, especially in the case of the sharp contrast between the mechanical properties of constituents. It is not our objective to determine which method is more appropriate for any given microstructure, but rather to develop a set of computational formulae implementing the schemes.

3.2. Mori–Tanaka scheme

Mori–Tanaka approach (Mori and Tanaka, 1973) as interpreted by Benveniste (1987) is based on the assumption that each inclusion is subjected to the remote stress that is equal to average stress σ_M in the

matrix phase of the RVE. Then, the contribution of the inclusion can be evaluated by substituting $\sigma^\infty = \sigma_M$ in Eq. (12), and the macroscopic strain in the RVE is

$$\varepsilon = S_M : \sigma^0 + \sum_k H^{(k)} : \sigma_M \quad (17)$$

Thus, the additional strain can be represented as $\Delta\varepsilon = H^{NI} : \sigma_M$. This yields the following equation for Mori–Tanaka approximation of the inclusion compliance contribution tensor H^{MT} :

$$H^{MT} : \sigma^0 = H^{NI} : \sigma_M \quad (18)$$

Using analysis of the average strain to express σ_M in terms of σ^0 , the formulae for H^{MT} and the effective compliance are obtained

$$\begin{aligned} H^{MT} &= H^{NI} : [f_M(S_I - S_M) + H^{NI}]^{-1} : (S_I - S_M) \\ S &= S_M + H^{MT} \end{aligned} \quad (19)$$

3.3. Self-consistent scheme

In this approximation (Kröner, 1958; Hill, 1965; Budiansky, 1965), each inclusion is assumed to be placed in the equivalent matrix having compliance of the overall composite S , and subjected to the remotely applied stress σ^0 . Formula (10) in this case is re-written as

$$H^{NI}(S, S_I) : \sigma^0 = f_I(S_I - S) : \sigma_I \quad (20)$$

where $H^{NI}(S, S_I)$ is the non-interaction approximation of H -tensor for the inclusions of compliance S_I placed in the matrix of compliance S . The inclusion compliance contribution tensor H^{SC} is found by substituting the expression for σ_I from Eq. (20) into

$$H^{SC} : \sigma^0 = f_I(S_I - S_M) : \sigma_I \quad (21)$$

Thus, self-consistent predictions of the H -tensor and the effective compliance are

$$H^{SC} = (S_I - S_M) : (S_I - S)^{-1} : H^{NI}(S, S_I) \quad (22)$$

$$S = S_M + (S_I - S_M) : (S_I - S)^{-1} : H^{NI}(S, S_I) \quad (23)$$

Note. If analytical formula for the inclusion compliance contribution tensor of a single inclusion is not available and the numerical approach to obtain H is used, the nonlinear equation (23) can be solved for S iteratively. In this case, repetitive calculations of H -tensor for the consecutive approximations of the matrix compliance are required. The iteration procedure would involve calculation of $H^{NI}(S_M, S_I)$, substitution of it into formula (23) to find S , calculation of $H^{NI}(S, S_I)$, substitution of it into Eq. (23) to find the new value of S and so on.

3.4. Differential scheme

Differential scheme (Salganik, 1973; McLaughlin, 1977) assumes that inclusions are incrementally added to the material until the final volume fraction f_I is reached. On each increment, a set of non-interacting inclusions is added to the homogeneous material with properties that are determined by the previously embedded inclusions. Since part of the volume where the “new” inclusions are placed is already occupied by the “old” ones, the volume fraction of inclusions f is increased by Δf when $\Delta f/(1-f)$ of “new” inclusions are added. This process is described by the following set of ordinary differential equations

$$\frac{d\mathbf{S}(t)}{dt} = \frac{1}{f_I(1-t)} \mathbf{H}^{\text{NI}}(\mathbf{S}(t), \mathbf{S}_I) \quad (24)$$

where $\mathbf{S}(t)$ is the compliance of the composite having inclusion volume fraction t , $\mathbf{H}^{\text{NI}}(\mathbf{S}(t), \mathbf{S}_I)$ is the compliance contribution tensor of the inclusions \mathbf{S}_I placed into the matrix \mathbf{S} . The initial condition (matrix material with no inclusion) is $\mathbf{S}(0) = \mathbf{S}_M$.

The differential equation and initial condition for the compliance contribution tensor are

$$\frac{d\mathbf{H}^{\text{DIFF}}(t)}{dt} = \frac{1}{f_I(1-t)} \mathbf{H}^{\text{NI}}(\mathbf{S}_M + \mathbf{H}^{\text{DIFF}}, \mathbf{S}_I), \quad \mathbf{H}^{\text{DIFF}}(0) = 0 \quad (25)$$

The authors are unaware of any inclusion shapes that would allow analytical solution of differential equations (24) or (25), unless special relationships between the elastic moduli of matrix and reinforcement are satisfied (same bulk modulus, same shear modulus, rigid inclusions or cavities). So, for most composites, the differential equations (24) or (25) must be integrated numerically. If analytical expression for \mathbf{H}^{NI} is not available, the numerical procedure requires consequent calculations of \mathbf{H} -tensor for different matrix materials.

3.5. Dvorak–Srinivas comparison medium schemes

As shown in Dvorak and Srinivas (1999), the effective elastic properties can be derived using the assumption that when the boundary of RVE is subjected to the displacement field $\mathbf{u} = \boldsymbol{\varepsilon}^0 \cdot \mathbf{x}$, the average strain in each inclusion is the same as in a single inclusion placed in the infinite *comparison medium* with remotely applied uniform strain $\boldsymbol{\varepsilon}^0$. Different choices of the comparison medium yield various predictions of the effective elastic moduli, for example, the self-consistent scheme is obtained when the comparison medium is assumed to have properties of the overall composite. The formulae for the inclusion compliance contribution tensor and effective compliance that implement the Dvorak–Srinivas approach have the same structure as Eqs. (22) and (23)

$$\mathbf{H}^{\text{DS}} = (\mathbf{S}_I - \mathbf{S}_M) : (\mathbf{S}_I - \mathbf{S}^*)^{-1} : \mathbf{H}^{\text{NI}}(\mathbf{S}^*, \mathbf{S}_I) \quad (26)$$

$$\mathbf{S}^{\text{DS}} = \mathbf{S}_M + \mathbf{H}^{\text{DS}} \quad (27)$$

where \mathbf{S}^* is the compliance tensor of the comparison medium. This tensor must satisfy certain conditions as described in Dvorak and Srinivas (1999). In the numerical examples provided in Section 4, we use the comparison medium having the average stiffness of the composite:

$$\mathbf{S}^* = [f_I \mathbf{S}_I^{-1} + (1 - f_I) \mathbf{S}_M^{-1}]^{-1} \quad (28)$$

4. Three-dimensional examples. Composites with spheroidal inclusions

4.1. Spherical inclusions

Traditionally, micromechanical models are tested by comparing their predictions for effective moduli of materials with spherical elastic inclusions. We have chosen to compare the \mathbf{H} -tensor based results with the analytical and numerical predictions reported in the following three publications. The book of Aboudi (1991) provides clear presentation of several micromechanical models with easy-to-use formulae for spherical inclusions. A unified approach to the self-consistent scheme, Mori–Tanaka model and Hashin–Shtrikman bounds is given by Dvorak and Srinivas (1999); they also propose a way to obtain new estimates by

selecting the appropriate comparison media. Böhm et al. (2004) have performed extensive finite element simulations for periodic unit cells with spherical, as well as elongated spheroidal and cylindrical inclusions. In this section, we determine the \mathbf{H} -tensor for spherical elastic inclusions using several micromechanical schemes, and compare their predictions for the effective elastic properties of SiC/Al composite. It is assumed that the matrix and inclusions are isotropic, so that their mechanical properties are described by either Young's moduli E_M , E_I and Poisson's ratios ν_M , ν_I , or by shear and bulk moduli μ_M , μ_I , k_M , k_I . Components of the compliance tensor are expressed as

$$S_{ijkl} = \frac{1-2\nu}{3E} \delta_{ij} \delta_{kl} + \frac{1+\nu}{2E} \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \frac{2}{3} \delta_{ij} \delta_{kl} \right) \quad (29)$$

and the moduli are inter-related as

$$k = \frac{E}{3(1-2\nu)}, \quad \mu = \frac{E}{2(1+\nu)}$$

Substitution of the corresponding Eshelby tensor (see, for example, Mura, 1987) into Eqs. (15) and (16) yields the following formula for the non-interaction approximation of the inclusion compliance contribution tensor

$$\mathbf{H}_{ijkl}^{\text{NI}} = f_I \left[h_1 \delta_{ij} \delta_{kl} + h_2 \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \frac{2}{3} \delta_{ij} \delta_{kl} \right) \right] \quad (30)$$

where

$$h_1 = \frac{(3k_M + 4\mu_M)(k_M - k_I)}{9k_M^2(3k_I + 4\mu_M)}, \quad h_2 = \frac{5(3k_M + 4\mu_M)(\mu_M - \mu_I)}{4\mu_M[3k_M(2\mu_I + 3\mu_M) + 4\mu_M(3\mu_I + 2\mu_M)]}$$

Expression (30) can be used to predict the effective properties using various micromechanical schemes as described in Section 3. For example, the Mori–Tanaka prediction is derived when Eq. (30) is substituted in Eq. (19). After some algebra, the expression for Mori–Tanaka approximation of \mathbf{H} -tensor is represented as

$$\mathbf{H}_{ijkl}^{\text{MT}} = f_I \left[h_3 \delta_{ij} \delta_{kl} + h_4 \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \frac{2}{3} \delta_{ij} \delta_{kl} \right) \right] \quad (31)$$

where

$$h_3 = \frac{(3k_M + 4\mu_M)(k_M - k_I)}{9k_M[4f_I\mu_M(k_I - k_M) + k_M(3k_I + 3\mu_M)]}$$

$$h_4 = \frac{5(3k_M + 4\mu_M)(\mu_M - \mu_I)}{4\mu_M[3k_M(2\mu_I + 3\mu^*) + 4\mu_M(3\mu_I + 2\mu^*)]}$$

and $\mu^* = (1-f_I)\mu_M + f_I\mu_I$.

This corresponds to the following predictions of the effective bulk and shear moduli

$$k^{\text{MT}} = \frac{k_M(3k_I + 4\mu_M) + 4f_I\mu_M(k_I - k_M)}{(3k_I + 4\mu_M) - 3f_I(k_I - k_M)} \quad (32)$$

$$\mu^{\text{MT}} = \frac{\mu_M[3k_M(2\mu_I + 3\mu_M) + 4\mu_M(3\mu_I + 2\mu_M)] + f_I\mu_M(\mu_I - \mu_M)(9k_M + 8\mu_M)}{[3k_M(2\mu_I + 3\mu_M) + 4\mu_M(3\mu_I + 2\mu_M)] - 6f_I(\mu_I - \mu_M)(k_M + 2\mu_M)} \quad (33)$$

Formulae (32) and (33) are equivalent to the results presented in Aboudi (1991) where they are given in a more compact form.

Similarly, application of the Dvorak–Srinivas micromechanical scheme (26) with the average stiffness comparison medium (28) produces inclusion compliance contribution tensor

$$\mathbf{H}_{ijkl}^{\text{DS}} = f_1 \left[h_5 \delta_{ij} \delta_{kl} + h_6 \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \frac{2}{3} \delta_{ij} \delta_{kl} \right) \right] \quad (34)$$

where $h_5 = \frac{(3k^* + 4\mu^*)(k_M - k_I)}{3k_M k^* (3k_I + 4\mu^*)}$, $h_6 = \frac{5(3k^* + 4\mu^*)(\mu_M - \mu_I)}{2\mu_M [3k^* (2\mu_I + 3\mu^*) + 4\mu^* (3\mu_I + 2\mu^*)]}$, and $k^* = (1 - f_1)k_M + f_1 k_I$, $\mu^* = (1 - f_1)\mu_M + f_1 \mu_I$. The effective elastic moduli are then found from Eq. (27).

The self-consistent and differential schemes do not allow immediate closed form expressions for \mathbf{H} -tensor, but numerical solutions are readily obtainable using Eqs. (22)–(25). Moreover, as shown by Hill (1965), the self-consistent formulation in the case of spherical inclusions can be reduced to a nonlinear algebraic equation for one variable.

We illustrate the results of this section by considering a SiC/Al composite with aluminum matrix ($E_M = 70$ GPa, $\nu_M = 0.3$) reinforced by silicon carbide spherical particles ($E_I = 450$ GPa, $\nu_I = 0.17$). Fig. 3 provides dependence of the composite Young's, bulk and shear moduli on the volume fraction f_1 of the inclusions. For comparison purposes, the range of change of f_1 is taken from 0 to 1, even though the first order micromechanical models considered in this paper are not appropriate for high inclusion densities. Also, there is an upper limit for possible values of f_1 in the case of the inclusions of finite size. (For spherical inclusions of the *same* size, for example, the maximum possible value is $f_1 \approx 0.74048$, see Hales, 1997).

As expected, micromechanical predictions for composites with spherical inclusions obtained using the corresponding \mathbf{H} -tensors are identical to results reported in Aboudi (1991), Dvorak and Srinivas (1999), and Böhm et al. (2004).

Note that the non-interaction predictions of the effective elastic moduli hyperbolically depend on the inclusion volume fraction. In the case of spherical inclusions that are stiffer than matrix, the “non-interaction” shear modulus tends to infinity when

$$f_1 \rightarrow \frac{3k_M(2\mu_I + 3\mu_M) + 4\mu_M(3\mu_I + 2\mu_M)}{5(3k_M + 4\mu_M)(\mu_M - \mu_I)} \quad (35)$$

For the bulk modulus, the corresponding critical value of the inclusion volume fraction is

$$f_1 = \frac{k_M(3k_I + 4\mu_M)}{(k_I - k_M)(3k_M + 4\mu_M)} \quad (36)$$

4.2. Needle-shaped elastic inclusions

We provide here the micromechanical predictions for composites with randomly oriented needle-shaped inclusions—elongated spheroids having one axis that is much greater than the other two. Eshelby tensor for such shapes is given, for example, in Walpole (1969). Randomly oriented reinforcement produces composites with overall isotropic elastic properties. The non-interaction approximation of the inclusion compliance contribution tensor in this case is

$$\mathbf{H}_{ijkl}^{\text{NI}} = f_1 \left[h_7 \delta_{ij} \delta_{kl} + h_8 \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \frac{2}{3} \delta_{ij} \delta_{kl} \right) \right] \quad (37)$$

where

$$h_7 = \frac{(k_M - k_I)(\mu_M(4k_I - k_M) + k_M(3k_I + \mu_I))}{9k_I k_M^2 (3k_I + \mu_I + 3\mu_M)}$$

$$h_8 = \frac{\mu_M - \mu_I}{5\mu_M} \left[\frac{2}{\mu_M + \mu_I} + \frac{6k_M + 8\mu_M}{3k_M \mu_I + 7\mu_I \mu_M + 3k_M \mu_M + \mu_M^2} - \frac{4\mu_I + k_I}{4\mu_I^2} + \frac{(3k_I + 4\mu_I)(k_I + \mu_I)}{4\mu_I^2 (3k_I + \mu_I + 3\mu_M)} \right]$$

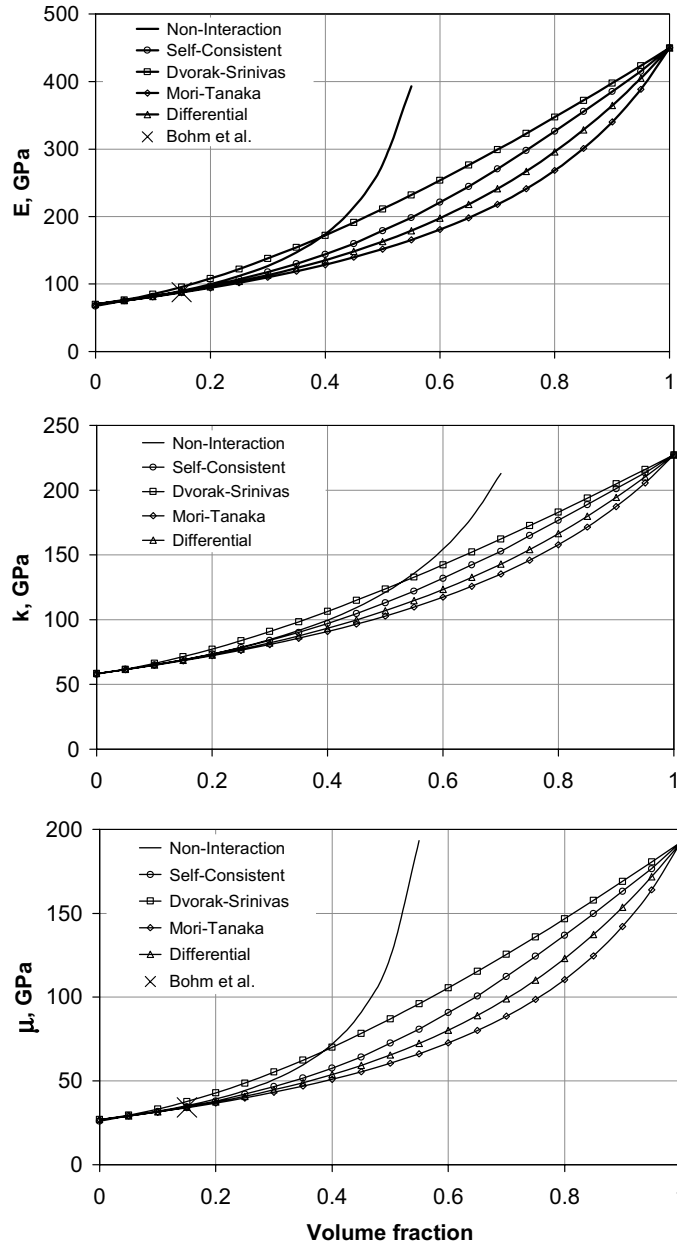


Fig. 3. Effective elastic moduli of SiC/Al composite. Spherical particles.

Predictions of other micromechanical schemes can be obtained from Eq. (37) by substituting this representation of \mathbf{H}^{NI} into Eqs. (19), (23)–(27). The resulting expression for Mori–Tanaka scheme is

$$\mathbf{H}_{ijkl}^{\text{MT}} = f_1 \left[h_9 \delta_{ij} \delta_{kl} + h_{10} \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \frac{2}{3} \delta_{ij} \delta_{kl} \right) \right] \quad (38)$$

where

$$h_9 = \frac{(k_M - k_I)(\mu_M(4k_I - k_M) + k_M(3k_I + \mu_I))}{9k_I k_M^2(3k_I + \mu_I + 3\mu_M) - 36f_I k_I k_M \mu_M(k_M - k_I)}, \quad h_{10} = h_8 \left(1 - f_I + f_I h_8 \frac{4\mu_M \mu_I}{\mu_M - \mu_I} \right)^{-1}$$

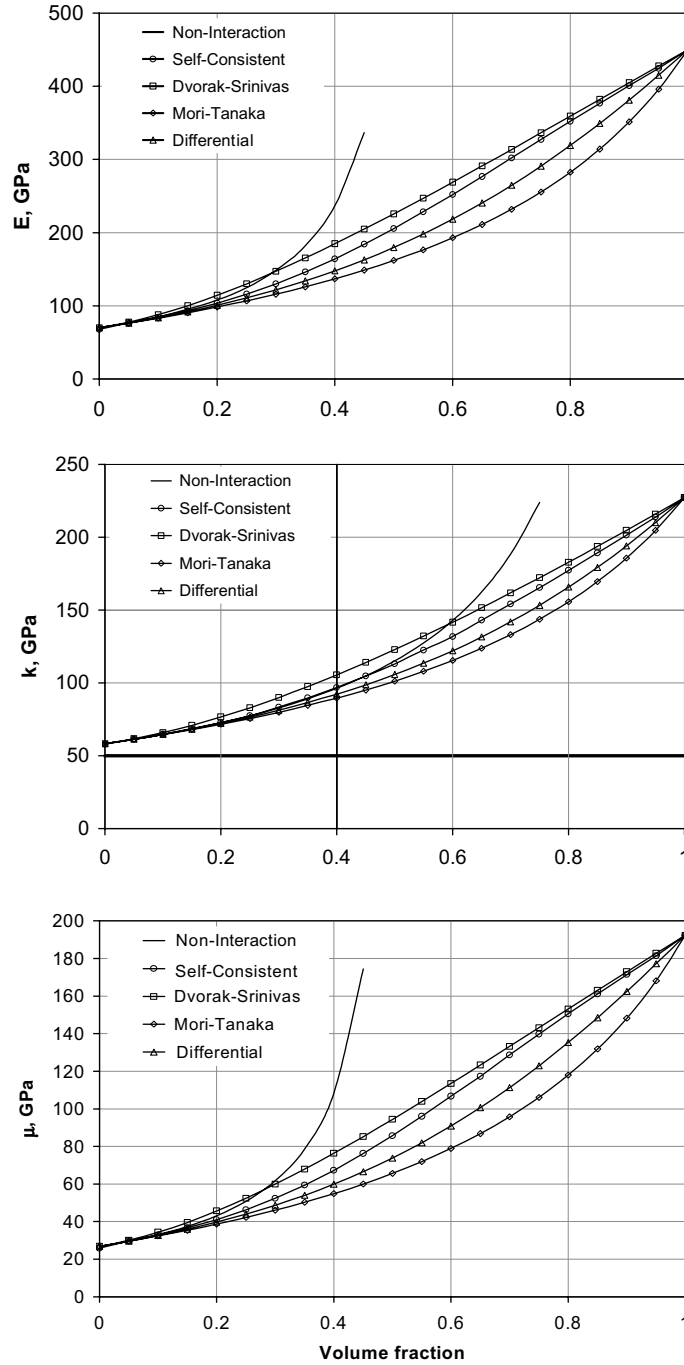


Fig. 4. Effective elastic moduli of SiC/Al composite. Randomly oriented needle-like inclusions.

The inclusion compliance contribution tensor for Dvorak–Srinivas micromechanical scheme with the average stiffness comparison medium is

$$\mathbf{H}_{ijkl}^{\text{DS}} = f_I \left[h_{11} \delta_{ij} \delta_{kl} + h_{12} \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \frac{2}{3} \delta_{ij} \delta_{kl} \right) \right] \quad (39)$$

where

$$h_{11} = \frac{(k_M - k_I)(3k^* + 3\mu^* + \mu_I)}{3k^* k_M (3k_I + 3k^* + \mu_I)}$$

$$h_{12} = \frac{\mu_M - \mu_I}{5\mu_M} \left[\frac{2}{\mu^* + \mu_I} + \frac{6k^* + 8\mu^*}{3k^* \mu_I + 7\mu_I \mu^* + 3k^* \mu^* + \mu^{*2}} + \frac{\mu^* + \mu_I}{4\mu_I \mu^*} + \frac{3k_I(\mu^* - \mu_I)^2 + \mu_I(\mu^{*2} - \mu_I^2)}{4\mu_I^2 \mu^* (3k_I + \mu_I + 3\mu^*)} \right]$$

and $k^* = (1-f_I)k_M + f_I k_I$, $\mu^* = (1-f_I)\mu_M + f_I \mu_I$. For self-consistent and differential schemes, the effective elastic properties are easily calculated numerically using representation (37) and formulae (22)–(25).

Fig. 4 depicts elastic moduli of SiC/Al composite with constituents having elastic properties described in Section 4.1. Needle-shaped inclusions are randomly oriented and perfectly bonded in the matrix material. As in the case of spherical inclusions, the \mathbf{H} -tensor based results for randomly oriented needle-like inclusions are in complete correspondence with known predictions (Wu, 1966; Walpole, 1969; Markov, 2000). Also, Mori–Tanaka estimates of the effective moduli are the lowest among all considered schemes. This behavior, pointed out by Dvorak and Srinivas (1999) for the case of spherical inclusions, holds for composites having inclusions that are stiffer than matrix.

5. Two-dimensional examples. Composites with irregularly shaped inhomogeneities

5.1. Rigid inclusions of triangular shape

Let us consider a 2D solid with absolutely rigid inclusions of the triangular type shape shown in Fig. 5. The matrix material is isotropic with Young's modulus E_M and Poisson's ratio ν_M . All formulae in this section are given for the case of plane stress. For plane strain, the expression $E/(1-\nu^2)$ should be substituted instead of Young's modulus E , and $\nu/(1-\nu)$ instead of Poisson's ratio ν . The representation of shear modulus μ in terms of E and ν remains the same for both cases. In 2D problems, the components of compliance tensor are expressed in terms of the engineering constants as

$$S_{ijkl} = \frac{1-\nu}{2E} \delta_{ij} \delta_{kl} + \frac{1+\nu}{2E} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \delta_{ij} \delta_{kl}) \quad (40)$$

First, we must obtain the inclusion compliance contribution tensor \mathbf{H} from the solution of a single inclusion problem. For the special case of an absolutely rigid inclusion, Eq. (13) reduces to

$$\mathbf{H} : \boldsymbol{\sigma}^\infty = -\mathbf{S}_M : (f_I \boldsymbol{\sigma}_I) \quad (41)$$

The triangular shape is isotropic (see Appendix A) so it is enough to consider a uniaxial tension of the infinite plate with the inclusion to find all components of \mathbf{H} -tensor. If tension P is applied in the direction of x_1 -axis, the solution can be found using results of Savin (1961) as

$$\boldsymbol{\sigma}_I = P(h_{13} \mathbf{e}_1 \mathbf{e}_1 + h_{14} \mathbf{e}_2 \mathbf{e}_2) \quad (42)$$

where $h_{13} = \frac{43+7\nu_M}{7(1+\nu_M)(3-\nu_M)}$, $h_{14} = \frac{7-29\nu_M}{7(1+\nu_M)(3-\nu_M)}$.

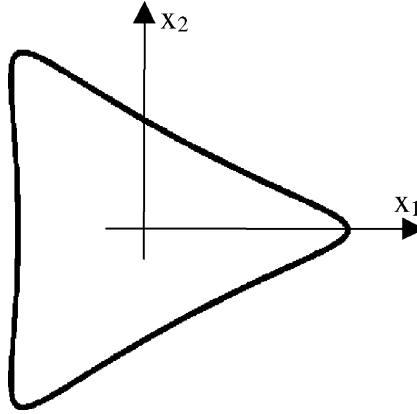


Fig. 5. Triangular-type rigid inclusion.

Then, the non-zero components of \mathbf{H} -tensor are obtained from Eq. (41) as

$$\begin{aligned} H_{1111} = H_{2222} &= -\frac{V_I}{\tilde{V}} \frac{h_{13} - v_M h_{14}}{E_M} \\ H_{1122} = H_{2211} &= -\frac{V_I}{\tilde{V}} \frac{h_{14} - v_M h_{13}}{E_M} \\ H_{1212} = H_{2121} = H_{1221} = H_{2121} &= -\frac{V_I}{\tilde{V}} \frac{(1 + v_M)(h_{13} - h_{14})}{2E_M} \end{aligned} \quad (43)$$

and components of \mathbf{H}^{NI} are found by direct summation of the inclusion contributions (43):

$$\mathbf{H}_{ijkl}^{\text{NI}} = f_I [h_{15} \delta_{ij} \delta_{kl} + h_{16} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \delta_{ij} \delta_{kl})] \quad (44)$$

where

$$h_{15} = -\frac{(1 - v_M)(h_{13} + h_{14})}{2E_M} \quad \text{and} \quad h_{16} = -\frac{(1 + v_M)(h_{13} - h_{14})}{2E_M}$$

The effective compliances of the solid with non-interacting rigid triangular inclusions are calculated using Eq. (16). The following expressions for the effective Young's modulus and Poisson's ratio are obtained:

$$\frac{E}{E_M} = [1 - (h_{13} - v_M h_{14})f_I]^{-1}, \quad v = \frac{E}{E_M} [v_M + (h_{14} - v_M h_{13})f_I] \quad (45)$$

For the interacting inclusions, Mori–Tanaka method (19) produces the following approximations of \mathbf{H} -tensor and effective elastic moduli:

$$\mathbf{H}_{ijkl}^{\text{MT}} = f_I [h_{17} \delta_{ij} \delta_{kl} + h_{18} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \delta_{ij} \delta_{kl})], \quad (46)$$

$$\frac{E}{E_M} = \frac{1}{1 + E_M(h_{17} + h_{18})f_I}, \quad v = \frac{v_M - E_M(h_{17} - h_{18})f_I}{1 + E_M(h_{17} + h_{18})f_I} \quad (47)$$

where

$$h_{17} = -\frac{(1 - v_M)(h_{13} + h_{14})}{2E_M[1 - f_I(1 - h_{13} - h_{14})]} \quad \text{and} \quad h_{18} = -\frac{(1 + v_M)(h_{13} - h_{14})}{2E_M[1 - f_I(1 - h_{13} - h_{14})]}$$

Predictions of self-consistent and differential schemes are obtained by substituting \mathbf{H}^{NI} into formulae (22)–(25). In the case of self-consistent scheme, the problem can be reduced to one nonlinear algebraic equation for the effective Poisson's ratio. Application of the differential scheme requires solution of two ordinary differential equations. These calculations have been performed numerically, and are illustrated in Fig. 6 for the case of aluminum matrix ($E_{\text{M}} = 70$ GPa, $\nu_{\text{M}} = 0.3$) with absolutely rigid inclusions of triangular-type shape shown in Fig. 5. The effective elastic properties are given in the range of inclusion concentration from 0 to

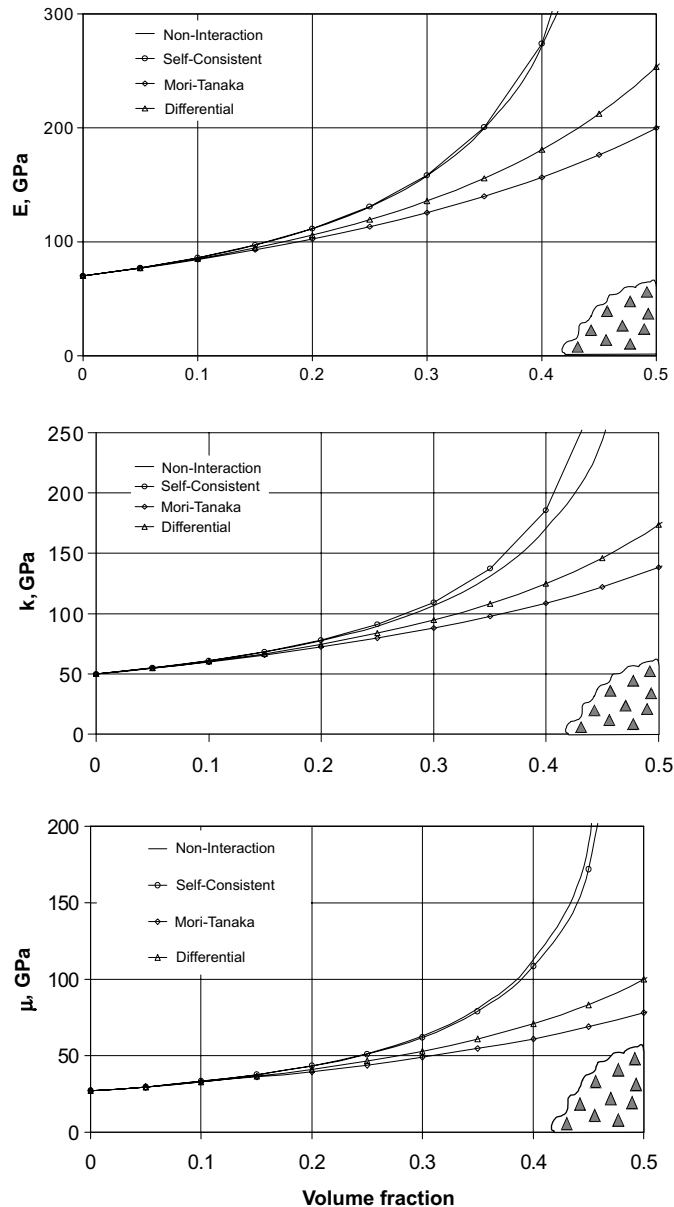


Fig. 6. Effective elastic moduli of the two-dimensional composite consisting of Al matrix ($E = 70$ GPa, $\nu = 0.3$) reinforced by rigid triangular inclusions.

0.5. As discussed in Jasiuk (1995), the self-consistent scheme predicts that percolation (elastic moduli go to infinity) for triangular type rigid inclusions occurs at $f_1 = 0.536$. Note that our results for the non-interaction and self-consistent schemes coincide with those of Jasiuk (1995).

5.2. Two-dimensional holes of irregular shape

Let us consider a two-dimensional solid with randomly oriented identical holes of irregular shape shown in Fig. 7. Holes of such shape were analyzed by Tsukrov and Novak (2002), and the hole compliance contribution tensor was found to be

$$\mathbf{H} = \frac{S}{AE_M} [3.74\mathbf{e}_1\mathbf{e}_1\mathbf{e}_1 + 6.9\mathbf{e}_2\mathbf{e}_2\mathbf{e}_2 - 0.96(\mathbf{e}_1\mathbf{e}_1\mathbf{e}_2 + \mathbf{e}_2\mathbf{e}_2\mathbf{e}_1) + 1.54(\mathbf{e}_1\mathbf{e}_1\mathbf{e}_2 + \mathbf{e}_1\mathbf{e}_2\mathbf{e}_1 + \mathbf{e}_1\mathbf{e}_2\mathbf{e}_1 + \mathbf{e}_2\mathbf{e}_1\mathbf{e}_1) + 1.16(\mathbf{e}_1\mathbf{e}_2\mathbf{e}_2 + \mathbf{e}_2\mathbf{e}_1\mathbf{e}_2 + \mathbf{e}_2\mathbf{e}_2\mathbf{e}_1 + \mathbf{e}_2\mathbf{e}_2\mathbf{e}_1) + 3.72(\mathbf{e}_1\mathbf{e}_2\mathbf{e}_1 + \mathbf{e}_1\mathbf{e}_2\mathbf{e}_1 + \mathbf{e}_2\mathbf{e}_1\mathbf{e}_2 + \mathbf{e}_2\mathbf{e}_1\mathbf{e}_2)] \quad (48)$$

where S is the area of the hole and A is the reference area.

The non-interacting approximation of \mathbf{H} for a solid with randomly oriented holes of this type is

$$\mathbf{H}^{NI} = \frac{f_1}{E_M} [5.44\mathbf{e}_1\mathbf{e}_1\mathbf{e}_1 + 5.44\mathbf{e}_2\mathbf{e}_2\mathbf{e}_2 - 0.75(\mathbf{e}_1\mathbf{e}_1\mathbf{e}_2 + \mathbf{e}_2\mathbf{e}_2\mathbf{e}_1) + 3.45(\mathbf{e}_1\mathbf{e}_2\mathbf{e}_1 + \mathbf{e}_1\mathbf{e}_2\mathbf{e}_1 + \mathbf{e}_2\mathbf{e}_1\mathbf{e}_2 + \mathbf{e}_2\mathbf{e}_1\mathbf{e}_2)] \quad (49)$$

This tensor is isotropic, and the approximate scheme predictions (19), (23) and (24) for the effective compliance tensor of the porous material can be simplified to the following expressions. For the Mori–Tanaka model,

$$\mathbf{S}^{MT} = \mathbf{S}_M + \frac{1}{1 - f_1} \mathbf{H}^{NI} \quad (50)$$

For the self-consistent scheme,

$$\mathbf{S}^{SC} = \mathbf{S}_M + \frac{1}{1 - f_1 h} \mathbf{H}^{NI} \quad (51)$$

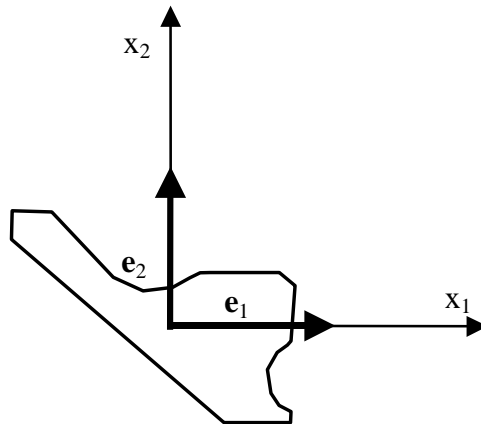


Fig. 7. Irregularly-shaped hole.

For the differential scheme,

$$\mathbf{S}^{\text{DIFF}} = \mathbf{S}_M + \frac{1}{f_1 h} \{ \exp[h \ln(1 - f_1)] - 1 \} \mathbf{H}^{\text{NI}} \quad (52)$$

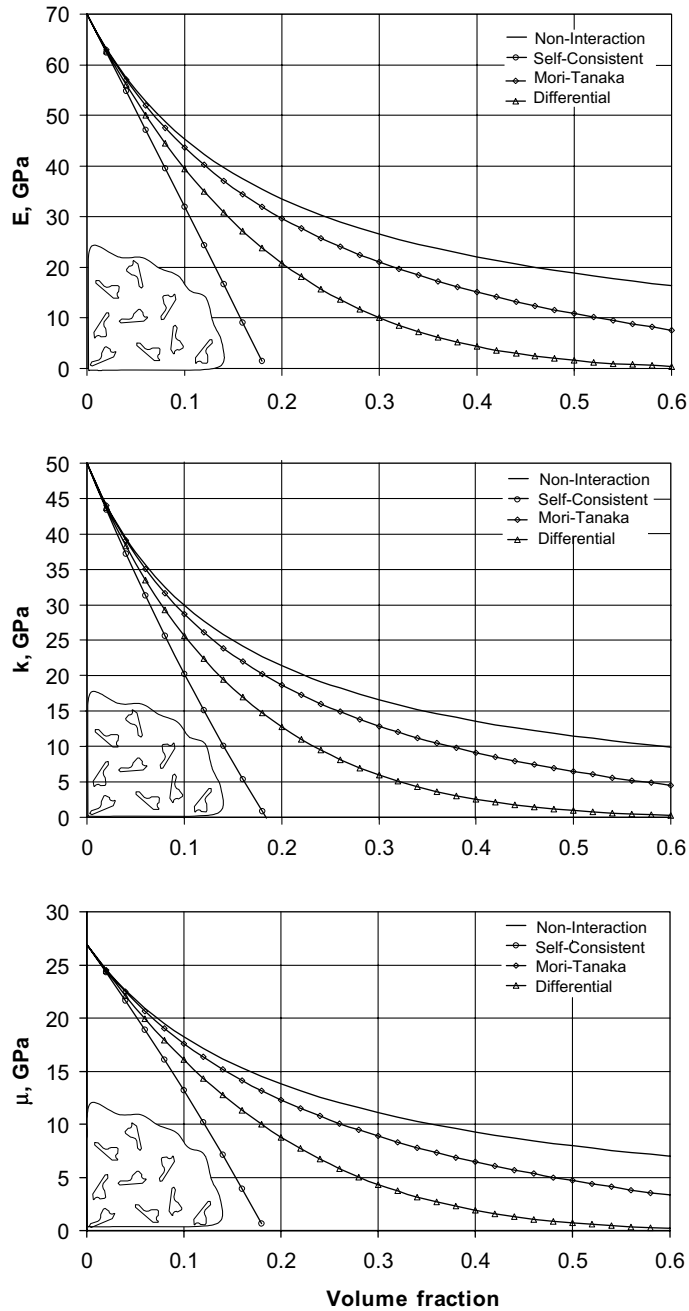


Fig. 8. Effective elastic moduli of Al plate ($E = 70$ GPa, $\nu = 0.3$) weakened by randomly oriented holes of the shape shown in Fig. 7.

In the equations above, the dimensionless parameter h depends on the geometry of holes only. It is related to the components of \mathbf{H}^{NI} as $h = E_{\text{M}} H_{1111}^{\text{NI}} / f_1$.

Fig. 8 shows how the predicted values of the effective elastic moduli of perforated aluminum plate change with porosity f_1 . It can be seen that even at $f_1 = 0.1$, the discrepancy in predictions is substantial. For example, the estimates of Young's modulus vary from $E = 43.6$ GPa (Mori–Tanaka) to 31.9 GPa (self-consistent). Thus, one has to be careful when making a decision on which micromechanical model to employ in the case of sharp contrast between the mechanical properties of constituents.

6. Conclusions

Effective elastic moduli of random two-phase particulate composites depend on mechanical properties of constituents, geometric shape and volume fraction of reinforcement, and interaction between reinforcement particles (inclusions). At small inclusion concentrations, the non-interaction approximation provides good accuracy. As volume fraction of reinforcement increases, more advanced micromechanical models are needed.

In this paper, we have considered several popular first-order approximate schemes that account for interaction between particles, namely, the self-consistent, Mori–Tanaka, differential, and Dvorak–Srinivas comparison medium estimates. All of these schemes are realizable on certain microgeometries. It was not our objective to determine when each of the above schemes must be used. Instead, we concentrated on derivation of the explicit set of computational formulae that combine the inclusion compliance contribution tensor with various micromechanical models to predict the effective moduli of the two-phase particulate composites.

The \mathbf{H} -tensor based formulae have been applied to the three-dimensional composites with spherical and needle-like elastic inclusions, and the two-dimensional solids with perfectly rigid inclusions and with holes. In all cases, the predictions of effective moduli are in complete correspondence with known results of other authors. The proposed procedure can be applied to composites with reinforcements of any shape for which the solution (analytical or numerical) of the single inclusion problem is available.

Appendix A. Elastically isotropic two-dimensional shapes

As has been noticed in the literature, the inclusions and holes of some regular polygonal shapes produce an isotropic contribution to the effective elastic properties (Kachanov et al., 1994; Jasiuk, 1995; Tsukrov and Novak, 2002). Let us show that any two-dimensional inclusion that can be mapped on itself by a rotation by angle θ different from multiples of $\frac{\pi}{2}$ is an “elastically isotropic” object, i.e. tensor \mathbf{H} that characterizes its contribution to the effective elastic properties is isotropic. (As everywhere in the paper, it is assumed that both the inclusion and the matrix are made of isotropic materials.)

It is well known that the rotation of coordinate system by angle φ results in the following transformation of components of the forth-rank tensor:

$$H'_{ijkl} = H_{oprs} Q_{io} Q_{jp} Q_{kr} Q_{ls} \quad (\text{A.1})$$

where Q_{ij} are the components of the second rank transformation tensor

$$\mathbf{Q} = \begin{pmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{pmatrix} \quad (\text{A.2})$$

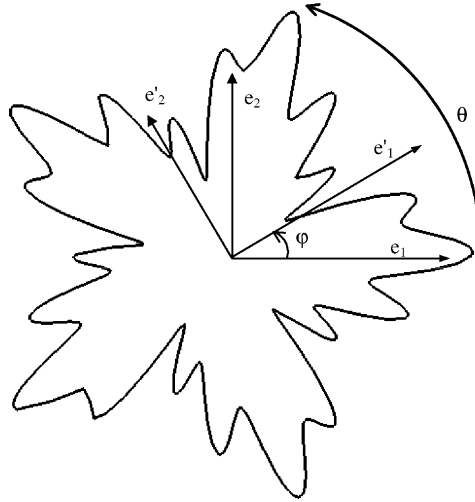


Fig. 9. Elastically isotropic inclusion.

that relates basic vectors of rotated and original coordinate systems $\mathbf{e}_i = \mathbf{Q} \cdot \mathbf{e}'_i$ ($i = 1, 2$), see Fig. 9.

Let us analyze the components of tensor \mathbf{H}' as functions of angle φ . Geometric symmetry requires these functions to be periodic with period θ . We will show that if $\theta \neq \frac{\pi}{2}, \pi, \frac{3\pi}{2}, \dots$, then H'_{ijkl} are constants, and thus tensor \mathbf{H} is isotropic. From representation (A.1) it follows that each component of \mathbf{H}' can be expressed as

$$H'_{ijkl} = A_1 \cos^4 \varphi + A_2 \cos^3 \varphi \sin \varphi + A_3 \cos^2 \varphi \sin^2 \varphi + A_4 \cos \varphi \sin^3 \varphi + A_5 \sin^4 \varphi \quad (\text{A.3})$$

where coefficients A_1 – A_5 are some linear combinations of H_{ijkl} . Expression (A.3) can be re-written using trigonometric identities as a Fourier polynomial:

$$H'_{ijkl} = a_0 + \sum_{m=1,2,4} a_m \cos m\varphi + \sum_{m=1,2,4} b_m \sin m\varphi \quad (\text{A.4})$$

where a_m, b_m are linear combinations of H_{ijkl} . But it is well known that the Fourier series expansion of a function with period θ must contain only terms $\cos \frac{2\pi m\varphi}{\theta}$ or $\sin \frac{2\pi m\varphi}{\theta}$. Thus, existence of φ -dependent terms in representation (A.4) is only possible when $\theta = \frac{\pi}{2}, \pi, \frac{3\pi}{2}, \dots$. For any other value of θ , we have $a_m = b_m = 0$ ($m = 1, 2, 4$), so all components H'_{ijkl} are constant, and tensor \mathbf{H} is isotropic.

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