On some background of micromechanics of random structure matrix composites

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Abstract:
We consider a linearly elastic composite medium, which consists of a homogeneous matrix containing statistically inhomogeneous random set of heterogeneities and loaded by inhomogeneous remote loading. The new general integral equation is obtained by a centering procedure without any auxiliary assumptions such as, e.g., effective field hypothesis implicitly exploited in the known centering methods. The method makes it possible to abandon the basic concepts of classical micromechanics such as effective field hypothesis, and the hypothesis of "ellipsoidal symmetry". The results of this abandonment leads to detection of some fundamentally new effects that is impossible in the framework of a classical background of micromechanics.

Keywords: A. microstructures, B. inhomogeneous material, B. elastic material.

1 Introduction

The final goals of micromechanical research of composites involved in a prediction of both the overall effective properties and statistical moments of stress-strain fields are based on the approximate solution of exact initial general integral equations connecting the random stress fields at the point being considered and the surrounding points. These equations are well-known for statistically homogeneous composite materials subjected to homogeneous boundary conditions. In the current paper, these known equations are generalized to the case of inhomogeneity of both the statistical microstructure and applied loading. The method is based on a centering procedure of subtraction from both sides of a known initial integral equation the statistical averages obtained without any auxiliary assumptions such as, e.g., effective field hypothesis implicitly exploited in the known centering methods.

A considerable number of methods are known in the linear elasticity theory of composites. Appropriate, but by no means exhaustive, references are provided by the book by Buryachenko.

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Nowadays, it appears that variants of the effective medium by Kröner [2] and mean field methods by Mori and Tanaka [3] are the most popular and widely used methods. Recently, a new method has become known, the multiparticle effective field method (MEFM) (see [1]). The MEFM is based on the theory of functions of random variables and Greens functions. Within this method one constructs a hierarchy of statistical moment equations for conditional averages of the stresses in the inclusions. The hierarchy is then cut by introducing the notion of an effective field. This way the interaction of different inclusions is taken into account. Buryachenko [1] has demonstrated that the MEFM includes as particular cases the well-known methods of mechanics of strongly heterogeneous media.

However, all mentioned methods are based on the effective field hypothesis (EFH, even if the term “effective field hypothesis” was not indicated) according to which each inclusion is located inside a homogeneous so-called effective field (see for references [1]). Effective field hypothesis is apparently the most fundamental, most prospective, and most exploited concept of micromechanics. This concept has directed a development of micromechanics over the last sixty years and made a contribution to their progress incompatible with any another concept. The idea of effective field dating back to Mossotti [4] was added by the hypothesis of “ellipsoidal symmetry” for the distribution of inclusions attributed to Willis [5]. However, we will show in this paper that the EFH (also called the hypothesis H1) is a central one and other concept plays a satellite role providing the conditions for application of the EFH. Moreover, we will show that all mentioned hypotheses are not really necessary and can be relaxed.

The outline of the study is as follow. In Section 2 we present the basic equation of thermoelasticity, notations, and statistical description of the composite microstructure. The new general integral equations are proposed in Section 3 for the case of statistically inhomogeneous structures of composite materials. These equations are obtained by a centering procedure of subtraction from both sides of a known initial integral equation the statistical averages obtained without any auxiliary assumptions such as, e.g., EFH implicitly exploited in the known centering methods. The new general integral equation is compared with the known ones. In Section 4 we recall the basic concepts defining the background of classical micromechanics. Explicit formulae for both effective elastic moduli and strain concentrator factor are presented. The new general integral equations presented in Section 5 through the operator form of the particular solutions for one heterogeneous in the infinite matrix subjected to inhomogeneous effective field. This equation is solved by the iteration method in the framework of the quasi-crystallite approximation but without basic hypotheses of classical micromechanics such as both the EFH and “ellipsoidal symmetry” assumption. In Section 5 we qualitatively explain the advantages of the new approach with respect to the classic ones and demonstrate the corrections of popular propositions obtained in the framework of the old background of micromechanics.

2 Description of the mechanical properties and geometrical structure of the components

Let a linear elastic body occupy an open bounded domain $w \subset \mathbb{R}^d$ with a smooth boundary
Γ and with a characteristic function \( W \) and space dimensionality \( d \) (\( d = 2 \) and \( d = 3 \) for 2-D and 3-D problems, respectively). The domain \( w \) contains a homogeneous matrix \( v^{(0)} \) and a statistically inhomogeneous set \( X = (v_i, V_i, x_i) \) of inclusions \( v_i \) with characteristic functions \( V_i \) and centers \( x_i \). It is assumed that the inclusions can be grouped into component (phase) \( v^{(1)} \) with identical mechanical and geometrical properties (such as the shape, size, orientation, and microstructure of inclusions). For the sake of definiteness, in the 2-D case we will consider a plane-strain problem. At first no restrictions are imposed on the elastic symmetry of the phases or on the geometry of the inclusions \(^1\).

We will consider the local basic equations of elastostatics of composites

\[
∇σ(x) = 0, \quad (2.1)
\]

\[
σ(x) = L(x)ε(x), \quad \text{or} \quad ε(x) = M(x)σ(x), \quad (2.2)
\]

\[
ε(x) = [\nabla \otimes u + (\nabla \otimes u)^\top]/2, \quad \text{Inc}ε(x) = 0, \quad (2.3)
\]

where \( \otimes \) denotes tensor product, and \((.)^\top\) denotes matrix transposition. \( L(x) \) and \( M(x) \equiv L(x)^{-1} \) are the known stiffness and compliance fourth-order tensors, and the common notation for contracted products has been employed.

In particular, for isotropic constituents the stiffness tensor \( L \) is given in terms of the local bulk modulus \( k \) and the shear modulus \( μ \) as: \( L = (dk, 2μ) ≡ dkN_1 + 2μN_2, N_1 = δ \otimes δ/d, N_2 = I - N_1 (d = 2 or 3); δ and \( I \) are the unit second-order and fourth-order tensors. The tensors \( g \) (\( g = L, M \)) of material properties are piecewise constant and decomposed as \( g = g^{(0)} + g_1(x) = g^{(0)} + g^{(1)}_1(x) \) where \( g^{(0)}\) = const, \( g(x) \equiv g^{(0)} \) at \( x \in V^0 \) and \( g^{(1)}_1(x) \equiv g^{(1)}_1 \) is a homogeneous function of the \( x \in V^{(1)} \):

\[
L^{(1)}_1(x) = L^{(1)}_1 \equiv \text{const. at } x \in V^{(1)}. \quad (2.4)
\]

The upper index of the material properties tensor put in parentheses shows the number of the respective constituent. The upper index \( (m) \) indicates the components and the lower index \( i \) indicates the individual inclusions; \( v^0 = w \backslash v, v \equiv v^{(1)}, V(x) = V^{(1)} = \sum V_i(x) \), and \( V^{(1)}(x) \) and \( V_i(x) \) are the indicator functions of \( v^{(1)} \) and \( v_i \), respectively.

The boundary conditions at the interface boundary will be considered together with the mixed boundary conditions on \( Γ \) with the unit outward normal \( n^Γ \)

\[
u(x) = u^Γ(x), \quad x \in Γ_u, \quad (5.5)
\]

\[
σ(x)n^Γ(x) = t^Γ(x), \quad x \in Γ_t, \quad (5.6)
\]

where \( Γ_u \) and \( Γ_t \) are prescribed displacement and traction boundaries such that \( Γ_u \cup Γ_t = Γ, Γ_u \cap Γ_t = \emptyset \). \( u^Γ(x) \) and \( t^Γ(x) \) are, respectively, prescribed displacement on \( Γ_u \) and traction on \( Γ_t \). Of special practical interest are the homogeneous boundary conditions

\[
u^Γ(x) = ε^Γx, \quad ε^Γ \equiv \text{const.}, \quad x \in Γ, \quad (5.7)
\]

\[
t^Γ(x) = σ^Γ n^Γ(x), \quad σ^Γ = \text{const.}, \quad x \in Γ, \quad (5.8)
\]

\(^1\)It is known that for 2-D problems the plane-strain state is only possible for material symmetry no lower than orthotropic (see e.g. [6]) that will be assumed hereafter in 2-D case.
where $\varepsilon^\Gamma(\mathbf{x}) = \frac{1}{2} \langle \nabla \otimes \mathbf{u}^\Gamma(\mathbf{x}) + (\nabla \otimes \mathbf{u}^\Gamma(\mathbf{x}))^\top \rangle$, $\mathbf{x} \in \Gamma$, and $\varepsilon^\Gamma$ and $\sigma^\Gamma$ are the macroscopic strain and stress tensors, i.e. the given constant symmetric tensors.

It is assumed that the representative macrodomain $w$ contains a statistically large number of realizations $\alpha$ of inclusions $v_i \in v$ (providing validity of the standard probability theory technique) of the constituent $v_i \in v$ ($i = 1, 2, \ldots$). A random parameter $\alpha$ belongs to a sample space $\mathcal{A}$, over which a probability density $p(\alpha)$ is defined (see, e.g., [7]). For any given $\alpha$, any random function $g(\mathbf{x}, \alpha)$ (e.g., $g = V, \sigma, \varepsilon$) is defined explicitly as one particular member, with label $\alpha$, of an ensemble realization. Then, the mean, or ensemble average is defined by the angle brackets enclosing the quantity $g$

$$\langle g \rangle(\mathbf{x}) = \int_{\mathcal{A}} g(\mathbf{x}, \alpha) p(\alpha) d\alpha. \quad (2.9)$$

No confusion will arise below in notation of the random quantity $g(\mathbf{x}, \alpha)$ if the label $\alpha$ is dropped for compactness of expressions unless such indication is necessary. One treats two material length scales (see, e.g., [8]): the macroscopic scale $L$, characterizing the extent of $w$, and the microscopic scale $a$, related with the heterogeneities $v_i$. Moreover, one supposes that applied field varies on a characteristic length scale $\Lambda$. The limit of our interests for both the material scales and field one is presented in an asymptotic sense

$$L \gg \Lambda \geq a, \quad (2.10)$$

as the scale of microstructure $a$ relative to the macroscale $L$ tends to zero. All the random quantities under discussion are described by statistically inhomogeneous random fields. For the alternative description of the random structure of a composite material let us introduce a conditional probability density $\varphi(v_i, \mathbf{x}_i|v_1, \mathbf{x}_1, \ldots, v_n, \mathbf{x}_n)$, which is a probability density to find the $i$-th inclusion with the center $\mathbf{x}_i$ in the domain $v_i$ with fixed inclusions $v_1, \ldots, v_n$ with the centers $\mathbf{x}_1, \ldots, \mathbf{x}_n$. The notation $\varphi(v_i, \mathbf{x}_i|v_1, \mathbf{x}_1, \ldots, v_n, \mathbf{x}_n)$ denotes the case $\mathbf{x}_i \neq \mathbf{x}_1, \ldots, \mathbf{x}_n$.

We will consider a general case of statistically inhomogeneous media with the homogeneous matrix (for example for so-called Functionally Graded Materials (FGM)), when the conditional probability density is not invariant with respect to translation: $\varphi(v_i, \mathbf{x}_i|v_1, \mathbf{x}_1, \ldots, v_n, \mathbf{x}_n) \neq \varphi(v_i, \mathbf{x}_i + \mathbf{x}|v_1, \mathbf{x}_1 + \mathbf{x}, \ldots, v_n, \mathbf{x}_n + \mathbf{x})$, i.e. the microstructure functions depend upon their absolute positions. In particular, a random medium is called statistically homogeneous in a narrow sense if its multi-point statistical moments of any order are shift-invariant functions of spatial variables. Of course, $\varphi(v_i, \mathbf{x}_i|v_1, \mathbf{x}_1, \ldots, v_n, \mathbf{x}_n) = 0$ for values of $\mathbf{x}_i$ lying inside the "excluded volumes" $\cup v_{m_i}^0$ (since inclusions cannot overlap, $m = 1, \ldots, n$), where $v_{m_i}^0 \supset v_m$ with characteristic function $V_{m_i}^0$ is the "excluded volumes" of $\mathbf{x}_i$ with respect to $v_m$ (it is usually assumed that $v_{m_i}^0 \equiv v_m^0$, and $\varphi(v_i, \mathbf{x}_i|v_1, \mathbf{x}_1, \ldots, v_n, \mathbf{x}_n) \to \varphi(v_i, \mathbf{x}_i)$ as $|\mathbf{x}_i - \mathbf{x}_m| \to \infty$, $m = 1, \ldots, n$ (since no long-range order is assumed). $\varphi(v_i, \mathbf{x})$ is a number density, $n = n(\mathbf{x})$ of component $v \ni v_i$ at the point $\mathbf{x}$ and $c^{(1)}(\mathbf{x})$ is the concentration, i.e. volume fraction, of the component $v_i \ni v$ at the point $\mathbf{x}$: $c^{(1)}(\mathbf{x}) = \langle V \rangle(\mathbf{x}) = \mathbf{\pi}_i n^{(1)}(\mathbf{x})$, $\mathbf{\pi}_i = \text{mes} v_i$; $i = 1, 2, \ldots$, $c^{(0)}(\mathbf{x}) = 1 - \langle V \rangle(\mathbf{x})$. Hereafter only if the pair distribution function $g(|\mathbf{x}_m - \mathbf{x}_i|) \equiv \varphi(v_i, \mathbf{x}_i|v_m, \mathbf{x}_m)/n^{(k)}$ depends on $|\mathbf{x}_m - \mathbf{x}_i|$ it is called the radial distribution function (RDF). The notations $\langle (\cdot) \rangle(\mathbf{x})$ and
that there are inclusions at the points \( \langle \cdot \rangle_i \) can be reduced to a symmetrized integral form after integrating by parts (see, e.g., Chapter 7 in [1]).

The ensemble of a statistically inhomogeneous field \( X = (v_i) \) at the point \( x \), on the condition that there are inclusions at the points \( x_1, \ldots, x_n \) and \( x_i \neq x_j \) if \( i \neq j \) \( (i,j = 1, \ldots, n) \). The notations \( \langle \cdot \rangle; v_1, x_1; \ldots; v_n, x_n \rangle(x) \) are used for the case \( x \notin v_1, \ldots, v_n \). The notation \( \langle (\cdot) \rangle_i(x) \) at \( x \in v_i \) means the average over an ensemble realization of surrounding inclusions (but not over the volume \( v_i \) of a particular inhomogeneity, in contrast to \( \langle (\cdot) \rangle_{(i)} \) at the fixed \( v_i \). Without loss of generality, we assume that the subdomains \( v^{(1)} \) do not touch the boundary \( \Gamma \); such subdomains are called floating subdomains. In other words, the body \( w \) is considered as one cut out from an infinite random medium and the inclusions \( v_i \) intersected with the boundary \( \Gamma \) are replaced by the matrix material.

We will use two sorts of conditional averages of some tensor \( g \) (e.g., \( g = \varepsilon, \sigma \)). At first, the conditional statistical average in the inclusion phase \( \langle g \rangle^{(q)}(x) \equiv \langle g^{V}(q) \rangle(x) \) (at the condition that the point \( x \) is located in the inclusion phase \( x \in v^{(q)} \) can be found as \( \langle g^{V}(q) \rangle(x) = \langle V^{(q)}(x) \rangle^{-1} \langle g V^{(q)} \rangle(x) \). Usually, it is simpler to estimate the second conditional averages of these tensors in the concrete point \( x \) of the fixed inclusion \( x \in v_q \). \( \langle g|v_q, x_q \rangle(x) \equiv \langle g \rangle_q(x) \). At first we built some auxiliary set \( v_q^1(x) \) with the boundary \( \partial v_q^1(x) \) formed by the centers of translated ellipsoids \( v_q(0) \) around the fixed point \( x \). We construct \( v_q^1(x) \) as a limit \( v_q^1 \rightarrow v_q^1(x) \) if a fixed ellipsoid \( v_q \) is shrinking to the point \( x \). Then we can get a relation between the mentioned averages \( [x = (x_1, \ldots, x_d)^T] \):

\[
\langle g \rangle^{(q)}(x) = \int_{v_q^1(x)} n^{(q)}(y) \langle g|v_q, y \rangle(x) \, dy. \tag{2.11}
\]

Formula (2.11) is valid for any material inhomogeneity of inclusions of any concentration in the macrodomain \( w \) of any shape (if \( v_q^1(x) \subset w \)). Obviously, the general Eq. (2.11) is reduced to the popular one \( \langle g \rangle^{(q)} = \langle g \rangle_q \) for statistically homogeneous media subjected to homogeneous boundary conditions.

### 3 General integral equation

Substituting the constitutive equation (2.1) and the Cauchy equation (2.3) into the equilibrium equation (2.1), we obtain a differential equation with respect to the displacement \( u \) which can be reduced to a symmetrized integral form after integrating by parts (see, e.g., Chapter 7 in [1])

\[
\varepsilon(x) = \varepsilon^0(x) + \int_w U(x - y) \tau(x) \, dy, \tag{3.1}
\]

where \( \tau(x) \equiv L_1(y)\varepsilon(y) \) is called the stress polarization tensor, and the surface integral is absent because the heterogeneous are assumed (without loss of generality) to be floating ones. The integral operator kernel \( U \) is an even homogeneous a generalized function of degree \(-d \) defined by the second derivative of the Green tensor \( G: U_{ijkl}(x) = [\nabla_j \nabla_k G_{ik}(x)]_{(ijkl)}, \) the parentheses in
indices mean symmetrization. $\mathbf{G}$ is the infinite-homogeneous-body Green's function of the Navier equation with an elastic modulus $\mathbf{L}^{(0)}$ defined by

$$
\nabla \left\{ \mathbf{L}^{(0)} \left[ \nabla \otimes \mathbf{G}^{(0)}(\mathbf{x}) + (\nabla \otimes \mathbf{G}^{(0)}(\mathbf{x}))^\top \right] \right\}/2 = -\delta \delta(\mathbf{x}),
$$

and vanishing at infinity ($|\mathbf{x}| \to \infty$), $\delta(\mathbf{x})$ is the Dirac delta function. The deterministic function $\varepsilon^0(\mathbf{x})$ is the strain field which would exist in the medium with homogeneous properties $\mathbf{L}^{(0)}$ and appropriate boundary conditions (see, e.g., Ref. [9]):

$$
\varepsilon^0_{pq}(\mathbf{x}) = \int_{\Gamma} \left[ G_{i(p,q)}(\mathbf{x} - \mathbf{s}) t_i^0(\mathbf{s}) - u_i^0(\mathbf{s}) L_{i,j,k\ell}^{(0)} G_{k(p,q)}^{(0)}(\mathbf{x} - \mathbf{s}) n_j(\mathbf{s}) \right] d\mathbf{s}, \tag{3.2}
$$

which conforms with the stress field $\mathbf{\sigma}^0(\mathbf{x}) = \mathbf{L}^{(0)} \varepsilon^0(\mathbf{x})$. The representation (3.2) is valid for both the general cases of the first and second boundary value problems as well as for the mixed boundary-value problem (see for references [1]). For simplicity we will consider only internal points $\mathbf{x} \in w$ of the microinhomogeneous macrodomain $w$ at sufficient distance from the boundary

$$
a \ll |\mathbf{x} - \mathbf{s}|, \quad \forall \mathbf{s} \in \Gamma. \tag{3.3}
$$

In so doing, some Cauchy data $[\mathbf{u}^0(\mathbf{s}), \mathbf{t}^0(\mathbf{s})]$ (3.2) (if they are not prescribed by the boundary conditions) will depend on perturbations introduced by all inhomogeneities, and, therefore $\varepsilon^0(\mathbf{x}) = \varepsilon^0(\mathbf{x}, \alpha)$.

Now we will center Eq. (3.1), i.e. from both sides of Eq. (3.1) their statistical averages are subtracted

$$
\varepsilon(\mathbf{x}) = \langle \varepsilon \rangle(\mathbf{x}) + \int \mathbf{U}(\mathbf{x} - \mathbf{y}) \tau(\mathbf{y}) - \langle \mathbf{U}(\mathbf{x} - \mathbf{y}) \tau \rangle(\mathbf{y}) d\mathbf{y} + \mathbf{T}_x^\Gamma. \tag{3.4}
$$

Without loss of generality, it is assumed the traction boundary conditions (2.6). Then $\mathbf{T}_x^\Gamma \equiv \varepsilon^0(\mathbf{x}, \alpha) - \langle \varepsilon^0 \rangle(\mathbf{x})$ defined by the integral (3.2) (containing only $\mathbf{u}^0(\mathbf{s})$) over the external surface $\mathbf{s} \in \Gamma$ can be dropped out, because this tensor vanishes at sufficient distance $\mathbf{x}$ from the boundary $\Gamma$ (3.3) (see for details, e.g., Ref. [10] and its applications Shermergor [11]; see also [1], [12] where the case of nonfloating subdomains is considered).

The integrals in Eqs. (3.4) converges absolutely for both the statistically homogeneous and inhomogeneous random fields $\mathbf{X}$ of inhomogeneities. Indeed, even for the FGMs, the term in the square brackets in Eq. (3.4) is of order $O(\mathbf{u}(\mathbf{x}) \cdot \mathbf{y})^{-2d}$ as $|\mathbf{x} - \mathbf{y}| \to \infty$, and the integral in Eq. (3.4) converges absolutely. Therefore, for $\mathbf{x} \in w$ considered in Eqs. (3.4) and removed far enough from the boundary $\Gamma$ (3.3), the right-hand side integrals in Eq. (3.4) does not depend on the shape and size of the domain $w$, and it can be replaced by the integrals over the whole space $\mathbb{R}^d$. With this assumption we hereafter omit explicitly denoting $\mathbb{R}^d$ as the integration domain in the equation

$$
\varepsilon(\mathbf{x}) = \langle \varepsilon \rangle(\mathbf{x}) + \int \mathbf{U}(\mathbf{x} - \mathbf{y}) \tau(\mathbf{y}) - \langle \mathbf{U}(\mathbf{x} - \mathbf{y}) \tau \rangle(\mathbf{y}) d\mathbf{y} + \mathbf{T}_x^\Gamma. \tag{3.5}
$$

It should be mentioned that a popular equality

$$
\langle \mathbf{U}(\mathbf{x} - \mathbf{y}) \tau(\mathbf{y}) \rangle(\mathbf{y}) = \mathbf{U}(\mathbf{x} - \mathbf{y}) \langle \tau(\mathbf{y}) \rangle(\mathbf{y}) \tag{3.6}
$$
is only asymptotically valid at $|x - y| \to \infty$. Then Eq. (3.5) is asymptotically reduced to the known one (see for details [1])

$$
\varepsilon(x) = \langle \varepsilon \rangle(x) + \int U(x - y)[\tau(y) - \langle \tau \rangle(y)]dy,
$$

(3.7)

which in turn coincides with the equation

$$
\varepsilon(x) = \langle \varepsilon \rangle + \int U(x - y)[\tau(y) - \langle \tau \rangle]dy,
$$

(3.8)

for statistically homogeneous media subjected to the homogeneous boundary conditions.

Let the inclusions $v_1, \ldots, v_n$ be fixed and we define two sorts of effective fields $\bar{\varepsilon}_i(x)$ and $\bar{\varepsilon}_1,\ldots,n(x)$ ($i = 1, \ldots, n; x \in v_1, \ldots, v_n$) by the use of the rearrangement of Eq. (3.6) in the following form (see for the earliest references of related manipulations [1]):

$$
\varepsilon(x) = \bar{\varepsilon}_i(x) + \int U(x - y)V_i(y)\tau(y)dy,
$$

$$
\bar{\varepsilon}_i(x) = \bar{\varepsilon}_1,\ldots,n(x) + \sum_{j \neq i} \int U(x - y)V_j(y)\tau(y)dy,
$$

$$
\bar{\varepsilon}_1,\ldots,n(x) = \langle \varepsilon \rangle(x) + \int \left\{ U(x - y)\tau(y)V(y; v_1, x_1; \ldots; v_n, x_n) - \langle U(x - y)\tau \rangle(y) \right\}dy,
$$

(3.9)

for $x \in v_i, i = 1, 2, \ldots, n$; here $V(y|v_1, x_1; \ldots; v_n, x_n)$ is a random characteristic function of inclusions $x \in v$ under the condition that $x_i \neq x_j$ if $i \neq j$ ($i, j = 1, \ldots, n$). Then, considering some conditional statistical averages of the general integral equation (3.5) leads to an infinite system of new integral equations ($n = 1, 2, \ldots$)

$$
\langle \varepsilon|v_1, x_1; \ldots; v_n, x_n\rangle(x) - \sum_{i=1}^{n} \int U(x - y)\langle V_i(y)\tau|v_1, x_1; \ldots; v_n, x_n\rangle(y)dy
$$

$$
= \langle \varepsilon \rangle(x) + \int \left\{ U(x - y)\langle \tau|v_1, x_1; \ldots; v_n, x_n\rangle(y) - \langle U(x - y)\tau \rangle(y) \right\}dy.
$$

(3.10)

Since $x \in v_1, \ldots, v_n$ in the $n$-th line of the system can take the values of the inclusions $v_1, \ldots, v_n$, the $n$-th line actually contains $n$ equations.

4 Background of analytical micromechanics

4.1 Approximate effective field hypothesis

In the current section 4, only statistically homogeneous media subjected to homogeneous boundary conditions (2.7) are considered. In order to simplify the exact system (3.10) we now
apply the so-called effective field hypothesis which is the main approximate hypothesis of many micromechanical methods:

**Hypothesis 1a, H1a.** Each inclusion \( v_i \) is located in the field (3.9)

\[
\varepsilon_i(y) \equiv \varepsilon(x_i) \quad (y \in v_i),
\]

which is homogeneous over the inclusion \( v_i \).

In some methods (such as, e.g., the MEFM) this basic hypothesis \( \text{H1a} \) is complimented by a satellite hypothesis [compare with (3.6)]:

**Hypothesis 1b, H1b.** The perturbation introduced by the inclusion \( v_i \) at the point \( y \notin v_i \) is defined by the relation

\[
\int U(y - x)V_i(x)\tau(x)dx = \bar{v}_i T_i(y - x_i)\tau_i.
\]

Hereafter \( \tau_i \equiv \langle \tau(x)\rangle_{(i)} \) is an average over the volume of the inclusion \( v_i \) (but not over the ensemble), \( \langle \cdot \rangle_{(i)} \equiv \langle \langle \cdot \rangle \rangle_{(i)} \), and \( (x, z \in v_i, x \notin v_i, x_j, y \in v_j) \)

\[
T_i(x - x_i) = \langle U(x - z)\rangle_{(i)}, \quad T_{ij}(x_j - x_i) = \langle T_i(y - x_i)\rangle_{(j)}.
\]

If \( x \in v_i \) then \( T_i(x - x_i) = -(\tau_i)^{-1}P_i \equiv \text{const.} \), where the tensor \( P_i \) is associated with the well-known Eshelby tensor by \( S_i = P_i L^{(0)} \). For a homogeneous ellipsoidal inclusion \( v_i \) the standard assumption (4.1) (see, e.g., [1]) yields the assumption (4.2), otherwise the formula (4.2) defines an additional assumption. The tensors \( T_{ij}(x_i - x_j) \) has an analytical representation for spherical inclusions of different size in an isotropic matrix (see for references [1]).

According to hypothesis \( \text{H1a} \) and in view of the linearity of the problem there exist constant fourth and second-rank tensors \( A_i(x), R_i(x) \), such that

\[
\varepsilon(x) = A_i(x)\varepsilon(x_i), \quad \tau(x) = R(x)\varepsilon(x_i), \quad x \in v_i,
\]

where \( v_i \subset v^{(i)} \) and \( R(x) = L_{i1}^{(1)} A_i(x) \). According to Eshelby’s [13] theorem there are the following relations between the averaged tensors (4.4) \( R = \tau_i P_i^{-1}(I - A_i) \), where \( g_i \equiv \langle g(x)\rangle_{(i)} \) (\( g \) stands for \( A_i, R \)). For example, for the homogeneous ellipsoidal domain \( v_i \) (2.4) we obtain

\[
A_i = \left(I + P_i L_{i1}^{(i)}\right)^{-1}.
\]

In the general case of coated inclusions \( v_i \), the tensors \( A_i(x) \) can be found by the transformation method by Dvorak and Benveniste [14] (see for references and details [1]).

### 4.2 Closing hypothesis
For termination of the hierarchy of statistical moment equations (3.10) we will use the closing EFH called the “quasi-crystalline” approximation by Lax [15] which in our notations has a form

**Hypothesis 2, “quasi-crystalline” approximation.** It is supposed that the mean value of the effective field at a point $x \in v_i$ does not depend on the stress field inside surrounding heterogeneities $v_j \neq v_i$:

$$
\langle \varepsilon_i(x) | v_i, x_i; v_j, x_j \rangle = \langle \varepsilon_i \rangle, \quad x \in v_i.
$$

(4.5)

In the framework of the hypothesis $H_1$, substitution of the solution (4.4) into the first equation of the system (3.9) at $n = 1$ and at the EFH $H_2$ leads to the solution ($x \in v_i$)

$$
\langle \varepsilon \rangle_i = R^{-1} Y R \langle \varepsilon \rangle,
$$

(4.6)

$$
\langle \tau \rangle_i(x) = R(x) R^{-1} Y R \langle \varepsilon \rangle,
$$

(4.7)

$$
L^* = L^{(0)} + Y R c^{(1)},
$$

(4.8)

where the matrix $Y$ determines the action of the surrounding inclusions on the considered one and has an inverse matrix $Y^{-1}$ given by

$$
(Y^{-1}) = I - \bar{v} R \int \left[ T_{iq}(x_i - x_q) \varphi(v_q, x_q; v_i, x_i) - T_i(x_i - x_q) n^{(1)} \right] dx_q.
$$

(4.9)

General case of the closing hypothesis taking $n$ interacting heterogeneities is considered in Chapter 8 in [1].

### 4.3 Hypothesis of “ellipsoidal symmetry” of composite structure

To make further progress, the hypothesis of “ellipsoidal symmetry” for the distribution of inclusions attributed to Willis [5] is widely used:

**Hypothesis 3, “ellipsoidal symmetry”.** The conditional probability density function $\varphi(v_j, x_j ; v_i, x_i)$ depends on $x_j - x_i$ only through the combination $\rho = ||(a_{ij}^0)^{-1}(x_j - x_i)||$:

$$
\varphi(v_j, x_j ; v_i, x_i) = h(\rho), \quad \rho \equiv ||(a_{ij}^0)^{-1}(x_j - x_i)||
$$

(4.10)

where the matrix $(a_{ij}^0)^{-1}$ (which is symmetric in the indexes $i$ and $j$, $a_{ij}^0 = a_{ji}^0$) defines the ellipsoid excluded volume $v_{ij}^0 = \{ x : ||(a_{ij}^0)^{-1}x||^2 < 1 \}$.

For spherical inclusions the relation (4.10) is realized for a statistical isotropy of the composite structure. It is reasonable to assume that $(a_{ij}^0)^{-1}$ identifies a matrix of affine transformation.
that transfers the ellipsoid $v^0_{ij}$ being the “excluded volume” (“correlation hole”) into a unit sphere and, therefore, the representation of the matrix $Y$ can be simplified:

$$(Y^{-1}) = I - \epsilon^{(i)} R P^0_{ij},$$

(4.11)

where for the sake of simplicity of the subsequent calculation we will usually assume that the shape of “correlation hole” $v^0_{ij}$ does not depend on the inclusion $v_j$: $v^0_{ij} = v^0_i$ and $P^0_{ij} = P^0_i \equiv P(v^0_i)$.

The concept of the EFH (even if this term is not mentioned) in combination with subsequent assumptions (e.g., mentioned above) totally dominates (and creates the fundamental limitations) in all four groups of analytical micromechanics in physics and mechanics of heterogeneous media: model methods, perturbation methods, self-consistent methods (e.g., Mori-Tanaka, MT, approach, and the MEFM), and variational ones (see for references [1]).

5 Background of computational analytical micromechanics

5.1 A single inclusion subjected to inhomogeneous prescribed effective field

In the current subsection we will consider a satellite problem whose solution will be used for estimation of effective properties of composites in Subsection 5.2. Namely, let the inclusions $v_i$ be fixed and loaded by the inhomogeneous effective field $\tau_i(x)$. Then we used the known regularized integral equation

$$\tau(x) = \tau_i(x) + \int K_i(x,y)[\tau(y) - \tau(x)]dy, \quad x \in v_i,$$

(5.1)

where $\tau_i(x) = E_i(x)\tau(x)$, $(x \in v_i)$ is called the effective stress polarization tensor in the inclusion $v_i$, and (no sum on $i$)

$$K_i(x,y) = E_i(x)U(x-y)V_i(y),$$

$$E_i(x) = L_1(x)[I + P^0_i(x)L_1(x)]^{-1}.$$

(5.2)

Here the tensor $P^0_i(x) = -\int V^0_i(y)U(x-y)dy$ can be estimated, e.g., by the FEA and assumed to be known.

We formally write the solution of Eq. (5.1) as

$$\tau = L_i + \tau_i,$$

(5.4)

where the inverse operator $L_i = (I - K_i)^{-1}$ will be constructed by the iteration method based on the recursion formula

$$\tau^{[k+1]} = \tau_i + K_i \tau^{[k]},$$

(5.5)

the convergence of which is analyzed in [1]. Here the integral operator $K_i$ has the kernel formally represented as

$$K_i(x,y) = K_i(x,y) - \delta(x-y)\int V_i(z)K_i(x,z)dz,$$

(5.6)
and one used an initial approximation
\[ \tau^{[0]}(x) = \tau_i(x), \quad (5.7) \]
which is exact for a homogeneous ellipsoidal inclusion subjected to remote homogeneous stress field \( \tau(x) \equiv \tau = \text{const.} \)

The solution (5.4) allows us to state that the linear operators \( \mathcal{L}^\epsilon \) and \( \mathcal{L}^\tau \) describing a perturbation of the strain fields inside and outside the inclusion \( v_i \ (x \in \mathbb{R}^d) \)
\[ \int U(x - y)V_i(y)\tau(y)dy = \epsilon(x) - \tau_i(x) = \mathcal{L}^\tau_i(\tau)(x), \quad (5.8) \]
\[ \mathcal{L}^\epsilon_i(\tau_i)(x) = \int U(x - y)\mathcal{L} \ast (E_i \tau)(y)V_i(y)dy, \quad (5.9) \]
\[ \mathcal{L}^\tau_i(\tau)(x) = \int U(x - y)\tau(y)V_i(y)dy. \quad (5.10) \]
are constructed.

5.2 Estimation of effective elastic moduli

The new general integral equation (3.5) can be rewritten in terms of the operator representation \( \mathcal{L}^\tau \) (5.8)
\[ \epsilon(x) = \langle \epsilon \rangle(x) + \int [\mathcal{L}^\tau(\tau)(x) - \langle \mathcal{L}^\tau(\tau) \rangle(x)]dy. \quad (5.11) \]

For statistically homogeneous media subjected to homogeneous boundary conditions (2.7) and in the framework of the quasi-crystalline approximation (4.5), conditional averaging of Eq. (5.11) can be solved by the iteration method
\[ \langle \tau \rangle_i^{[n+1]}(x) = \langle \epsilon \rangle + \int \mathcal{L}^\tau_q(\langle \tau \rangle_i^{[n]}(x)) \varphi(v_q,x_q;v_i,x_i) - \tau_i^{[n]}(x_q)d\tau_q, \]
\[ \langle \epsilon \rangle^{[n+1]}_i(x) = \mathcal{R}_q \ast \langle \epsilon \rangle_q^{[n+1]}(x), \quad (5.12) \]
where \( \mathcal{R}_q = \mathcal{L}^{(1)}_i(I + \mathcal{L}^{*}_q) \). Generalization of Eq. (5.12) to the cases of both the statistically inhomogeneous media and other multiparticle closing assumptions (see [1]) is obvious. A convergence of the sequence \( \langle \tau \rangle_i^{[n]}(x) \) (5.12) is analyzed analogously to the sequence (5.5). An initial approximation \( \langle \tau \rangle_i^{[0]}(x) \) is defined by the classical approach (4.7) and (4.11). It suggests the Neumann series form for the solution \( \langle \tau \rangle_i^{[n]}(x) \) (as \( n \to \infty \)) of (5.12) and
\[ \langle \tau \rangle_i^{[n]}(x) = \mathcal{L}_i \ast (E_i \langle \tau \rangle_i^{[n]})(x): \]
\[ \langle \tau \rangle_i(x) \equiv \lim_{n \to \infty} \langle \tau \rangle_i^{[n]}(x) = \mathcal{R}_i \langle \epsilon \rangle, \quad (5.13) \]
which yields the final representations for the effective properties
\[ \mathbf{L}^* = \mathbf{L}^{(0)} + \langle \mathbf{R}^* \mathbf{V} \rangle. \quad (5.14) \]
6 Qualitative comparison of the classical and new approaches

The hypothesis **H1** is widely used (explicitly or implicitly) for the majority of the methods of micromechanics even if the term “effective field hypothesis” is not indicated. For example, Buryachenko [1] demonstrated that hypothesis **H1** is exploited in the effective medium method, generalized self-consistent method, differential methods, Mori-Tanaka method, the MEFM, conditional moments method, variational methods, and others. These are a lot of other methods using the hypothesis **H1** differ one from another by some additional specific assumptions used at the analysis of the initial integral equations either Eqs. (3.5), (3.7), or (3.8).

The differences of Eqs. (3.5), (3.7), and (3.8) are fundamental for subsequently solving the truncated hierarchy (3.10) involving a rearrangement of each appropriate equation before it is solved. The most successful rearrangement are those which make the right-hand side of the coupled equations reflect the detailed corrections to that basic physics. So, Eq. (3.8) was obtained by subtracting the difficult state at infinity from equation (3.1), i.e. roughly speaking the constant force-dipole density expressed through an alternative technique of the Green’s function. This dictates the fundamental limitation of a possible generalization of Eq. (3.8) to both the FGMs and inhomogeneous boundary conditions. The mentioned deficiency of Eq. (3.8) was resolved by Eq. (3.7) which the renormalizing term provides an absolute convergence of the integral in Eq. (3.7) at \(|x - y| \to \infty\) for the general cases of the FGMs. However, the same term in Eq. (3.7) is used in a short-range domain \(|x - y| < 3a\) in the vicinity of the point \(x \in w\). A fundamental deficiency of Eq. (3.7) is a dependence of the renormalizing term \(U(x - y)\tau(y)\) [obtained in the framework of the asymptotic approximation (3.6)] only on the statistical average \(\langle \tau(y) \rangle\) while the renormalizing term \(U(x - y)\tau(y)\) in Eq. (3.5) explicitly depends on on details distribution \(\tau|v_q, x_q(y)\) \((y \in v_q)\). What seems to be only a formal trick [abandoning the use of the approximations (3.6)] is in reality a new background of micromechanics [defining a new field of micromechanics called computational analytical micromechanics, CAM] which yields the discovery of fundamentally new effects even in the theory of statistically homogeneous media subjected to homogeneous boundary conditions. So, the final classical representation of the effective properties (4.8) depends only on the average strain concentrator factor \(A_i\) while the effective properties (5.14) implicitly depend on the inhomogeneous tensor \(A_i(x)\). Moreover, the detected dependence of the effective properties (5.14) on the detailed strain concentrator factors \(A_i(x)\) rather than on the average values \(A_i\) allows us to abandon the hypothesis **H1b** whose accuracy is questionable for the noncanonical inclusions. In such a case the statistical average effective field estimated by Eq. (5.12) is found to be inhomogeneous that discards the hypothesis **H1a**. Thus, the CAM does not involve the hypotheses **H1a**, **H1b**, and **H3** as contrasted to the classical analytical micromechanics. Only the closing assumption **H2** (or its multiparticle generalizations, see [1]) is exploited in CAM.

It should be mentioned, that the domain of the operator \(\mathcal{L}^c_q(\langle \xi_q^{[n]} \rangle(x) (5.12)\) is a whole space \(x \in R^d\), and, because of this, some points of the area \(x \in v_i\) in Eq. (5.12) can be uncovered by the heterogeneities \(v_q\) and, therefore, the effective strain \(\langle \xi_i^{[n+1]} \rangle(x) (5.12)\) will depend on the strain perturbations \(\mathcal{L}^c_q(\langle \xi_q^{[n]} \rangle(x)\) in the vicinity \(x \in v_q\) of the area \(v_q\) rather than only
on stress distributions in the inhomogeneity $v_q$. In particular, for well-stirred approximation of the binary correlation function $\varphi(v_q, x_q | v_i, x_i)$ of ellipsoidal inclusions, $v_q^{\oplus}$ is expressed by the Minkowski addition $v_q^{\oplus} = v_q^0 \oplus v_i$ while for the spherical inclusions $v_q^{\oplus} = \{x | |x - x_q| < 3a\}$. Thus, we obtain a fundamental conclusion that effective moduli (5.14) in general depend not only on the strain distribution inside the inhomogeneities but also on the strains in the vicinities of heterogeneities. Then the size of the excluded volume as well as the RDF will impact on the effective field (5.12) even in the framework of hypothesis $H_3$. Indeed, if the radius of the excluded volume $v_q^0$ for the spherical inclusions increases from $2a$ to $3a$ then the long distance of the influence zone $v_q^{\oplus}$ of the inhomogeneity $v_q$ on the effective field $\langle \sigma \rangle_i(x)$ will increase from the value $|x - x_q| = 3a$ to $|x - x_q| = 4a$. A larger difference between the backgrounds (3.5) and (3.8) was obtained for composites reinforced by either nonellipsoidal or inhomogeneous inclusions demonstrating essentially inhomogeneous stress distribution inside isolated heterogeneities even in the framework of the hypothesis $H_1$.

Quantitative estimations of the analyses presented above are under progress for some particular cases of fiber composites and will be considered in other publications.

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